Algebraic localisation of linear response in networks with algebraically decaying interaction, and application to discrete breathers in dipole–dipole systems

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Abstract. Networks of units for which the coupling decreases algebraically with distance between them are studied. It is proved that the linear response to an algebraically localised force is algebraically localised if the response exists and is unique. Applications are given to equilibria of networks of bistable units and to breathers in networks of oscillating dipoles.

1 Introduction

The response of a network with exponentially decaying interaction to an exponentially localised force is itself exponentially decaying, provided the response exists and is unique (by response we always mean bounded response) (for a proof in a general setting, see [1]). Many systems of physical interest, however, have algebraically decaying interaction. For example, the potential energy of dipole–dipole interaction decays like the inverse cube of their separation, and that of van der Waals forces (due to correlations in dipole moment fluctuations) like the inverse sixth power. Is there an analogous result for algebraically decaying interaction? In this paper we give an affirmative answer.

Our interest in this problem was stimulated by work on "discrete breathers" in a monolayer of carbon monoxide molecules adsorbed on the surface of ruthenium [2]. Discrete breathers are spatially localised time-periodic vibrations of a network of oscillators. In this

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case, the oscillators are the $C-O$ stretches and they are considered to be coupled by dipole–dipole interaction, the ruthenium substrate being regarded as rigid. The strategy of [3] can be easily adapted to the space ℓ_1 of spatially summable perturbations from equilibrium and hence to prove existence of ℓ_1-breathers, i.e. whose oscillation amplitudes are summable over space, which implies spatial decay to equilibrium but with no particular rate (as the decay could be lacunary). The question arises whether a better spatial decay result can be proved.

In this paper, we prove algebraic upper bounds for the linear response to an algebraically localised force for a network with algebraically decaying coupling (provided the response exists and is unique), give a general application to continuation problems, and apply it to the dipole–dipole breather problem. We conclude by assessing how close our results are to optimal.

2 Basic result

Let (S,d) be a countable metric space. For each $s \in S$, let X_s and Y_s be Banach spaces, with norms $|.|_{X_s}$, $|.|_{Y_s}$, respectively. Let $X = \{x \in \times_{s\in S} X_s : \|x\|_X < \infty\}$ for some norm $\|.\|_X$ based on $(|.|_{X_s})_{s\in S}$, and suppose it is complete. Define Y similarly. We will drop the subscripts on the symbols for the norms when the context makes them clear. Let $L : X \to Y$ be a bounded linear map of matrix type[2], i.e. one which can be written as

$$(Lx)_r = \sum_{s\in S} L_{rs} x_s,$$

with respect to components in $\times_{r\in S} Y_r$ and $\times_{s\in S} X_s$. Let $\alpha \geq 0$.

Definition: A linear map $L : X \to Y$ of matrix type is said to be *α-algebraically local* if there exists $\zeta > 0$ such that the modified operator L^ζ defined by

$$L^\zeta_{rs} = (1 + \zeta\, d(r,s))^\alpha\, L_{rs}$$

is a bounded operator from X to Y.

Definition: A configuration $y \in Y$ is said to be *α-algebraically localised* about site $o \in S$, if there exists $\zeta > 0$ such that y^ζ, defined by

$$y^\zeta_s = (1 + \zeta\, d(o,s))^\alpha\, y_s,$$

is also in Y. Similarly for $x \in X$.

Note that if L^ζ and y^ζ are bounded for some $\zeta > 0$ then so are L^z and y^z for all $z \geq 0$: for $z < \zeta$ use $1 + zd \leq 1 + \zeta d$ (recall $d \geq 0$), and for $z > \zeta$ use $1 + zd \leq (z/\zeta)(1 + \zeta d)$.

[2]We are grateful to Mark Johnston for pointing out that we should have stated this assumption explicitly in [1] also.

Theorem 1 *If $L : X \to Y$ is α-algebraically local, $y \in Y$ is α-algebraically localised about $o \in S$, L is invertible, and $x = L^{-1}y$, then x is α-algebraically localised about $o \in S$. In fact, $\|L^z - L\| < \|L^{-1}\|^{-1}$ for z small enough, and for such z,*

$$\|x^z\| \leq \frac{\|y^z\|}{\|L^{-1}\|^{-1} - \|L^z - L\|}.$$

Lemma 1 *If L is α-algebraically local then L^z depends continuously on $z \in \mathcal{R}_+$.*

Proof: We treat separately the two cases $\alpha \geq 1$ and $0 \leq \alpha < 1$.

Suppose $\alpha \geq 1$. If $0 \leq p < q$ then

$$q^\alpha - p^\alpha \leq (q-p)\alpha q^{\alpha-1}.$$

Given $0 \leq a < b$, choose $c \geq b$. Given $r, s \in S$, write d for $d(r,s)$. Then

$$\begin{aligned} |L^b_{rs} - L^a_{rs}| &= \left[\left(\frac{1+bd}{1+cd}\right)^\alpha - \left(\frac{1+ad}{1+cd}\right)^\alpha\right] |L^c_{rs}| \\ &\leq (b-a)d\alpha \frac{(1+bd)^{\alpha-1}}{(1+cd)^\alpha} |L^c_{rs}| \\ &\leq \frac{b-a}{c}\alpha \left|L^c_{rs}\right|. \end{aligned}$$

Thus

$$\|L^b - L^a\| \leq \frac{b-a}{c}\,\alpha\, \|L^c\|.$$

If $0 \leq \alpha < 1$ and $0 \leq p < q$ then $(1+q)^\alpha - (1+p)^\alpha \leq q^\alpha - p^\alpha$. Given $0 \leq a < b$, choose $c \geq b$. Then

$$\begin{aligned} |L^b_{rs} - L^a_{rs}| &\leq \frac{(b^\alpha - a^\alpha)\, d^\alpha}{(1+cd)^\alpha} |L^c_{rs}| \\ &\leq \frac{b^\alpha - a^\alpha}{c^\alpha} |L^c_{rs}|. \end{aligned}$$

Thus

$$\|L^b - L^a\| \leq \frac{b^\alpha - a^\alpha}{c^\alpha} \|L^c\|. \qquad \square$$

Lemma 2 *If $o, r, s \in S$ and $z \geq 0$, then $\frac{1+z\,d(r,o)}{1+z\,d(s,o)} \leq 1 + z\,d(r,s)$.*

Proof: We treat separately the two cases $d(r,o) \geq d(s,o)$ and $d(r,o) < d(s,o)$.

If $d(r,o) \geq d(s,o)$ then since d is a metric, $d(r,s) \geq d(r,o) - d(s,o)$, and so

$$1 + z\,d(r,s) \geq 1 + z\,d(r,o) - z\,d(s,o).$$

It follows that

$$\begin{aligned}(1+z\,d(s,o))(1+z\,d(r,s)) &\geq (1+z\,d(s,o))(1+z\,d(r,o)-z\,d(s,o))\\ &= 1+z\,d(r,o)+z^2\,d(s,o)(d(r,o)-d(s,o))\\ &\geq 1+z\,d(r,o),\end{aligned}$$

and hence the desired result.

If $d(r,o) < d(s,o)$ then $\frac{1+z\,d(r,o)}{1+z\,d(s,o)} < 1 \leq 1+z\,d(r,s)$. □

Proof of Theorem 1: If $Lx = y$ then

$$\sum_{s\in S} L_{rs}\left(\frac{1+z\,d(r,o)}{1+z\,d(s,o)}\right)^{\alpha} x_s^z = y_r^z\,.$$

So

$$\left(L+\hat{L}^z\right)x^z = y^z, \tag{2.1}$$

where

$$\hat{L}_{rs}^z = \left[\left(\frac{1+z\,d(r,o)}{1+z\,d(s,o)}\right)^{\alpha} - 1\right] L_{rs}\,.$$

If $z \geq 0$ and $d(r,o) \geq d(s,o)$, then applying Lemma 2, we obtain

$$|\hat{L}_{rs}^z| \leq |L_{rs}^z - L_{rs}|. \tag{2.2}$$

If $d(r,o) < d(s,o)$, interchanging the roles of r and s in Lemma 2 and taking the reciprocal yields

$$\frac{1+z\,d(r,o)}{1+z\,d(s,o)} \geq \frac{1}{1+z\,d(r,s)}\,.$$

Using the standard inequality $x + 1/x \geq 2$, this leads to

$$1-\left(\frac{1+z\,d(r,o)}{1+z\,d(s,o)}\right)^{\alpha} \leq (1+z\,d(r,s))^{\alpha} - 1.$$

Hence (2.2) holds for $d(r,o) < d(s,o)$ also. Thus

$$\|\hat{L}^z\| \leq \|L^z - L\|.$$

But L^z depends continuously on z by Lemma 1, and $L^0 = L$, so

$$\|L^z - L\| < \|L^{-1}\|^{-1}$$

for z near 0. Thus $\left(L+\hat{L}^z\right)$ is invertible for such z and the theorem follows from (2.1).□

3 Application to continuation problems

As was done in [1] for exponential decay, we now show that under suitable conditions the continuation of a non-degenerate algebraically localised solution of a 1-parameter family of problems remains algebraically localised.

Suppose $G : \mathcal{R} \times X \to Y$, $(\varepsilon, x) \mapsto G_\varepsilon(x)$, is C^1. We adopt the notation D for the derivative with respect to $x \in X$ and $\partial/\partial\varepsilon$ for the derivative with respect to $\varepsilon \in \mathcal{R}$, unless ε is the only variable in which case we write $d/d\varepsilon$.

Given a solution x_0 of $G_0(x) = 0$ at which DG_0 is invertible then by the implicit function theorem there is a neighbourhood of $0 \in \mathcal{R}$ on which $G_\varepsilon(x) = 0$ has a unique solution $x(\varepsilon)$ near 0, and this solution satisfies

$$\frac{dx}{d\varepsilon} = -L_\varepsilon^{-1} \frac{\partial G_\varepsilon}{\partial \varepsilon}(x(\varepsilon)) \tag{3.1}$$

where $L_\varepsilon = DG_\varepsilon(x(\varepsilon))$. The solution can be continued with respect to ε as long as L_ε remains invertible.

We suppose a "reference state" in X, which we shall shift to the origin and hence denote by 0. We say a family of linear operators $P(\mu)$, μ in a set M, is uniformly α-algebraically local if there exists $\zeta > 0$ and $p \in \mathcal{R}$ such that $\|P^z(\mu)\| \le p$ for all $\mu \in M$.

Theorem 2 *If $x(0)$ is α-algebraically localised about site $o \in S$ (with respect to reference state 0), with continuation $x(\varepsilon)$ for $\varepsilon \in [0, \varepsilon_1]$ with L_ε invertible and α-algebraically local there, $Q = \frac{\partial G_\varepsilon}{\partial \varepsilon}(0)$ is α-algebraically localised about o for $\varepsilon \in [0, \varepsilon_1]$, $G \in C^2$ and $P = \frac{\partial}{\partial \varepsilon} DG$ is uniformly α-algebraically local for $\varepsilon \in [0, \varepsilon_1]$ and $\|x\| \le sup\{\|x(\varepsilon)\| : 0 \le \varepsilon \le \varepsilon_1\}$, then $x(\varepsilon)$ is α-algebraically localised about o for all $\varepsilon \in [0, \varepsilon_1]$.*

Proof: Choose $z > 0$ so that $\|L^z - L\| < \|L^{-1}\|^{-1}$. By compactness of $[0, \varepsilon_1]$ there are common bounds, $\|Q^z\| \le q$, $\|L^{-1}\|^{-1} - \|L^z - L\| \ge c^{-1} > 0$, and by the assumption on P, $\|P^z\| \le p$. For $x \in X$, let

$$\|x\|_z = \|x^z\|.$$

Then $\|x(0)\|_z < \infty$ and our aim is to prove that $\|x(\varepsilon)\|_z < \infty$ for all $\varepsilon \in [0, \varepsilon_1]$.

First we show that $\frac{\partial G_\varepsilon}{\partial \varepsilon}(x)$ is algebraically localised whenever x is. Now

$$\frac{\partial G_\varepsilon}{\partial \varepsilon}(x) = Q(\varepsilon) + \int_0^1 P(\varepsilon, tx)\, x\, dt.$$

Using Lemma 2, $\|Px\|_z \le \|P^z\| \|x^z\|$, so $\left\| \frac{\partial G_\varepsilon}{\partial \varepsilon}(x) \right\|_z \le q + p\|x\|_z$.

Next we use (3.1) and Theorem 1 to obtain

$$\left\| \frac{dx}{d\varepsilon} \right\|_z \le c\,(q + p\|x\|_z).$$

Integrating this differential inequality from $x(0)$ we obtain

$$\|x(\varepsilon)\|_z \leq \|x(0)\|_z\, e^{cp\varepsilon} + (e^{cp\varepsilon} - 1)\,\frac{q}{p} < \infty,$$

so $x(\varepsilon)$ remains α-algebraically localised. □

Extension to multi-dimensional parameter spaces is easy to achieve by taking one-dimensional paths.

4 Breathers in dipole–dipole networks

We recall from [3,4] that in many networks of oscillators, time-periodic solutions of compact support at the uncoupled limit can be continued to a range of weak coupling. The continuation process does not necessarily impose any spatial decay on the resulting solutions. Instead of performing the continuation in a space with some a priori spatial decay properties, we prefer to deduce spatial decay properties afterwards. This is because the continuation process often works equally well starting from solutions of the uncoupled network with no spatial decay properties, and yields interesting solutions like multi-breathers. But if the solution at the uncoupled limit is spatially localised then we can often deduce spatial decay of the continuation. For example, exponential decay was obtained in [3] for the continuation of solutions of compact support for 1D nearest neighbour chains and results were quoted there extending this conclusion to a variety of situations. Subsequently, using the idea of [1], this result was generalised in [4] to all networks with exponentially decaying interaction.

Here we apply Theorem 2 to prove algebraic decay in space for time-periodic solutions of some dipole–dipole networks obtained by continuation of solutions of compact support at the uncoupled limit.

Suppose S is a $\mathcal{Z}^D$ -lattice with Euclidean metric, and suppose interaction potential

$$\varepsilon W(x) = \sum_{r \neq s} \frac{\varepsilon\,(x_r - x_s)^2}{2d(r,s)^K} \tag{4.1}$$

and let

$$U_\varepsilon(x) = \sum_r V(x_r) + \varepsilon\, W(x) \tag{4.2}$$

for some local potential V.

For simplicity, instead of breathers we begin by considering the problem of continuing equilibria of U_ε from $\varepsilon = 0$, for V with (at least) two non-degenerate critical points, without loss of generality at $x = 0$ and 1. So we consider the implicit function problem

$$G_\varepsilon(x) := DU_\varepsilon(x) = 0.$$

Then $L = D^2W$ has off-diagonal elements

$$L_{rs} = \varepsilon\, d(r,s)^{-K}.$$

Use the ℓ_p metric, any $p \in [1, \infty]$, for the spaces X and Y. Then L is bounded iff $K > D$ (independently of p). We will assume this inequality, else the energy due to displacing a single site is infinite. The modified operator L^z is bounded iff $\alpha < K - D$. Thus we see that L is algebraically local if $K > D$, and we can choose any $\alpha \in [0, K - D)$ and any $z > 0$. For interacting dipoles ($K = 3$) on a surface ($D = 2$) we can take any $\alpha \in [0, 1]$, for example $\alpha = 0.99$.

Applying Theorem 2 to an initial equilibrium with $x_o = 1, x_r = 0$ for $r \neq o$, we obtain $||x(\varepsilon)||_z < \infty$. For $p = \infty$ this says that

$$|x_r(\varepsilon)| \leq \frac{C}{(1 + z\, d(r, o))^\alpha},$$

which is an algebraic decay result, though not as fast as for the coupling. Stronger results, however, are obtained with $p < \infty$. In particular, $p = 1$ gives

$$\sum_r |x_r(\varepsilon)|(1 + z\, d(r, o))^\alpha < \infty. \tag{4.3}$$

If $x(\varepsilon)$ is “full”, in the sense that $|x_r|$ lies between two positive constants times a decreasing function of distance, then this implies that $|x_r| \leq Cd(r, o)^{-K}$, but our method does not guarantee that $x(\varepsilon)$ is full so in general (4.3) is the strongest bound that we obtain. In the next section we give examples where the true solution has $|x_r| \sim Cd(r, o)^{-K}$. Thus our use of Lemma 2 must be throwing away a lot in the cases $p > 1$. This merits further investigation.

To prove algebraic localisation of breathers for a network with potential (4.2), instead of having two critical points we just require V to have a non-degenerate local minimum, without loss of generality at 0. We study the implicit function problem $G_{\varepsilon,T}(x) = 0$, where $G_{\varepsilon,T} : C^2_p(S^1_T, \mathcal{R}^S) \to C^0_p\left(S^1_T, \mathcal{R}^S\right)$ is defined by

$$\left[G_{\varepsilon,T}(x)\right]_r(t) = \ddot{x}_r(t) + \frac{\partial U_\varepsilon}{\partial x_r}(x(t)),$$

and $C^k_p(S^1_T, \mathcal{R}^S)$ is the space of C^k functions from a circle S^1_T of length T to $\mathcal{R}^S$, with the norm

$$\|x\|^p = \sum_{s \in S} |x_s|^p_k\,,$$

for $1 \leq p < \infty$, or $\|x\| = \sup_{s \in S} |x_s|_k$ for $p = \infty$, where $|.|_k$ is the C^k-norm, and then we will apply Theorem 2 (cf. [4]).

It can be checked that $L := DG_{\varepsilon,T,x}$ is bounded if $K > D$ and is α-algebraically local for all $\alpha < K - D$. If $x(0)$ is a breather for $\varepsilon = 0$ with only one site $s = o$ excited and L is invertible there then by the implicit function theorem we obtain a breather $x(\varepsilon)$ for ε small. Using Theorem 2, for all ε to which the breather can be continued with L invertible and z small enough, we deduce that $\|x(\varepsilon)\|_z < \infty$. Hence $x(\varepsilon)$ is α-algebraically localised about site o.

Again the strongest result is obtained for $p = 1$, though approximate analysis below suggests that it is not quite optimal.

The same analysis applies to problems with algebraically decaying interaction of more than just two body form.

5 True decay

For networks with algebraically decaying interaction, our theorems give upper bounds on the spatial decay of linear responses and of solutions of nonlinear problems obtained by continuation from localised solutions. For comparison, we compute here the asymptotics of the decay for some simple 1D problems.

Let
$$L_\varepsilon = I - \varepsilon\Delta : \mathcal{R}^{\mathcal{Z}} \to \mathcal{R}^{\mathcal{Z}},$$
where
$$\Delta_{rs} = |r-s|^{-K} \quad \text{for} \quad r \neq s,\ \Delta_{ss} = 0,$$
for some $K \in \mathcal{N}$, and use ℓ_1 norm. The operator Δ is bounded if $K > 1$, so L_ε is α-algebraically local for all $\alpha < K-1$ and L_ε is invertible for $\varepsilon < \|\Delta\|_1^{-1}$. Given $y \in \ell_1$ and $k \in S^1_{2\pi}$, let
$$\hat{y}(k) = \frac{1}{2\pi}\sum_r y_r e^{-ikr},$$
so
$$y_r = \int_{-\pi}^{\pi} \hat{y}(k) e^{ikr} dk.$$
Then the solution $x \in \ell_1$ of $L_\varepsilon x = y$ is given by
$$\hat{x}(k) = \frac{\hat{y}(k)}{\lambda(k,\varepsilon)},$$
where
$$\begin{aligned}\lambda(k,\varepsilon) &= 1 - \varepsilon \sum_{n\neq 0} |n|^{-K} e^{ikn} \\ &= 1 - 2\,\varepsilon\, g_K(k),\end{aligned}$$
where
$$g_K(k) = \sum_{n\geq 1} n^{-K} \cos nk.$$
For example, for $K = 2$, we have
$$g_2(k) = \frac{\pi^2}{6} + \frac{k^2}{4} - \frac{\pi\, k}{2} \quad \text{for} \quad 0 \leq k \leq 2\pi$$
and then repeated periodically. In particular, g_K is C^{K-2} and piecewise C^{K-1} with jumps in the $(K-1)$st derivative.

Now suppose $y_0 = 0$, $y_r = |r|^{-P}$ for $r \neq 0$, some $P \in \mathcal{N}$, then $y \in \ell_1$ for $P > 1$ and is α-algebraically localised about $r = 0$ for $\alpha < P - 1$. The Fourier transform

$$\hat{y}(k) = \frac{1}{\pi}\, g_P(k).$$

Hence

$$\hat{x}(k) = \frac{1}{\pi} \frac{g_P(k)}{(1 - 2\,\varepsilon\, g_K(k))}.$$

For $\varepsilon \neq 0$, this function is C^{N-2} and piecewise C^{N-1} with jumps in the $(N-1)$st derivative, where $N = \min(K, P)$. Thus by Fourier analysis (e.g. [5]), there exists $C \neq 0$ such that $|x_r| \sim C|r|^{-N}$.

Compare our bound

$$\sum_{r \in \mathcal{Z}} (1 + z|r|)^{\alpha} |x_r| \leq C'(\alpha, z) \quad \text{for all} \quad \alpha < N - 1,$$

which is slightly weaker.

Next we consider continuation of equilibria for the 1D case of the example (4.2). The equilibria are given by

$$V'(x_r) + \varepsilon \sum_{s \neq r} |r - s|^{-K} (x_r - x_s) = 0.$$

We know that the continuation of the initial solution $x_0 = 1, x_r = 0\,(r \neq 0)$ is in ℓ_1 for $K > 1$, thus $|x_r| \to 0$ as $|r| \to \infty$, and so it makes sense to separate the linearised part of the equation about 0 from the remainder:

$$\omega_0^2\, x_r + \varepsilon \sum_{s \neq r} |r - s|^{-K}\, (x_r - x_s) = y_r := \omega_0^2\, x_r - V'(x_r) = O(x_r^2)\,,$$

where $\omega_0^2 = V''(0)$. It follows that

$$\hat{x}(k) = \frac{\hat{y}(k)}{\omega_0^2 + 2\varepsilon\, (g_K(k) - g_K(0))}.$$

Now $y_r = O(x_r^2)$ implies that y_r decays more rapidly than x_r with r and hence that $\hat{y}$ is strictly smoother than $\hat{x}$ (a little more work is required to give a rigorous statement here). Hence we deduce that the smoothness of $\hat{x}$ is that of the denominator, i.e. $\hat{x}$ is C^{K-2} and piecewise C^{K-1} with jumps in the $(K-1)$st derivative. It follows that there exists $C(\varepsilon) \neq 0$ such that

$$x_r \sim C(\varepsilon)|r|^{-K}.$$

The same sort of argument can be attempted to find the asymptotics of the spatial decay for breathers in this model. We recall that in the case of finite range interactions in a translation invariant lattice, the decay in space of each time-Fourier component of a breather is asymptotically exponential with exponent given in the simplest cases by the smallest imaginary part of the roots k of the continuation of the dispersion relation for linearised solutions about equilibrium to complex wave number [6] (strictly speaking, the analysis given there needs extending to estimate the effect of the nonlinear remainders, including interaction of different time-Fourier harmonics, and this effect can lead to different results for the spatial decay of some of the harmonics, as was realised in [7]; a rigorous analysis can be obtained by bounding the spatial Fourier transform of the m^{th} harmonic in a strip $|\mathrm{Im}\, k| \leq \delta_m$).

In the case of algebraically decaying interactions, the dispersion relation does not have an analytic continuation to complex wave numbers, and in any case the problem always reduces to a linear inhomogeneous one rather than linear homogeneous, because of the infinite range of the interaction. We can write the equations of motion as

$$\ddot{x}_r + \omega_0^2\, x_r + \varepsilon \sum_{s \neq r} |r-s|^{-K} \left(x_r - x_s\right) = y_r := \omega_0^2\, x_r - V'\left(x_r\right) = O\left(x_r^2\right).$$

If the breather has frequency ω_b, its time-Fourier harmonics separate on the left but are mixed on the right. We obtain for the m^{th} time-Fourier component x^m of the breather

$$\hat{x}^m(k) = \frac{\hat{y}^m(k)}{\omega_0^2 - m^2\omega_b^2 + 2\,\varepsilon\, \left(g_K(k) - g_K(0)\right)}.$$

It is not easy to make a rigorous argument in this case, but it is plausible that y^m decays in space faster than x^m, at least for the fundamental ($m = 1$), and hence the smoothness of $\hat{x}^m$ would be given by the denominator again, so the oscillation amplitude would decay in space like $C|r|^{-K}$.

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