Discrete Breathers: Classical and Quantum

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Abstract

Discrete breathers are time-periodic spatially localised motions in networks of oscillators. Their occurrence in three principal contexts is reviewed: (i) autonomous Hamiltonian or reversible systems, (ii) autonomous forced damped systems, and (iii) time-periodically forced systems. The main proposed area of application, however, is to molecular crystals, where quantum effects must be taken into account. Thus an idea for a theory of quantum discrete breathers is also presented, though some details remain to be worked out.

Key words: Localisation; Nonlinear Dynamics; Spectral Projection; Discrete Breather
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1 Introduction

Discrete Breathers (DB), also known as Intrinsic Localized Modes, or Nonlinear Localised Excitations, are an important new phenomenon in physics, with potential applications of sufficient significance to rival or surpass the Soliton of integrable partial differential equations. They occur in networks of oscillators rather than spatially continuous media, and are time-periodic spatially localised solutions. The three principal classical contexts in which they arise are:

(1) Autonomous Hamiltonian or reversible systems;
(2) Autonomous forced damped systems;
(3) Time-periodically forced systems.

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The conditions under which they occur in each of these contexts will be reviewed, together with their principal properties and some connections with experiments.

The main proposed area of application, however, is to molecular crystals, where quantum effects must be taken into account. Thus an idea for a theory of Quantum Discrete Breathers will also be presented.

Before commencing, here are a few comments on terminology.

(1) "Network" includes all crystalline lattices and also quasicrystal and amorphous arrays. Mathematically, it is a countable metric space (S, d). Note that the word "countable" includes the finite case.
(2) "Oscillator" includes rotors (e.g. [108]) and spins (e.g. [70]). The important mathematical feature is that they possess periodic orbits. They differ only in the topology of the state space $(\mathbb{R}^2, \mathbb{R} \times S^1, S^2)$.
(3) The meaning of "spatially localised" will depend on the context, but the default is exponential localisation, i.e. the amplitude of oscillation at site s is bounded by $C\lambda^{d(s,o)}$ for some site o and constants $C > 0$ and $\lambda \in (0, 1)$.

2 Discrete Breathers in Autonomous Hamiltonian or Reversible Systems

The central class of system for which the idea of discrete breather was developed is autonomous spatially discrete Hamiltonian models. Many of these also possess a time-reversal symmetry, which can simplify the analysis, and indeed can substitute for the Hamiltonian property, so we treat the two cases in parallel. For some other surveys on breathers in the Hamiltonian or reversible case, see [104,47,9].

The class of autonomous Hamiltonian or reversible networks can be arranged in a hierarchy of increasing physical relevance and mathematical difficulty. We start with the simplest case.

2.1 Discrete Self-Trapping networks

The simplest type of autonomous Hamiltonian or reversible network system is a discrete nonlinear Schrödinger (DNLS) network

$$\mathrm{i}\dot{\psi}_s = \omega_0 \psi_s + |\psi_s|^2 \psi_s + \varepsilon \sum_{r \in S} \Delta_{rs} (\psi_r - \psi_s). \qquad (1)$$

and generalisations called discrete self-trapping (DST) equations (e.g. [101]). In addition to a Hamiltonian structure ($i\dot{\psi} = \frac{\partial}{\partial\bar{\psi}} H(\psi, \bar{\psi})$) and a time-reversal symmetry (complex conjugation), they have a global phase rotation symmetry, which implies that there are solutions of the form $\psi_s(t) = u_s \, e^{-i\omega t}$ provided u satisfies (for DNLS):

$$(\omega - \omega_0) u_s = |u_s|^2 u_s + \varepsilon \sum_{r \in S} \Delta_{rs} (u_r - u_s). \tag{2}$$

In particular, if Δ is real, $\omega > \omega_0$ and ε is small enough, there are real solutions u close to any configuration $\sigma \in \{0, \pm\sqrt{\omega - \omega_0}\}^S$ (a simple application of [81]). If Δ_{rs} decays suitably with $d(r,s)$, those solutions with only finitely many of the σ_s non-zero are spatially localised (apply [17] or [18]). Thus, one obtain DBs, as found numerically in [34]. They are very special DBs, however, having only a single Fourier harmonic in time.

2.2 Klein-Gordon networks

The next simplest type of system of this class can be called *Klein-Gordon networks*. They include the DNLS networks but are much more general since global phase rotation symmetry is not imposed. They are Hamiltonian systems consisting of one degree of freedom anharmonic Hamiltonian oscillators coupled weakly in a network. "Anharmonic" means that the frequency of oscillation varies non-trivially with amplitude [2]. The simplest type of coupling is nearest neighbour and linear.

A basic example of a Klein-Gordon network is a 1D chain of Morse oscillators connected by springs, whose Hamiltonian is:

$$H(p, q) = \sum_{n \in \mathbb{Z}} \frac{1}{2} p_n^2 + V(q_n) + \frac{\varepsilon}{2} (q_{n+1} - q_n)^2, \tag{3}$$

where

$$V(q) = \frac{1}{2} (1 - e^{-q})^2. \tag{4}$$

For the Morse oscillator, the frequency of oscillation is given by

$$\omega = 1 - I, \tag{5}$$

[2] A better word is "non-isochronous", but it seems not to be used much in physics. Note that there are other isochronous potentials besides parabolae, even analytic ones [26].

where $I = \frac{1}{2\pi}\oint p.dq$, integrating around the periodic orbit. The frequency decreases as the amplitude of oscillation increases, so the oscillator is called "soft" (the opposite case, called "hard", can be treated equally well).

Klein-Gordon models (in common with DST equations) have the additional feature that they are time-reversible: there is a "reversor", that is an involution of phase space (in this case, $p \mapsto -p$) which reverses the flow.

For $\varepsilon = 0$ there are trivial DBs: simply choose to put one unit, say $n = 0$, on a periodic orbit, and the remainder at equilibrium $q_n = 0$. Denote the frequency of the chosen orbit by ω_b and the frequency of linearised oscillations about the equilibria by ω_0 (which is 1 for our normalised Morse oscillator). If the *non-resonance* condition $m\omega_b \neq \omega_0$ holds for all $m \in \mathbb{Z}$ (which is easy to achieve) then there is an $\varepsilon_0 > 0$ such that the DB persists for all $|\varepsilon| < \varepsilon_0$, uniformly in the size of the network. Furthermore, for nearest neighbour or exponentially decaying coupling, the amplitude of oscillation of the DB is bounded by an exponential decay in space, uniformly in the system size.

The proof of the above result given in [80] uses both the Hamiltonian and time-reversible structure, but it is indicated there that one or other structure would suffice. A proof using only the Hamiltonian structure is given in [103] (another proof is sketched in [23] and given in more detail in [92]). The reversible structure alone suffices provided the chosen orbit is symmetric under the reversor. Sometimes a different reversor can be found to render a given periodic orbit symmetric; for example, rotary motion of a pendulum is not symmetric under $p \mapsto -p$ but is symmetric under $q \mapsto -q$ which is also a reversor. Also the spatial localisation result in [80] is just for the 1D nearest neighbour case, but in [103] a general result for exponentially decaying interactions [17] is used. Power law decay can also be treated [18], which is relevant to dipole-dipole and van der Waals interactions, and leads to power law localisation (results confirmed numerically in [42]).

The existence of DB in Klein-Gordon networks contrasts with two other situations:

(1) In the linearised problem for a 1D nearest neighbour chain, every localised initial condition disperses, because the solution can be written as $q_n(t) = \int dk A(k)\, \mathrm{e}^{\mathrm{i}(kn-\omega(k)t)}$ with $\omega(k) = \omega_0^2 + 4\varepsilon \sin^2 k/2$, and $\omega'(k)$ is not constant.
(2) The continuum limit problem $q_{tt} = q_{xx} - V'(q)$ has a breather if and only if V is a sinusoid [65].

In the Hamiltonian case, these DB are stable for small coupling, provided the stronger non-resonance condition $m\omega_b \neq 2\omega_0$ holds for all $m \in \mathbb{Z}$. More precisely, there is an $\varepsilon_1 > 0$ (depending on the model and the distance from resonance) such that they are ℓ_2-linearly stable for $\varepsilon < \varepsilon_1$ [82]. Stability in the reversible non-Hamiltonian case remains to be investigated [3].

Modulo the effect of damping, DB can be demonstrated in chains of pendula connected by torsion springs, e.g. [97] [4]. They are also believed to occur in DNA, where the local oscillators are the hydrogen-bonded base pairs and the coupling is provided by dipole-dipole interaction and via the phospho-diester helices (see [49] and the evidence for local openings in [71]).

By starting with several units excited at $\varepsilon = 0$, one can make "multibreathers". The chosen oscillations at $\varepsilon = 0$ should be in rational frequency ratio, and unless all the oscillators are excited, the non-resonance condition is required on ω_b, now defined to be the largest number which divides all the excited frequencies integrally. If the system is reversible and the chosen oscillations are symmetric then there are two choices of initial phase (0 and π) for each excited oscillator which give a symmetric periodic orbit; each configuration of phases 0 and π on the excited sites gives rise to a persisting symmetric periodic orbit. If either of those assumptions fail but the system is Hamiltonian and the number N of excited units is finite [5], then one can still prove existence of at least 2^{N-1} nearby periodic orbits for small coupling, corresponding to phase relations which make an "effective Hamiltonian" stationary, but they do not necessarily move continuously with ε (the idea was mentioned in [80] and fleshed out in [9] and [5]). In general, phase differences other than 0 and π lead to an average energy flow between the excited units, hence most non-symmetric multi-breathers are transporting energy (a simple rigorous example was given in [80], followed by numerics in [9]). If the phase relations do not correspond to a critical point of the effective Hamiltonian, there still exist "generalised multibreather" solutions, which look like multibreathers but have slowly evolving relative phases [5].

Numerical experiments (e.g. [94]) indicate that in a certain range of energy density e, DBs (or some approximate superposition of them, some of them quasiperiodic) form spontaneously. This appears to contradict the above stability result, because that applies equally well in backwards time. The resolution of the paradox is that the formation of DBs occurs in ℓ_∞ (bounded perturbations) whereas the stability result is only in ℓ_2 (finite energy perturbations). There are interesting interactions between breathers and phonons, e.g. [30], which are relevant to the formation process and breather life-times under perturbation.

An interesting question is whether one can predict the number of DBs which

[3] Is there an analogue of symplectic signature?

[4] This reference concentrates on travelling DB, but the same apparatus has been used to demonstrate standard DB too.

[5] It would be interesting to address the case with infinitely many excited oscillators, where it is non-trivial to use energy conservation.

form, and their distribution of energies. A first attempt was made in [75]. The answer should be given by the canonical ensemble $Z(\beta)^{-1}\,\mathrm{e}^{-\beta H}\,d\mu$, where μ is Liouville measure, $Z(\beta) = \int \mathrm{e}^{-\beta H}\,d\mu$, and the inverse temperature $\beta = 1/T$ is related to e by

$$e = -\frac{1}{N}\frac{\partial}{\partial\beta}\log Z(\beta). \tag{6}$$

The only difficulty is to assign to each point in phase space a configuration of DBs. For weak coupling ε, a crude criterion is that there is a DB on a site s if its action I_s exceeds $C\varepsilon$, where C is a constant depending on anharmonicity and the form of coupling, since this is the range of existence given by our proof and is plausibly the right order of magnitude. Using this, the probability of seeing a DB on a given site is

$$P(DB) = \int_{C\varepsilon}^{\infty} \mathrm{e}^{-\beta H(I)}\,dI \Big/ \int_{0}^{\infty} \mathrm{e}^{-\beta H(I)}\,dI \tag{7}$$

For example, for the chain of Morse oscillators with T and ε small, C should be chosen of order 1 and then $P(DB) \sim \mathrm{e}^{-\beta C\varepsilon}$. It would be interesting to test this numerically.

One might be tempted to speculate that DBs can be continued as long as the frequency remains non-resonant with the phonon spectrum, that is the set of frequencies for bounded solutions of the coupled linearised system, but localised modes can also appear on breathers [85], and their Floquet multipliers can approach $+1$ and lead to breather bifurcation (investigated further in [16], a paper that we did not yet publish because we wanted in addition to predict the number of localised modes). These localised modes can lead to approximate quasiperiodic (QP) breathers, but it is conjectured that true QP breathers do not exist in general. Exact QP breathers are easy to make in DNLS networks, however, as pointed out in [80], by using the above construction to make a non-trivial multibreather (i.e. with more than one Fourier coefficient) for some modified value ω_1 of ω_0 and then phase rotating at rate $\omega_0 - \omega_1$ to make a solution for the original problem; if this rate is incommensurate with the chosen frequency, the result is quasiperiodic.

The estimates in the theorems can be made quantitative. In particular, a rigorous domain of existence of DB for the 1D Morse chain in the space of (ω_b, ε) has been obtained in [59].

There is no limit on the dimensionality of the lattice, provided that the vector field remains uniformly C^1. There is no need even for a regular lattice. One just requires a condition on the coupling that the force on one unit due to displacing the others by a bounded amount is bounded. An interesting conjecture, however, is that in two or more dimensions there is a positive minimum energy for a breather [44] (proved in [114] for DNLS), which could have important physical consequences.

There is also no need to suppose that all the oscillators are identical. It is enough to require uniform bounds on the local dynamics. The non-resonance condition just becomes that there exists $K > 0$ such that for all $m \in \mathbb{Z}$ and i non-excited, $|m\omega_b - \omega_i| \geq K$, and the stability result requires the existence of a $K' > 0$ such that $|\omega_i + \omega_j - m\omega_b| \geq K'$ for all i, j non-excited and $m \in \mathbb{Z}$ [82]. A simple application would be to DNA, where there are two types of oscillator: the C-G and A-T base pairs. If the nonlinearity is reduced as the disorder is increased, interesting connections with the theory of Anderson localisation can be made, e.g. [8,66].

Similarly, the theory generalises to oscillators with more than one degree of freedom. All that is required is a normally non-degenerate family of periodic orbits [103].

2.3 Optic DB in Euclidean invariant systems

Klein-Gordon models, while important, are still quite a special type of Hamiltonian or reversible network, having only "optic" phonons. A crucial extension is to allow the "optic" degrees of freedom to interact with "acoustic modes". A key feature of such models is "piezoactivity": presence of an oscillation can lead to a change in the mean lengths of some bonds and hence a distortion of the mean configuration in addition to the localised vibration (e.g. [67,64]).

An example of such a system is a diatomic FPU chain, with masses 1 and M and interparticle potential $W(u) = \frac{1}{2}u^2 + k_3u^3 + k_4u^4$ depending on the separation u. For M large, existence of DB was proved, including an associated kink defect in the mean configuration when $k_3 \neq 0$ [74] [6]. An interesting feature for $k_4 > 0$ and k_3 large enough is that the kink distortion lowers the local frequency, allowing DB with frequencies below the optic band as well as above it [7]. Another simple example is a model for vibrations of a DNA chain allowing for acoustic waves [49]. I sketched how to prove existence of DB in this model during a conference in Crete in September 1995. A third example is treated numerically in [45].

[6] Actually, we inserted a linear term rather than a cubic one, but the effects are equivalent.

[7] An open problem, probably straightforward, is to prove rigorously the stability results of [99] and extend them to the case $k_3 \neq 0$.

One approach towards a more general result was developed in [10], but it requires a periodic lattice and harmonic acoustic degrees of freedom, coupled linearly to the optic ones. At a workshop in Dresden in April 97, however, I proposed a general strategy to treat DB in Euclidean invariant systems, whose cornerstone is a treatment of the statics problem of defects in Euclidean invariant systems [77]. The application to DB is given in [78].

2.4 Acoustic DB in Euclidean invariant systems

Numerics [105,91] and approximate theory (e.g. [32,98]) on monatomic FPU chains and other Euclidean invariant systems strongly suggest that "acoustic DB" can also occur, meaning ones which do not have an approximate description as a vibration of a molecule but instead are an analogue of the continuum sine-Gordon breathers, which are better thought of as the end result of modulational instability of a standing wave. Existence of DB can be proved for FPU chains with pure power potential ([91,41], details completed in [83]), but the question of extension to other potentials remains open (though Friesecke and I are hopeful that it can be treated by constrained minimisation methods).

2.5 Travelling breathers

A challenging open problem is to explain numerics (e.g. the numerous references surveyed in section 9.1 of [47] and the recent paper [13]) indicating the existence of travelling breathers in certain systems. An example with explicit travelling breather solutions was given in [1], but the existence of such solutions with tails going exactly to zero is unlikely to be general. Instead, there can be "nanopterons" [9] (for some rigorous results, see [57]). A proposal for a theory of approximate moving breathers is given in [5], which we are in the process of putting on a firm footing.

3 Discrete Breathers in Autonomous Forced Damped Systems

As a basic example here, consider a chain of pendula, with angles θ_n to the vertical, each with constant torque Γ and damping ν, coupled by torques of the form $\varepsilon \sin(\theta_{n+1} - \theta_n)$. For (ν, Γ) in the regions I and II of parameter space indicated in Figure 1, the phase portrait of a single unit has both an attracting equilibrium and an attracting (rotating) periodic orbit (Figure 2).

For $\varepsilon = 0$, we can make a DB by putting one pendulum on the periodic orbit and the rest at equilibrium. A result of [103] implies that it persists

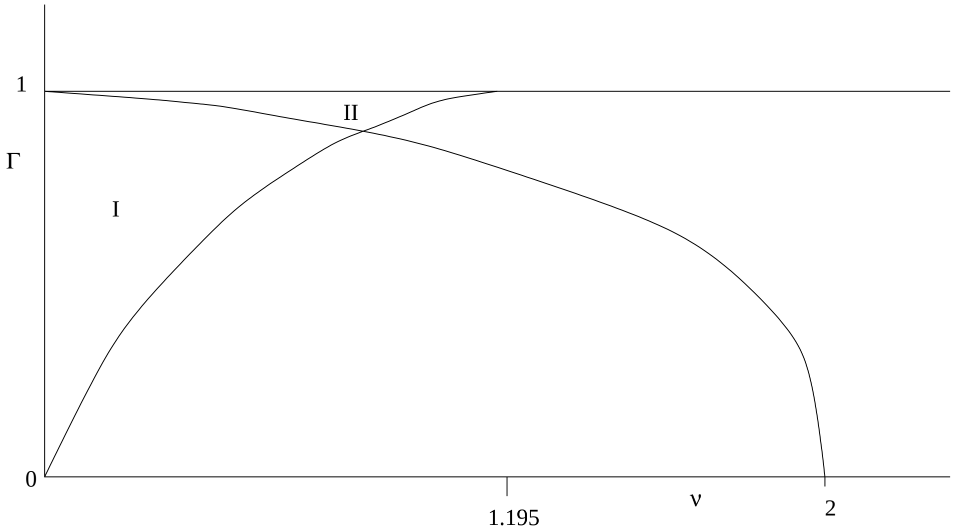

Fig. 1. The bistable region of parameter space for the pendulum with damping ν and torque Γ, separated into underdamped (I) and overdamped (II) cases.

for a range of ε uniformly in the length of the chain, the amplitude of motion decays exponentially with distance from the rotating pendulum and it attracts an ℓ_∞-neighbourhood.

Experimental demonstrations of these DB have recently been given in Josephson junction ladders (whose equations are very close to those for chains of damped pendula with torque) [109,25].

Multibreathers can also be obtained in such systems, under certain conditions

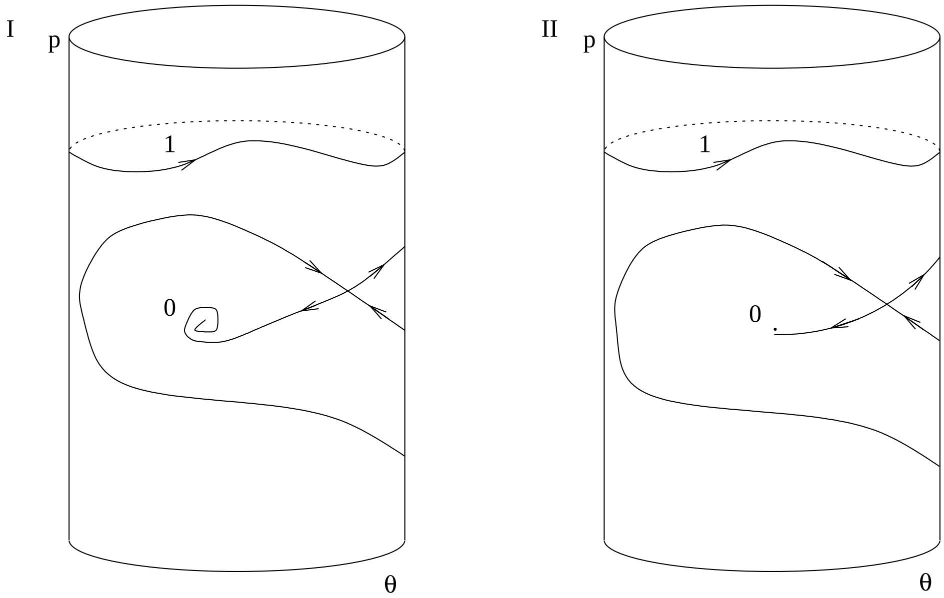

Fig. 2. The phase portraits for the bistable cases I and II of the forced damped pendulum.

[4]. A more general result is that the normally hyperbolic N-tori corresponding to N sites being on the periodic orbit, persist for small coupling uniformly in the size of the network (to be written up), but the dynamics on them need not contain periodic orbits close to any of the uncoupled case, nor even any periodic orbits at all. The flow on a 2-torus can not be chaotic but may be quasiperiodic, and the flow on an N-torus with $N \geq 3$, for arbitrarily weak coupling, can exhibit remarkably complex behaviour including chaotic, e.g. [15]. The solutions could be called "dissipative generalised multibreathers". Ignoring the dynamics on them, however, these N-tori could be used for coding. Indeed, one can reinterpret some of the proposed strategies for Josephson supercomputer memory in these terms, though the latest favourite seems to be to trap and eject flux quanta [73].

4 Discrete Breathers in Time-periodically forced systems

Time-periodic forcing is a common experimental scenario to probe a system. In periodically forced networks of oscillators, DB can occur whose period is commensurate with the forcing [96]. The theory of DB is easier for this case than for autonomous systems, as there is no longer any phase-shift degeneracy. The existence theory applies equally well to Hamiltonian and non-Hamiltonian systems. The stability theory, however, is better developed for non-Hamiltonian systems (I am not aware of a publication on the stability of DB for periodically forced Hamiltonian systems, but it could be treated along similar lines to [82]).

The time-T map of a network of units forced at period T in time is a coupled map lattice. If the coupling for the ODEs is exponentially decaying in space then the same holds for the map, though in general with a weaker exponent [16] (this reference treats only the linearised problem, but that is the key step). So for this section let us consider coupled map lattices F.

Suppose the local dynamics for each unit has a fixed point O and some other periodic orbit P, period $p \geq 1$. In the uncoupled case, we can put one unit on P and the rest on O. This gives a DB. If P has no multiplier $+1$ and O has no multiplier a p^{th} root of unity, then there exists $\varepsilon_0 > 0$ such that the DB persists uniformly in the system size for $\varepsilon < \varepsilon_0$ (mentioned in one sentence in [76] by analogy to the case of equilibria which is treated in detail there). It is exponentially localised if the coupling is, and it uniformly exponentially attracts an ℓ_∞ neighbourhood if O and P are linearly attracting.

The last statement perhaps requires some justification, as it was not proved in [76]. Without loss of generality take $p = 1$ and put the uncoupled fixed point at 0. The idea is to construct an adapted norm on a neighbourhood which is contracted by the linearisation A_0 of F_0. If the multipliers of O and P are contained in the disc of radius $r < 1$ then for any $\mu \in (r, 1)$ and any initial norm $||.||$,

$$||x||_\mu := \sum_{n \geq 0} \mu^{-n} ||A_0^n x|| \tag{8}$$

defines an equivalent norm

$$||x|| \leq ||x||_\mu \leq C(\mu)||x||, \tag{9}$$

where $C(\mu) = \sum_{n\geq 0} \mu^{-n}||A^n|| < \infty$, and it is contracted by A_0:

$$||A_0 x||_\mu = \mu(||x||_\mu - ||x||). \tag{10}$$

Let $\kappa = \mu/C(\mu)$. If the coupled map lattice F_ε is locally uniformly C^1 on ℓ_∞, then in a local chart there exists $\delta > 0, \varepsilon_1 > 0$ such that

$$||F_\varepsilon(x) - F_\varepsilon(y) - A_0(x - y)|| \leq \kappa ||x - y|| \tag{11}$$

for $||x||_\mu, ||y||_\mu \leq \delta$ and $|\varepsilon| \leq \varepsilon_1$, and $||F_\varepsilon(0)|| \leq (1 - \mu)\delta$ for $|\varepsilon| \leq \varepsilon_1$. Hence

$$||F_\varepsilon(x) - F_\varepsilon(y)||_\mu \leq ||A_0(x - y)||_\mu + C(\mu)\kappa||x - y|| = \mu||x - y||_\mu \tag{12}$$

for $||x||_\mu \leq \delta$ and $|\varepsilon| \leq \varepsilon_1$. So F_ε is a μ-contraction on $||x||_\mu \leq \delta$ with respect to the adapted norm[8]. Thus it has a unique fixed point on this ball and it attracts the whole ball at rate at least μ.

Similarly, there are multibreathers: put some units on P and the rest on O.

A recent experiment which can be interpreted in these terms is reported in [100]. I suspect that the experiments of [72] on periodically forced vibrations of model solar sails can also be interpreted in these terms, though non-uniformities are clearly also important there because the system always chooses the same places to localise the vibrations.

In the periodically forced context, one can also obtain localised chaos quite easily. Start with individual units having a hyperbolic fixed point O (no multipliers on the unit circle) and a uniformly hyperbolic set Λ, and put one unit

[8] There are alternative constructions of adapted norms $||.||_*$ such that instead of (10), $||A_0 x||_* \leq \mu||x||_*$, but still $||x|| \leq ||x||_* \leq C||x||$, for some $\mu \in (r, 1)$ and $C \geq 1$, and then one can choose any $\kappa < (1-\mu)/C$ and obtain contraction constant $\mu + C\kappa < 1$ on a neighbourhood, by similar analysis.

on Λ and the rest on O. Then there exists $\varepsilon_0 > 0$ such that for $\varepsilon < \varepsilon_0$ there is a continuation of the invariant set, with topologically equivalent dynamics [76]. We call solutions on this invariant set, *chao-breathers*. Multi-chao-breathers can be constructed by starting with several units on Λ. If the coupling decays exponentially, then the effect of the chaos dies away exponentially in space from the excited units. If O and Λ are attracting, then the resulting invariant sets are uniformly ℓ_∞ exponentially attracting. The argument is an elaboration of the case of an attracting periodic orbit dealt with above, but if one is content just to prove existence of a uniform ℓ_∞ neighbourhood of attraction, it suffices to choose neighbourhoods of attraction for O and Λ, small enough that all η-pseudo-orbits in them are also uniformly hyperbolic for some $\eta > 0$, and take their product. Then this is also a neighbourhood of attraction for all $|\varepsilon| < \varepsilon_1$, some $\varepsilon_1 > 0$, and the intersection of its forward images is precisely the continued invariant set above.

Persistence of isolated invariant sets, without necessarily preserving topologically equivalent dynamics (cf. numerics of [87,28]), follows more generally from Conley index theory, an extension of the above idea of persistence of neighbourhoods of attraction to invariant sets which are not necessarily attractors nor necessarily uniformly hyperbolic, but are maximal for some neighbourhood. For a review of the basics of Conley index theory and an application to a network problem, see [22] [9] . To establish persistence of some form of chaos, one needs to extend the application of Conley index theory to connection matrices, as in [88].

5 Quantum Discrete Breathers

5.1 Introduction

The principal proposed applications of autonomous Hamiltonian or reversible DB are to motion at the atomic scale, for example:

- Molecular crystals [90], e.g. $H - H$ stretches [55] and rotations in solid H_2 or D_2 [33], $C = O$ stretches and bends in solid CO_2, $C = O$ stretches in acetanilide [35], proton motion along hydrogen bonds in N-methylacetamide and polyglycine I [62], $KHCO_3$ [38] and benzoic acid, rotations of a methyl group in 4-methyl pyridine [39], bond angle vibrations in $NaNO_2$ [60], and vibrations in CS_2 [51] and NH_4Cl [52].

[9] Note that the application given there is not uniform in the system size, because it involves a tensor product, but probably the method of Section 5.2 of the present paper could be used to obtain results uniform in the system size.

- Other crystals with narrow optic bands, like mica [86], $PtCl$ ethylenediamine chlorate [106], and NaI [64] (proposals for DB in diamond turned out to be incorrect, as shown by [110]).
- Biomolecules with weakly coupled degrees of freedom, like the $C = O$ stretches in globular proteins [101], in particular myoglobin [115], and the hydrogen bonds between base pairs in DNA, e.g. [49], and possibly the operation of some biomotors [11].
- Other polymers, like polyacetylene [112,111].
- Quasicrystals, e.g. $Al_{62}Cu_{25.5}Fe_{12.5}$ (section III.G.3 of [95]).
- Adsorbed gases on surfaces, e.g. CO on Ruthenium [58], and H on Silicon [27].
- Magnetic spin systems, e.g. the review [70].
- Amorphous solids, e.g. spectral hole burning [11], and interstellar hydrogenated carbon (Aubry, private communication).

There is experimental evidence for DB in many of these, but

(1) Few of the experiments observe spatial localisation, though see figure 4 of [40] and the previously mentioned reference [71] on DNA experiments;
(2) These systems are highly quantum mechanical so the classical theory does not really apply.

In an attempt to rectify the first of these problems, I looked at $PtCl$ ethylenediamine chlorate by neutron scattering instead of the Raman scattering of [106], using the MARI instrument on the ISIS facility at Rutherford Appleton Laboratory [79]. In contrast to light, the neutrons used have a wavelength comparable to interatomic distances, so their scattering could in principle provide information about spatial correlations of vibrations. The material contains long chains of $ClPt^{IV}Cl - Pt^{II} - ClPt^{IV}Cl - Pt^{II} \ldots$, and the suspected DB are symmetric stretches of the $ClPt^{IV}Cl$ "molecules". Unfortunately, we were not able to detect the $ClPt^{IV}Cl$ stretches among the many other modes of vibration with similar energies excited by the neutrons, let alone obtain sufficiently well resolved wave-number dependence of the scattering to infer their spatial structure. I proposed instead to try solid O_2. In the β-phase [56] (the stable form from 23.9K to 43.6K), there is just one molecule per rhombohedral unit cell, which makes it simple. The neutron scattering from oxygen is entirely coherent, thus correlations between motions of different O_2 molecules are maximally observable. From [6], however, the intermolecular coupling (even at normal pressures) appears to be stronger than the 0.75% anharmonicity of the O_2 stretch, so DB are unlikely. Perhaps it would be better to try solid D_2, though it has four molecules per unit cell, and except at low temperature it is rotationally disordered (which will allow critics to say the localisation is due to randomness!).

There have been several approaches to rectify the second problem, some of which even predate the theory of DB. In particular, the idea that interacting phonons might form a bound state has been around for a long time (e.g. see the reviews [2,3] and [68,69]). Explicit "quantum lattice solitons" have been found in some special quantum models, e.g. [102] plus the review in [101]. Numerics have been performed on (small) quantum systems (and theory on even smaller ones) which suggest narrow bands which have been assigned the name "quantum breather", e.g. [113]. Einstein-Brillouin-Keller (EBK) quantisation can be applied to classical DB [9], and more sophisticated local mean-field approximations have been developed [93]. Coherent state and path integral approximations have been applied, e.g. [107,48]. I have not, however, found a general rigorous theory about quantum analogues of DB, so I am attempting to develop one. If it works, its scope will be much broader than just quantum DB, having applications to spin systems, electron-phonon systems and many others. The basic idea is to obtain a persistence result for spectral projections; the strategy is outlined below, but the details are not yet finalised.

5.2 Persistence of spectral projections for networks of quantum units

Suppose we have a network S of quantum units. The network has large but finite size $N = |S|$. The quantum unit at site $s \in S$ has local complex Hilbert space U_s, which for purposes of presentation we take to be of finite dimension $d_s \geq 2$, and a local Hermitian operator V_s with eigenvalues $E_s^0 < E_s^1 \leq E_s^2 \leq \ldots \leq E_s^{d_s-1}$ and eigenbasis $0_s, 1_s, 2_s, \ldots, d_s - 1$ (we suppose at least the lowest eigenvalue to be simple). The simplest example is a two-level unit, representing a spin-$\frac{1}{2}$ particle in a magnetic field. For the application to quantum DB, we take one degree of freedom anharmonic quantum oscillators (but truncate the spectrum). For example, the Morse oscillator has eigenvalues $E^n = (n+\frac{1}{2})\hbar - \frac{1}{2}(n+\frac{1}{2})^2\hbar^2, 0 \leq n \leq \frac{1}{\hbar} - \frac{1}{2}$ [89], where $\hbar$ is Planck's constant (followed by continuous spectrum $[\frac{1}{2}, \infty)$). Without loss of generality, by shifting the zeroes of energy we take $E_s^0 = 0$ for all s. The principal feature that we want for the anharmonic units is that $E_s^2 \neq 2E_s^1$. For concreteness, we shall suppose

$$0 = E_s^0 < E_s^1 < E_s^2 < 2E_s^1 < E_s^3 \tag{13}$$

(soft but not too soft).

The state of the whole network is an element of the tensor product $\otimes_{s \in S} U_s$, i.e. the set of multilinear maps $\psi : \times_{s \in S} U_s^* \to \mathbb{C}$, where U^* is the dual of U. To make an orthogonal basis B for the tensor product one can take the set of configurations $\sigma = (\sigma_s)_{s \in S}$ where for each s, σ_s ranges over the local basis of U_s, and for each configuration σ define the basis element $|\sigma>$ to be the unique multilinear map such that $|\sigma>(\alpha) = 1$ if $\alpha_s = \sigma_s$ for all s and $|\sigma>(\alpha) = 0$

for all other choices of α_s from the bases of U_s.

Consider Hermitian coupling operators Δ^{rs} on the tensor product $U_r \otimes U_s$ (more than two-body interactions can also be considered, but two suffices for illustration). We suppose that

$$\sup_{s \in S} \sum_{r \in S} ||\Delta^{rs}|| \leq K. \tag{14}$$

Consider a Hermitian operator $H^\varepsilon = V + \varepsilon\Delta$ on $\otimes_{s\in S} U_s$, where $V = \sum_{s\in S} V_s$ and $\Delta = \sum_{r,s\in S} \Delta^{rs}$, each term being applied to the tensor product in the natural way.

For $\varepsilon = 0$, the bottom of the spectrum of H^0 is illustrated in Table 1, assuming all units to be identical for simplicity (some non-uniformity could be allowed, in which case we would consider the spectral projections corresponding to groups of nearby eigenvalues). For each eigenvalue, the table indicates typical eigenvectors, its multiplicity, and a name for its spectral projection. Recall that a *spectral projection* is a projection P onto a subspace corresponding to an isolated subset of the spectrum, whose complementary projection $Q = I - P$ projects onto the subspace corresponding to the complement of the spectrum. The *spectral gap* for a spectral projection P is $g = \inf\{|E_P - E_Q| : E_P \in \mathrm{spec} H_P, E_Q \in \mathrm{spec} H_Q\}$, where H_P, H_Q are the restrictions of H to the ranges of P and Q respectively.

Table 1
The bottom of the spectrum for an uncoupled network of identical units with (13).

eigenvalue	typical eigenvector	multiplicity	spectral projection
$2E^1$	$110\ldots0$	$N(N-1)/2$	$P^{(1,1)}$
E^2	$200\ldots0$	N	$P^{(2)}$
E^1	$100\ldots0$	N	$P^{(1)}$
0	$000\ldots0$	1	$P^{(0)}$

I wish to prove persistence of these spectral projections for some range of ε, uniformly with respect to N. This is not straightforward, however.

The usual norm on a tensor product of Hilbert spaces can be written as $||\psi|| = \sqrt{\sum_{\sigma\in B} |\psi_\sigma|^2}$, where ψ_σ is the component of ψ in basis direction $|\sigma>$. The associated norm on operators (as used for Δ^{rs} above) is $||\Delta|| = \sup_{\psi\neq 0} ||\Delta\psi||/||\psi||$ (which for Hermitian operators is equal to the largest eigenvalue in absolute value). For typical coupling Δ, however, $||\Delta||$ is of order N, so standard results on persistence of spectral projections, e.g. [61], apply only for $\varepsilon < c/N$ for some c of order 1. This is useless for applications to solid-state physics where N is of the order of 10^{23}.

There is a genuine problem: a typical perturbation of a network of quantum units turns the groundstate nearly orthogonal to its initial position as soon as $\varepsilon > c/\sqrt{N}$ for some c of order 1. A simple illustration is to take V to be two-level quantum units for which the groundstate $|\mathbf{0}>$ consists of each unit in its groundstate, and to take the perturbation, instead of coupling, to be simply a simultaneous rotation C_ε of all the bases by angle ε (physically, this is spin-$\frac{1}{2}$ particles in a magnetic field at angle ε). So $H^\varepsilon = C_\varepsilon V C_\varepsilon^{-1}$. Then the new groundstate is simply $C_\varepsilon|\mathbf{0}>$ and its overlap with the original groundstate $<\mathbf{0}|C_\varepsilon|\mathbf{0}> = \cos^N \varepsilon$ which decreases through $\frac{1}{2}$ at ε of order $1/\sqrt{N}$ and is exponentially small in N for any fixed $\varepsilon > 0$. Thus the groundstate does not move uniformly in N with respect to ε in the usual norm on the tensor product.

Note also that for typical perturbations, the energies move at rate proportional to N with respect to ε. A simple illustration of this is to take $H^\varepsilon = \sum_{s\in S}(V_s + \varepsilon I_s)$, where I_s is the identity on U_s, again a perturbation which does not perform any coupling but instead just shifts the local energy levels. Then the energy levels for the network each shift by $N\varepsilon$, which is of order 1 as soon as $\varepsilon = 1/N$. Thus for more general perturbation it is not at all obvious that any spectral gaps will persist for a range of ε independent of N.

The problem is easy to treat in systems which reduce to independent particles on the network: one simply does standard perturbation theory for the single particle problem and then superposes the results to deduce the spectrum for the full problem (for an example, see [19]). But as soon as the Hamiltonian is not quadratic in creation and annihilation operators, because of anharmonicity for example, it is very unlikely to be reducible to independent particles. Persistence of non-degenerate ground-state and its spectral gap has been proved by [63], using cluster expansions for the partition function at non-zero temperature, but they do not obtain that it moves smoothly in any sense, nor does their proof look easy to extend to higher spectral projections. A "size consistent" approach to treating electron correlation is proposed in [24], but it is not clear to me how to use it. Thus I have been trying a new technique.

My proposed solution is to use new norms[10] on the set of projections P on a tensor product. These norms are defined via the density matrices of infinitesimal changes to P for subsets of the network. For an operator A on $\otimes_{s\in S}U_s$ and a subset $\Lambda \subset S$, the *density matrix* A^Λ is the operator $Tr_{S\setminus\Lambda}A$ on $\otimes_{s\in\Lambda}U_s$. The partial trace is defined using a basis of the form B, so that $A^\Lambda_{\rho,\rho'} = \sum_\tau A_{\rho\tau,\rho'\tau}$ where ρ, ρ' are configurations on Λ and τ runs over configurations on $S \setminus \Lambda$. For an introduction to density matrices, see [37], but note that I do not normalise to $TrA = 1$, nor do I require $A^\dagger A$ non-negative. The importance

[10] It is commonplace nowadays to feel free to choose whatever norm is convenient, but some physicists have been happy to do this for many years, e.g. [7].

of density matrices goes back to [31], and was emphasised for example in [29].

For positive integer r, let $\mathbb{M}_r$ be the set of orthogonal projections P (i.e. $P^2 = P = P^\dagger$) of rank r on $\otimes_{s\in S} U_s$. It is a smooth manifold (a Grassmannian) of real dimension $2r(\prod_{s\in S} d_s - r)$. Define the *0-norm* on tangent vectors π to $\mathbb{M}_r$ at P by (it is easy to check that it has the defining properties of a norm)

$$|||\pi|||_0 = \sup_{\Lambda\subset S, \Lambda\neq\emptyset} ||\pi^\Lambda||/|\Lambda|. \tag{15}$$

For example, taking $r = 1$ and P_ε to be the projection onto the groundstate of our spin-$\frac{1}{2}$ system in a magnetic field at angle ε, and $\pi = \frac{\partial P_\varepsilon}{\partial \varepsilon}$, then $||\pi^\Lambda|| = |\Lambda|$, so $|||\pi|||_0 = 1$, uniformly in N, which suggests that the 0-norm is a good idea.

For a quantum system governed by Hermitian operator H, the evolution of any operator A is given by Heisenberg's equation $\dot{A} = \mathrm{i}[H, A]$, where $[H, A]$ denotes the commutator $HA-AH$. In particular, this equation defines a vector field $\dot{P} = F_H(P) = \mathrm{i}[H, P]$ on each of the manifolds $\mathbb{M}_r$ (it is easy to check that $\mathrm{i}[H, P]$ is tangent to $\mathbb{M}_r$).

Now it turns out that every non-degenerate equilibrium of F_H on $\mathbb{M}_r$ (i.e. P such that $F_H(P) = 0$ and the derivative $DF_H(P)$ is invertible) is a spectral projection of rank r with gap at least $|||DF_H^{-1}|||_0^{-1}$, and for an uncoupled network any spectral projection is a non-degenerate equilibrium with $|||DF_H^{-1}|||_0^{-1}$ equal to the spectral gap. To show these results, we use that $DF_H\pi = \mathrm{i}[H, \pi]$ and $T\mathbb{M}_{r,P} = \{\pi : \pi^\dagger = \pi, \pi P = Q\pi\}$, so in a basis for which $P = \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix}$ and $Q = \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}$, then π has the form

$$\pi = \begin{bmatrix} 0 & \alpha \\ \alpha^\dagger & 0 \end{bmatrix}, \tag{16}$$

and so if $[H, P] = 0$ then $H = \begin{bmatrix} H_Q & 0 \\ 0 & H_P \end{bmatrix}$ and

$$DF_H\pi = \mathrm{i}\begin{bmatrix} 0 & H_Q\alpha - \alpha H_P \\ H_P\alpha^\dagger - \alpha^\dagger H_Q & 0 \end{bmatrix}. \tag{17}$$

So at a spectral projection of an uncoupled network with gap g bounded away from zero, DF_H is invertible uniformly in N in the 0-norm.

Now $\frac{\partial F_{H^\varepsilon}}{\partial \varepsilon}(P) = \mathrm{i}[\Delta, P]$, so it can be shown that

$$|||\frac{\partial F}{\partial \varepsilon}|||_0 \leq \sup_s \sum_r ||\Delta^{rs}||, \tag{18}$$

which is bounded by K. Unfortunately, in general DF fails to be continuous in (P, ε) uniformly [11] in N. Otherwise we could use the implicit function theorem to deduce that a non-degenerate equilibrium of F_H persists for an interval of ε, with estimates uniform in N, giving a smooth continuation P_ε of the spectral projection P_0 for H^0, moving with velocity $\frac{dP}{d\varepsilon} = -DF_{H^\varepsilon}^{-1} \frac{\partial F_{H^\varepsilon}}{\partial \varepsilon}(P_\varepsilon)$, bounded uniformly in N.

In fact, such a result can not hold without using more features of our problem, like non-degeneracy of the groundstates of the individual units, otherwise it would imply contradictions with the known behaviour of some models like the half-filled 1D Hubbard model, for which the gap between the "Heisenberg antiferromagnet band" and the "charge excitations" closes at an electron hopping amplitude of around $1/\sqrt{N}$. An even easier counterexample is to take $E_s^0 = E_s^1 = 0, E_s^2 = 1$ and $\Delta = \sum_{s \in S} \Delta^s$ with $\Delta^s = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, for which the spectrum of H^ε is $\{0, \varepsilon, \ldots, N\varepsilon, 1, 1+\varepsilon, \ldots, 1+(N-1)\varepsilon, \ldots\}$, and so the spectral gap for the spectral projection continuing that onto the groundstates of $\varepsilon = 0$ closes [12] at $\varepsilon = 1/N$. Thus we must use the assumption of non-degenerate groundstate.

Another basic problem with the strategy so far is that DF is not bounded uniformly in N: typically, its 0-norm grows linearly with N. So there is no reason that DF should remain invertible for small changes in (P, ε). To take care of this problem, we define the *1-norm* on tangent vectors π at P_0 by

$$|||\pi|||_1 = ||||[H^0, \pi]||||_0 \tag{19}$$

[11] A family of functions $G : X \to Y$ between metric spaces all depending on N is continuous *uniformly in* N if there exists a function $\omega : \mathbb{R}_+ \to \mathbb{R}_+$ independent of N with $\omega(r) \to 0$ as $r \to 0$ and $d(G(x), G(x')) \leq \omega(d(x, x'))$ for all $x, x' \in X$.

[12] In generic one-parameter families, gaps do not close exactly, but for generic perturbations of these two examples the continuations of the spectral projections would cease to be uniformly smooth around these parameter values.

(it is a norm since P_0 is a spectral projection for H^0), and regard F_H as mapping $\mathbb{M}_r$ endowed with a metric induced by the 1-norm (in a manner to be explained shortly), to $T\mathbb{M}_r$ with the 0-norm [13]. Then the norm of DF_H becomes

$$|||DF_H|||_{1\to 0} = \sup_{\pi\neq 0} \frac{|||[H,\pi]|||_0}{|||[H^0,\pi]|||_0} = 1 + |\varepsilon| \sup_{\pi\neq 0} \frac{|||[\Delta,\pi]|||_0}{|||[H^0,\pi]|||_0}, \tag{20}$$

which, at the spectral projections of Table 1 under hypothesis (13), is at most $1+|\varepsilon|K/g$, where K was defined in (14). Such a bound does not hold if E_s^0 is not required to be simple, because Δ can link pairs of states, one in the range of P_0 and the other in the range of Q_0, with amplitude of order N, for which in contrast the unperturbed energy difference is of order 1.

The next problem is that $\mathbb{M}_r$ is not a linear space so we need to understand how to compare tangent vectors at different points, which is implicit in any discussion of how DF_H varies with position and is now crucial because we defined the 1-norm only at P_0. To resolve this, we define a diffeomorphism $\mathbb{P}$ from a neighbourhood of 0 in $T\mathbb{M}_{r,P_0}$ to a neighbourhood of P_0 in $\mathbb{M}_r$, and use it to transport everything back to $T\mathbb{M}_{r,P_0}$.

To define $\mathbb{P}$, let $J = Q_0 - P_0$, and given $\pi \in T\mathbb{M}_{r,P_0}$, let $\mathbb{P}(\pi) = e^{J\pi}P_0e^{-J\pi}$, which is a unitary transformation of P_0 and hence remains in $\mathbb{M}_r$ (the exponential can be defined by power series or as the solution after time 1 of the differential equation $\dot{U} = J\pi U$ on the unitary group starting at the identity). Furthermore, the derivative of $\mathbb{P}$ at 0 is easily seen to be the identity, so $\mathbb{P}$ is a local diffeomorphism.

For $k \in \{0,1\}$, let M_k denote $T\mathbb{M}_{r,P_0}$ with the k-norm. Then, in place of the vector field F_H on $\mathbb{M}_r$, we define a map between linear spaces $G_H : M_1 \to M_0$ by

$$G_H(\pi) = \mathrm{i}e^{-J\pi}[H,\mathbb{P}(\pi)]e^{J\pi} = \mathrm{i}[A_\pi(H), P_0], \tag{21}$$

where

$$A_\pi(H) = e^{-J\pi}He^{J\pi}. \tag{22}$$

[13] This is analogous to the treatment of differential operators in functional analysis: for a function ρ, the map $u \mapsto (\rho u)_x$ on functions u of x is considered as mapping C^1 to C^0, the space C^1 being defined by applying the C^0-norm to the result of the standard differential operator $u \mapsto u_x$. Here, I use the uncoupled Hamiltonian H^0 to define the 1-norm.

Note that $G_H(\pi)$ is of the form (16) with $\alpha = A_\pi(H)_{QP}$, the block which maps the range of P_0 to the range of Q_0, so we will often represent π and $G_\pi(H)$ by just this block, and define the k-norm of such a block to be the k-norm of the full matrix (16).

We have to bound the derivatives $\frac{\partial G}{\partial \varepsilon}$ and DG, check that DG is invertible at $(0,0)$ and show that DG depends continuously on (π, ε), all uniformly in N. Firstly,

$$\frac{\partial G}{\partial \varepsilon} = \mathrm{i} A_\pi(\Delta)_{QP}. \tag{23}$$

At $\pi = 0$ this is simply Δ_{QP}, and as before, $|||\Delta_{QP}|||_0 \leq K$. We leave discussion of the case $\pi \neq 0$ for later.

Secondly, to evaluate DG we need the derivative of $e^{J\pi}$ with respect to π. Using the differential equation acting on a variation σ, this is

$$\frac{\partial}{\partial \pi} e^{J\pi}(\sigma) = e^{J\pi} B_\pi(\sigma), \tag{24}$$

where

$$B_\pi(\sigma) = \int_0^1 A_{\pi t}(J\sigma)\ dt. \tag{25}$$

Then

$$DG_{H,\pi}(\sigma) = \mathrm{i}[A_\pi(H), B_\pi(\sigma)]_{QP}. \tag{26}$$

At $\pi = 0$, we have $B_\pi(\sigma) = J\sigma$, so

$$DG(\sigma) = \mathrm{i}[H, J\sigma]_{QP} = \mathrm{i}(H_Q \sigma - \sigma H_P). \tag{27}$$

Now the 1-norm of σ is defined to be the 0-norm of $\mathrm{i}[H^0, \sigma] = \mathrm{i}(H^0_Q \sigma - \sigma H^0_P)$. Thus at $\varepsilon = \pi = 0$, we have $|||DG|||_{1\to 0} = |||DG^{-1}|||_{0 \to 1} = 1$.

Thirdly, for $\pi = 0$, we have

$$\frac{\partial DG}{\partial \varepsilon}(\sigma) = \mathrm{i}[\Delta, J\sigma]_{QP} = \mathrm{i}(\Delta_Q \sigma - \sigma \Delta_P), \tag{28}$$

so $|||\frac{\partial DG}{\partial \varepsilon}|||_{1\to 0} \leq K/g$, at the spectral projections of Table 1 assuming (13).

The question remaining is how DG and $\frac{\partial G}{\partial \varepsilon}$ vary with π (including at $\varepsilon \neq 0$), and this is the point at which my work is incomplete. It is most simply tackled by looking at their derivatives with respect to π. Now

$$
\begin{aligned}
D^2G(\sigma,\tau) = & \,\mathrm{i}[[A_\pi(H), B_\pi(\tau)], B_\pi(\sigma)]_{QP} \\
& + \mathrm{i}[A_\pi(H), \int_0^1 [A_{\pi t}(J\sigma), B_{\pi t}(\tau)]\ dt]_{QP}.
\end{aligned} \tag{29}
$$

To achieve a uniform bound on D^2G, the size of this needs measuring in the 0-norm and comparing to the product of the 1-norms of σ and τ. I expect it to be bounded, but I have not yet analysed this. Similarly, at general π,

$$
\frac{\partial DG}{\partial \varepsilon}(\sigma) = \mathrm{i}[A_\pi(\Delta), B_\pi(\sigma)]_{QP}, \tag{30}
$$

whose 0-norm I also expect to be bounded in terms of the 1-norm of σ.

I hope to check these two matters in the near future, but if we assume uniform bounds "β" on D^2G and $\frac{\partial DG}{\partial \varepsilon}$ then we would deduce that each spectral projection of H^0 persists uniformly in N to a spectral projection of H^ε for a range of ε depending only on the "strength" K of the coupling, the initial spectral gap g and the bounds β. In particular, the spectral projections $P^{(0)}, P^{(1)}, P^{(2)}, P^{(1,1)}$ for H^0 would persist to spectral projections $P_\varepsilon^{(0)}, P_\varepsilon^{(1)}, P_\varepsilon^{(2)}, P_\varepsilon^{(1,1)}$ for H^ε for $\varepsilon < \varepsilon^{(0)}, \varepsilon^{(1)}, \varepsilon^{(2)}, \varepsilon^{(1,1)}$ respectively, all positive, uniformly in N.

5.3 Definition of quantum discrete breathers

Let us suppose that bounds β of the previous subsection exist for the anharmonic quantum network. Then we can define quantum discrete breathers (QDB).

Definition 1 *Non-zero vectors in the ranges of $P_\varepsilon^{(0)}, P_\varepsilon^{(1)}, P_\varepsilon^{(2)}, P_\varepsilon^{(1,1)}$ are called groundstate, first excited QDB, second excited QDB, $(1,1)$-multiQDB, respectively.*

Extension to more highly excited QDB and multiQDB is obvious, but the range of coupling over which they persist is likely to be smaller.

It remains to justify the names. First we show that the parts of the spectrum associated with these spectral projections come in the same order as for the uncoupled case. In considering the vector field F_H on $\mathbb{M}_r$ we lose track of the absolute position of the spectrum of H, but we do retain information about the signed spectral differences between $specH_P$ and $specH_Q$ for $P \in \mathbb{M}_r$. Even though $\mathbb{M}_r$ is not a complex manifold ($P^\dagger = P$ is not a complex equation), there is a natural complex structure on the tangent space $T\mathbb{M}_{r,P}$ at P, because it is parametrised by the complex $(\prod_s d_s - r) \times r$ matrices α of (16). Now the linearised vector field at an equilibrium in an eigenbasis for H is

$$\dot{\alpha}_{qp} = i(E_q - E_p)\alpha_{qp}, \tag{31}$$

with q labelling eigenstates of H_Q and p labelling those of H_P. So the $\mathbb{C}$-eigenvalues of the linearised vector field are $\mathrm{i}(E_q - E_p)$. The spectrum of the equilibrium would move continuously with ε if the bounds β hold (apply standard analysis to the resolvent $[DF_{H^\varepsilon}(P_\varepsilon) - \lambda]^{-1}$ for λ not in the spectrum, e.g. [61]), and is always on the imaginary axis, thus as long as the equilibrium remains non-degenerate, none of its spectrum can cross 0. Hence the signs of the spectral differences remain constant. In particular the groundstate remains the groundstate and the spectrum associated with $P_\varepsilon^{(0)}, P_\varepsilon^{(1)}, P_\varepsilon^{(2)}, P_\varepsilon^{(1,1)}$ and their total complement remain in order.

Secondly, we show that the range of $P_\varepsilon^{(1)}$ looks like one unit first excited and the rest in their groundstates. This is not true of all elements of the range nor necessarily of the eigenstates; for example, in a translation invariant system, the eigenstates can be chosen to be Bloch waves. But it is true of the subspace taken as a whole, in the sense that the density matrix for $P_\varepsilon^{(1)}$ on a single site s has the form

$$(P_\varepsilon^{(1)})^{\{s\}} = \left[\begin{array}{cc|c} N-1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 0 \end{array}\right] + O(\varepsilon) \tag{32}$$

in the basis $0_s, 1_s|2_s, \ldots$, where the remainder above is measured in the norm for the single unit. It is standard that the expectation of a density matrix in a state, divided by its trace, is interpreted as the probability of being in that state. The trace of any density matrix of a projection operator is simply its rank, so N in this case. Thus in the range of $P_\varepsilon^{(1)}$ the probability of seeing unit s in state 0_s is $1 - (1 + O(\varepsilon))/N$, that for state 1_s is $(1 + O(\varepsilon))/N$ and that summed over all other basis states of unit s is $O(\varepsilon)/N$. Thus indeed we have a probability close to $1/N$ of seeing any given unit in its first excited state. We can strengthen the statement by analysing the density matrix for a pair of states:

$$(P_\varepsilon^{(1)})^{\{r,s\}} = \left[\begin{array}{ccc|c} N-2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right] + O(2\varepsilon) \tag{33}$$

in the basis $0_r0_s, 1_r0_s, 0_r1_s|1_r1_s, \ldots$. Thus the probability of seeing the pair r, s is state 0_r0_s is near $1 - 2/N$, those for 1_r0_s and 0_r1_s are near $1/N$ and the probability of any other basis state, in particular 1_r1_s, is near zero. Thus there is a strong anticorrelation in range $P_\varepsilon^{(1)}$ for two excitations. Similarly, the range of $P_\varepsilon^{(2)}$ looks like one unit second excited and the rest in their groundstate, and the range of $P_\varepsilon^{(1,1)}$ looks like two units first excited and the rest in their groundstate.

To justify the name of QDB fully, I would like to show a stronger spatial localisation result, if the coupling matrix Δ has finite range or exponential decay with distance $d(r, s)$ between units. Namely, for the range of $P_\varepsilon^{(2)}$ I conjecture that the probability of seeing units r, s in state 1_r1_s is less than $C\varepsilon\lambda^{d(r,s)}$ for some $C > 0$ and $\lambda < 1$ independent of N (though in general dependent on ε), and analogous results for the other spectral projections, but this will have to wait for a future publication.

5.4 Discussion

At the conference, the above concept of QDB generated some controversy, so some discussion could be helpful. The apparent problem is that it would apply even to translation invariant systems, where all eigenstates are extended (Bloch waves). It is important to understand, however, that I am not claiming that the eigenstates are localised. What I am claiming (modulo establishing the bounds β of section 5.2) is that there is a range of weak coupling, independent of system size, for which there are spectral projections whose density matrices show strong anticorrelations between the positions of excitations. Note that this would hold even for what is traditionally called the "phonon band", namely my first excited QDB (a point not mentioned in [113] or [101]). I believe that my definition of QDB fits with the goal of all those previous attempts to formalise it which were listed in subsection 5.1.

One way of looking at the situation was understood by chemists in small systems since the 70s. They had found that spectroscopic measurements on benzene, for example, were much better interpreted in terms of localised C-H stretches and bends rather than normal modes. Even though all the eigenstates are extended, they resolved the paradox by estimating that the time it would take for a localised initial disturbance to tunnel to a different site was longer than the radiative decay time (see a nice discussion of this story in [101]). Our method is probably not required for benzene (N is only 6), though it could be expected to lead to a factor 6 extension of the range of electron hopping allowed for the validity of the local mode picture there.

A second question that has been raised is what about permutation symmetry for indistinguishable particles? In the setting treated here, however, the sites of the network are regarded as distinguishable, so I do not think the issue arises. Nonetheless, the method can easily be applied to problems with permutation symmetry, by restricting the tensor product to its odd or even subspace as appropriate.

Note that if a model has symmetries then these can be exploited to obtain more information about the spectrum. For example, in a crystal with a lattice of translation symmetries, pseudo-momentum vector $\mathbf{k}$ is a good quantum number, so one can treat each subspace of given $\mathbf{k}$ separately (Bloch waves), leading to a decomposition of the spectral projections as integrals over $\mathbf{k}$.

The programme of subsection 5.2 is likely to have many other applications than to QDB. For example, it would show that an array of spin-$\frac{1}{2}$ particles in a magnetic field interacting weakly with neighbours has a unique groundstate, a first excited part of spectrum corresponding to one spin being misaligned, a second excited part corresponding to two spins being misaligned, etc.. An interesting extension is that $A_{\pi_\varepsilon}(H^\varepsilon)_P$ would define an exact effective Hamiltonian for the dynamics on the range of the spectral projection P_ε.

The method would also allow us to extend results on existence of bipolarons in the adiabatic Holstein model [12,19–21] to the Holstein-Hubbard model, firstly in the adiabatic limit and secondly with quantum phonons. We sketch the idea for the first extension. When the electron hopping is zero, one can put each site into any of the electronic states $\emptyset, \uparrow, \downarrow, \uparrow\downarrow$ and obtain an equilibrium of the local optic degree of freedom $u_s = 0, -1, -1, -2$, respectively. Given a configuration of the $(u_s)_{s\in S}$ near the values 0 and -2, there is a non-degenerate groundstate consisting of $\emptyset$ on sites with u_s near 0 and $\uparrow\downarrow$ on sites with u_s near -2, and a gap to the rest of the spectrum. The method of this paper would prove that this groundstate and gap persist uniformly under changes in u and electron hopping amplitude. This is the key step that is required to prove persistence of the equilibrium configurations with $u_s \in \{0, -2\}$.

Perhaps the method could also be applied to excitons in polyphenylvinylene [53]. This is a material in which localised excitations can be created by passing a current, which decay by emitting visible light. Cambridge Display Technologies are producing flat screen displays using it, but they would like to know what determines the spatial size of the exciton.

I believe the method would find many other uses in quantum many body theory on lattices and simplify a lot of the calculations: no Feynman diagrams appear, there are no infinities to cancel, and no cluster expansions (contrast [84,54,14,36,50] for example) – just the standard implicit function theorem with novel norms.

I think also that an ℓ_1 version of the method will apply to problems in probability theory, such as the effect of weak coupling of many Markov processes into a network, where very similar issues to tensor products occur but the basic norm is the total variation norm (ℓ_1) rather than Hilbert (ℓ_2).

6 Conclusion

Discrete breathers are a widespread phenomenon in networks of oscillators, whether the dynamics is autonomous Hamiltonian or reversible, autonomous forced damped, time-periodically forced, or quantum. Discrete breathers are likely to provide explanations for many puzzling problems in physics and the basis for exciting new technology. For a recent conference proceedings on the subject, see [46], and for many further references, see the webpage [43]. A general method to prove persistence of spectral projections in quantum many body problems is proposed, with which it is hoped to put quantum discrete breathers onto a rigorous foundation, and if successful it is likely to have many other applications in solid-state physics.

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