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RESEARCH ARTICLE

Persistence of supersonic periodic solutions for chains with anharmonic interaction potentials between neighbours and next to nearest neighbours

Christine R. Venney[a*] and Johannes Zimmer[a]

[a]*Department of Mathematical Sciences, University of Bath, Bath BA2 7AY, UK*
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We consider an infinite chain of particles with nearest neighbour (NN) and next to nearest neighbours (NNN) being coupled by nonlinear springs. To mimic the Lennard-Jones potential, the NN and NNN springs act against each other. We prove that in contrast to the NN interaction case, there are supersonic periodic solutions.

Keywords: lattice dynamics; infinite-dimensional Hamiltonian dynamics; existence of periodic travelling waves; linking geometry; next to nearest neighbour interaction; advancedelay equation

MCS/CCS/AMS Classification/CR Category numbers: 37K60; 34A33; 34C15; 74J30

1. Introduction

Lattice models for solids involving nearest neighbour (NN) interaction have been studied with a variety of mathematical methods (to name a few studies, we refer the reader to [4, 8, 15]). In this paper we present mathematical results for a one-dimensional chain with springs linking anharmonic nearest neighbours and anharmonic next to nearest

*Corresponding author. Email: crv20@bath.ac.uk

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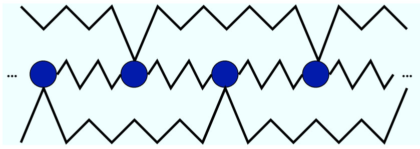

Figure 1. Springs with nearest neighbour (NN) and next to nearest neighbour (NNN) interaction.

neighbours (NNN), see Fig. 1. Specifically, we show that if the NN and NNN springs pull against each other with a ratio suggested by the harmonic model, then there exist slightly supersonic periodic waves, in contrast to the NN situation, where periodic waves are strictly confined to the subsonic regime.

The motivation for this paper is the analysis by Wattis [17], who finds subsonic solitary waves with oscillatory decay for the model considered here, using methods from asymptotic analysis. Again, this results suggests that the NNN interaction leads to phenomena not present in models with a pure NN interaction.

The inclusion of NNN springs can be seen as a poor man's version of a Lennard-Jones potential $a\left(-\left(\frac{b}{r}\right)^6+\left(\frac{b}{r}\right)^{12}\right)$, which is, if the distance between two atoms is r (in suitable units), a common physical model of interacting atoms. In physical reality, all atoms interact with each other. This is captured in the Lennard-Jones potential, but neither in the NN nor in the NNN model. Yet, the NNN model, in the regime we consider, has attractive and repulsive parts as the Lennard-Jones potential (unlike the simple NN model), which makes it an important step towards the analysis of fully-interacting systems. We remark that the chain with NNN interaction can also be seen as a one-dimensional model which captures long-range effects of higher-dimensional NN lattices [2, 12].

The effect of the inclusion of NNN springs has been studied for various applications. Charlotte and Truskinovsky [2] study a lattice model to examine surface relaxation; to this behalf, they consider a finite chain of atoms. Conventional models, which are limited to NN interaction, do not capture surface relaxation effects. The inclusion of NNN interaction (or further interactions) is shown to remedy the situation in the sense that experimental observations can be reproduced [7]. A detailed study by Charlotte and Truskinovsky [2] includes the NNN interaction to obtain a hyper-pre-stress; it is then shown that an exponential surface boundary layer is formed. The NN springs and the NNN springs are here incompatible in terms of their reference length. Surface relaxation in the presence of NNN interaction has also been reviewed by Salje [13].

Remarkably, there seems to be very little mathematical existence theory available for chains with NNN interactions even though this interaction is typically present in any physical system. Long-range interaction is also used to model biological systems; for example, Gaeta *et al.*s [5] describe the three-dimensional helicoidal structure of DNA approximately with a planar description which includes interactions with fifth neighbours. Calleja and Sire [1] use a centre manifold analysis to study combined NN and NNN interaction for the Frenkel-Kontorova chain, but with the two kinds of springs pulling in the same direction. Other analytical results we are aware of are by Percy Makita [10] (see also [9]). The system studied there includes some effects of NNN interaction, but for a different type of potential from that considered here. In particular, the competition of NN and NNN springs, which mimics the effect of a Lennard-Jones potential, is not studied in [9]. Numerical investigations can be found in [3]. The mathematical model is as follows.

For a chain of atoms, let u_j denote the position of atom j, with $j \in \mathbb{Z}$. We follow the convention to call quadratic potentials *harmonic* and anharmonic potentials *nonlinear*.

We examine the following equation of motion (obtained from the physical model using the travelling wave ansatz).

$$c^2 \ddot{u}(t) = U_1'\left(u(t+1) - u(t)\right) - U_1'\left(u(t) - u(t-1)\right) + g\left[U_2'\left(u(t+2) - u(t)\right) - U_2'\left(u(t) - u(t-2)\right)\right] . \quad (1)$$

Here U_1 is an anharmonic potential for the nearest neighbour interaction and U_2 is a (possibly harmonic) potential for the next-to-nearest neighbour interaction.

The stability of harmonic infinite chains with NNN interaction has been known for a long time [6]. Charlotte and Truskinovsky [2] provide an excellent synopsis of further related results. Here we consider a nonlinear context and prove under suitable conditions the persistence of periodic waves for all subsonic speeds and also, more unexpectedly, for a small range of supersonic speeds.

2. The mathematical setting

We are looking for periodic solutions of the equation (1). We write

$$U_1(r) = \frac{1}{2} c_0^2 r^2 + V(r) \quad (2)$$

and

$$U_2(r) = \frac{1}{2} c_0^2 r^2 + W(r) \; , \quad (3)$$

where $V(r)$ and $W(r)$ are higher order terms.

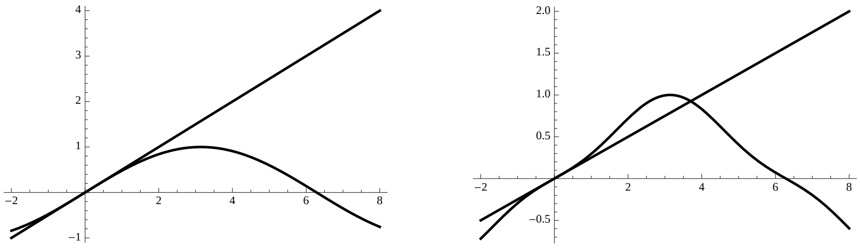

Figure 2. Plots of $\frac{1}{\sqrt{\mu}}\frac{q}{2}$ and $\sin\left(\frac{q}{2}\right)\sqrt{1+4g\cos^2\left(\frac{q}{2}\right)}$, for $g=0$ (left) and $g=-\frac{1}{8}$ (right) and $\mu=\frac{1}{1+4g}$. Intersections of the graphs correspond to roots of the dispersion relation, giving rise to periodic solutions for purely NN interaction (left) and including NNN interaction (right).

Equation (1) then becomes

$$\begin{aligned} c^2\ddot{u}(t) &= c_0^2[u(t+1)-2u(t)+u(t-1)] \\ &\quad + V'(u(t+1)-u(t)) - V'(u(t)-u(t-1)) \\ &\quad + g\big\{c_0^2[u(t+2)-2u(t)+u(t-2)] \\ &\quad + W'(u(t+2)-u(t)) - W'(u(t)-u(t-2))\big\} \,. \end{aligned}$$

We are interested in g such that

$$-\frac{1}{4} < g < -\frac{1}{16}$$

as, for this range of g, the purely harmonic potentials give supersonic periodic solutions with mean zero. Precise conditions on V and W are given in Subsection 2.1.

The inclusion of NNN interaction with the opposite sign has quite noticeable effects, as can already be seen from the linearisation of Equation (1). Attempting to solve the linearisation with e^{iqt} leads to the dispersion relation

$$\frac{1}{\sqrt{\mu}}\frac{q}{2} = \sin\left(\frac{q}{2}\right)\sqrt{1+4g\cos^2\left(\frac{q}{2}\right)}\,, \tag{4}$$

where $\mu=\frac{c_0^2}{c^2}$ and $c_0=\sqrt{U_1''(0)}$ is what we call the *NN sound speed*; the dispersion relations for the NN interaction and the NNN interaction are plotted in Fig. 2. We point out that the terminology "speed of sound" is ambiguous; from a macroscopic viewpoint, it is reasonable to give this name to the maximal group velocity, as this describes the speed of of information or energy. In this terminology, the waves found in this paper would be subsonic but still have a larger speed than the velocity $c_0\sqrt{(1+4g)}$ of linear long waves. However, we follow the terminology of [17] and call the latter velocity, that is, the speed of linear waves in the linearised model, the speed of sound. So in this terminology, the speed of sound for the lattice with NNN interaction is $c_0\sqrt{(1+4g)}$.

An examination of (4) and Fig. 2 explains the range of values considered for g. Clearly we need $-\frac{1}{4} < g$. Supersonic solutions for the linearisation arise when the graph on the right in Fig. 2 is convex for small positive q. Expressing the right-hand side of (4) as a series for small q gives

$$\sin\left(\frac{q}{2}\right)\sqrt{1+4g\cos^2\left(\frac{q}{2}\right)} = \frac{1}{1+4g}\left[\frac{q}{2}+\left(-\frac{1+16g}{48(1+4g)}\right)q^3+\dots\right] .$$

The coefficient of q^3 is positive (giving the required convexity) for $g < -\frac{1}{16}$.

We discuss $2k$ periodic solutions, with $k \geq 2$. We are interested in periodic solutions with zero mean and thus seek solutions of (1) in the Hilbert space

$$H^1_{k,0} = \left\{u \in H^1_{\mathrm{loc}}(\mathbb{R}) \;\middle|\; u(t+2k) = u(t), u(0) = 0, u(t) \text{ has zero mean}\right\} \tag{5}$$

with the inner product

$$\langle u, v\rangle_k := \int_{-k}^{k} u'(t)v'(t)\,\mathrm{d}t$$

and norm $\|u\|_k = \left(\int_{-k}^{k} |u'(s)|^2\,\mathrm{d}s\right)^{\frac{1}{2}}$.

We also define

$$\widehat{H^1_{k,0}} = \left\{u \in H^1_{\mathrm{loc}}(\mathbb{R}) \;\middle|\; u(t+2k) = u(t), u(t) \text{ has zero mean}\right\}$$

The argument is variational, in that we consider in $H^1_{k,0}$ the action functional

$$J_k(u) := \int_{-k}^{k}\left[\frac{1}{2}c^2u'(t)^2 - U_1(u(t+1)-u(t)) - gU_2(u(t+2)-u(t))\right]\mathrm{d}t$$

and show that it has the linking geometry.

2.1. Assumptions on the interaction potentials and main result

We make following assumptions for U_1 and U_2.

(1) U_1 is of the form (2) with $V \in C^1(\mathbb{R})$ and $V(0) = V'(0) = 0$; further $V(r) > 0$ for $r \neq 0$ and $V'(r) = o(|r|)$ as $r \to 0$.

(2) There exists $\theta > 2$ such that, for all $r \in \mathbb{R}$,

$$0 \leq \theta V(r) \leq rV'(r) .$$

(3) U_2 is of the form (3) with $W \in C^1(\mathbb{R})$ and $W(0) = W'(0) = 0$; further $W'(r) = o(|r|)$ as $r \to 0$. So, if W is not identically zero, it has superquadratic growth.

(4) There exists θ_2 with $2 < \theta_2 < \theta$ such that, for all $r \in \mathbb{R}$,

$$0 \le \theta_2 W(r) \le r W'(r) \ .$$

We remark that Assumption (2) implies that there exists a $C_\theta > 0$ such that

$$V(r) \ge C_\theta \, |r|^\theta \qquad \text{for all } r \ . \tag{6}$$

(5) The growth of W is bounded by the growth of V in the sense that

$$\begin{aligned} 0 \le r W'(r) \le \theta W(r) &\qquad \text{and} \\ W(r) \le \frac{C_\theta}{2^{\theta-2}} \, |r|^\theta &\qquad \text{for all } r \in \mathbb{R} \ . \end{aligned} \tag{7}$$

The $2^{\theta-2}$ term in the denominator is a normalising factor.

The main result of this paper is the following.

Theorem 2.1 *Let $V(r)$ satisfy Assumptions (1) and (2). Assume that $W(r)$ satisfies Assumptions (3), (4) and (5). Let $-1/4 < g < -1/16$. Then there exists an $\eta_g > 0$ depending on g and c_0 such that, if $c^2 < c_0^2(1+4g) + \eta_g$, Equation* (1) *has periodic solutions. The smallest period, $2k_0$, for which these solutions exist depends on c and increases as $c^2 \to c_0^2(1+4g) + \eta_g$. Once a solution exists with period $2k_0$ for a given g, c_0 and c, solutions exist with period $2k$ for any $k > k_0$.*

The proof is given in Section 3; in Subsection 2.2, we collect some results which are standard in similar contexts.

2.2. Auxiliary statements

We define the finite difference operators $A, B \colon H^1_{k,0} \to \widehat{H^1_{k,0}}$ by

$$(Au)(t) := u(t+1) - u(t) = \int_t^{t+1} u'(s) \, \mathrm{d}s \ ,$$

$$(Bu)(t) := u(t+2) - u(t) = \int_t^{t+2} u'(s) \, \mathrm{d}s \ .$$

Lemma 2.2 *The operators A and B are linear bounded operators from $H^1_{k,0}$ to $L^2(-k,k) \bigcap L^\infty(-k,k)$ satisfying*

$$\|Au\|_{L^\infty(-k,k)} \le \|u\|_k \,, \qquad \|Bu\|_{L^\infty(-k,k)} \le \sqrt{2}\, \|u\|_k$$

and

$$\|Au\|_{L^2(-k,k)} \leq \|u\|_k\,, \qquad \|Bu\|_{L^2(-k,k)} \leq 2\,\|u\|_k\ .$$

Proof: The statement is standard (at least for A) and follows from the Cauchy-Schwarz inequality. For the reader's convenience, we prove the second statement:

$$\begin{aligned}\int_{-k}^{k} |u(t+j)-u(t)|^2\,\mathrm{d}t &\leq j\int_{-k}^{k}\int_{t}^{t+j} |u'(s)|^2\,\mathrm{d}s\,\mathrm{d}t \\ &= j\int_{-k}^{k}\int_{s-j}^{s} |u'(s)|^2\,\mathrm{d}t\,\mathrm{d}s \\ &= j\int_{-k}^{k} |u'(s)|^2 \int_{s-j}^{s}\mathrm{d}t\,\mathrm{d}s \\ &= j^2\,\|u\|_k^2\ .\end{aligned}$$

□

The two propositions that follow are straightforward generalisations of the corresponding results in [15].

PROPOSITION 2.3 *For $U_1, U_2 \in C^1(\mathbb{R})$, the functional J_k is well defined on $H^1_{k,0}$, moreover J_k is C^1 and*

$$\left\langle J_k'(u), h\right\rangle = \int_{-k}^{k}\left[c^2u'(t)h'(t) - U_1'(Au(t))Ah(t) - gU_2'(Bu(t))Bh(t)\right]\,\mathrm{d}t\ . \tag{8}$$

PROPOSITION 2.4 *Any critical point of J_k is a classical (i.e., C^2) solution of* (1) *satisfying $u'(t+2k) = u'(t)$ for all $t \in \mathbb{R}$.*

We close this subsection with an argument that is genuine to the interaction of NN and NNN springs as considered here. The next lemma gives a lower bound for the anharmonic part of the potential energy (for $g < 0$). This bound will be used to show that the action functional has the Palais-Smale property.

LEMMA 2.5 *Under the assumptions of Subsection 2.1 and for $-\frac{1}{4} < g < -\frac{1}{16}$, there exists a constant $C_\theta > 0$ such that*

$$\int_{-k}^{k}\left[V(Au) + gW(Bu)\right]\,\mathrm{d}t \geq C_\theta(1+4g)\,\|Au\|^\theta\ . \tag{9}$$

Proof: The argument uses the bounds (6) and (7) and that $g < 0$. Namely,

$$\begin{aligned}\int_{-k}^{k} V(Au) + gW(Bu)\,\mathrm{d}t &\geq \int_{-k}^{k} C_\theta\,|Au|^\theta + g\frac{C_\theta}{2^{\theta-2}}\,|Bu|^\theta\ \mathrm{d}t \\ &\geq C_\theta\,\|Au\|_{L^\theta}^\theta + g\frac{C_\theta}{2^{\theta-2}}\,\|A(u(t+1)+Au(t)\|_{L^\theta}^\theta \\ &\geq C_\theta\,\|Au\|_{L^\theta}^\theta + g\frac{C_\theta}{2^{\theta-2}}\,(\|A(u(t+1)\|_{L^\theta} + \|Au(t)\|_{L^\theta})^\theta \\ &\geq C_\theta\,\|Au\|^\theta + g\frac{C_\theta}{2^{\theta-2}}2^\theta\,\|Au\|^\theta \\ &\geq C_\theta(1+4g)\,\|Au\|^\theta\ .\end{aligned}$$

□

3. Existence proof via linking

In this section, we first consider the linear part of (1) as an operator and show that its eigenfunctions span $H_{k,0}^1$. These eigenfunctions divide into a finite set with nonpositive eigenvalues and an infinite set with positive eigenvalues, suggesting the use of a linking theorem.

We show that $J_k(u)$ has the linking geometry, as described in the Appendix with $\alpha = 0$, on the spaces spanned by these two sets of eigenfunctions. Finally we show that that $J_k(u)$ satisfies the Palais-Smale condition in $H_{k,0}^1$ and so we can use Theorem A.3 to deduce the existence of a critical point for $J_k(u)$ and hence a solution of (1).

3.1. The associated linear operator and its spectrum

Consider the operator defined in $L^2(-k,k)$ by

$$\begin{aligned}Lu := -c^2u'' + c_0^2\,[u(t+1) - 2u(t) + u(t-1)] \\ + c_0^2g\,[u(t+2) - 2u(t) + u(t-2)] \quad (10)\end{aligned}$$

with $2k$ periodic boundary conditions. (It is easy to see that this operator is self adjoint.)

The eigenfunctions of L in $L^2(-k,k)$ are given by $u(t) = t$ and $u(t) = a$, where a is constant, with the associated eigenvalue 0, and $u(t) = \exp(\pm in\pi t/k)$ with $n \in \mathbb{N}$, with

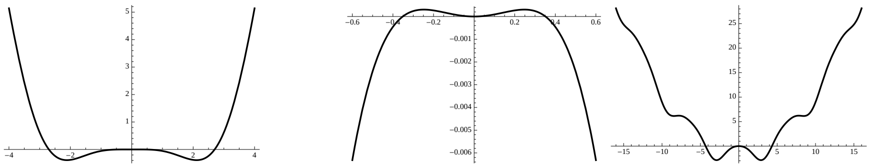

Figure 3. Plots of y for typical values of c for Case (2) (left panel, and zoom around the origin in middle panel) and Case (3) (right panel). Shown are plots for $c_0 = 1$ and $g = -\frac{1}{8}$.

the associated eigenvalue

$$c^2\left(\frac{n\pi}{k}\right)^2 + 2c_0^2\left(\cos\left(\frac{n\pi}{k}\right) - 1\right) + 2c_0^2 g\left(\cos\left(\frac{2n\pi}{k}\right) - 1\right)$$
$$= c^2\left(\frac{n\pi}{k}\right)^2 - 4c_0^2\sin^2\left(\frac{n\pi}{2k}\right)\left(1 + 4g\cos^2\left(\frac{n\pi}{2k}\right)\right) .$$

In $H^1_{k,0}$, the eigenfunctions are $u(t) = \sin(n\pi t/k)$ with $n = 1, 2, \ldots$. To understand the distribution of eigenvalues, we examine the function

$$y = c^2\left(\frac{x\pi}{k}\right)^2 - 4c_0^2\sin^2\left(\frac{x\pi}{2k}\right)\left(1 + 4g\cos^2\left(\frac{x\pi}{2k}\right)\right)$$
$$= c^2z^2 - 4c_0^2\sin^2\left(\frac{z}{2}\right)\left(1 + 4g\cos^2\left(\frac{z}{2}\right)\right) ;$$

the eigenvalues are the values of y for $x = 0, 1, 2, 3, \ldots$. There may be a finite number of negative eigenvalues and the positive eigenvalues have a limit point at infinity.

We recall that we focus on the regime $-1/4 < g < -1/16$. For each g, a graphical investigation shows that there exists $\eta_g > 0$ such that we have the three following cases.

(1) For $c^2 \geq c_0^2(1 + 4g) + \eta_g$, the function is always nonnegative.
(2) For $c_0^2(1 + 4g) < c^2 < c_0^2(1 + 4g) + \eta_g$ the function is positive in the immediate neighbourhood of zero, but then is negative on at least one finite interval either side of zero before tending to positive infinity.
(3) For $c^2 \leq c_0^2(1+4g)$ there is at least one finite interval either side of zero where the function takes negative values.

We can put an initial estimate on the value of η_g as follows. We look at

$$y(z) = c^2z^2 + 2c_0^2(\cos z - 1) + 2c_0^2 g(\cos z - 1)$$

and estimate it by its Taylor polynomial of degree 6, $p(z)$, (i.e., a polynomial of sufficient degree to capture the behaviour of $y(z)$ near zero in Case (2)),

$$p(z) = (c^2 - c_0^2(1 + 4g))z^2 + \frac{c_0^2(1 + 16g)}{12}z^4 - \frac{c_0^2(1 + 64g)}{360}z^6$$

We can use the zeros of $p(z)$ to estimate the zeros of $y(z)$. Both functions have a double zero at the origin. The remaining zeros of $p(z)$ are given, if they exist, by

$$z^2 = \frac{\frac{-c_0^2(1+16g)}{12} \pm \sqrt{\frac{c_0^4(1+16g)^2}{144} + \frac{c_0^2(1+64g)(c^2-c_0^2(1+4g))}{90}}}{\frac{-c_0^2(1+64g)}{180}} \tag{11}$$

For these zeros to exist and be distinct, remembering that $(1+64g) < 0$, we must have

$$0 < \frac{c_0^4(1+16g)^2}{144} + \frac{c_0^2(1+64g)(c^2 - c_0^2(1+4g))}{90}$$

$$\text{that is,} \qquad c^2 < c_0^2(1+4g) + \frac{-5c_0^2(1+16g)^2}{8(1+64g)} \ .$$

The second term on the right-hand side gives an estimate of $\eta_g > 0$.

Increasing k stretches the function in the x direction. So if the function y is negative on a non-empty interval, for k sufficiently large, this interval will contain at least one integer value and we have a finite number of negative eigenvalues, for k large enough. Also, once k is large enough for the interval containing negative eigenvalues to be of length 1, negative eigenvalues will continue to exist for greater k and the same c and g. Equation (11) could be used to estimate the length of the intervals on which $y(z)$ is negative and hence a minimum value for k for any particular values of c, c_0 and g.

For Case (2) ($c_0^2(1+4g) < c^2 < c_0^2(1+4g) + \eta_g$) and fixed c_0 and g, the value of k for which negative eigenvalues first appear depends on the wave speed c and increases as $c \to c_0(1+4g) + \eta_g$.

Negative eigenvalues can occur for values of x only if the straight line $y = \left|\frac{cx\pi}{c_0 2k}\right|$ lies beneath the curve $y = \left|\sin\frac{x\pi}{2k}\right| \sqrt{1+4g\cos^2\frac{x\pi}{2k}}$ (see Fig. 2). Notice that this is impossible if x is a multiple of $2k$. This fact is important for the proof of Lemma A.1 in Appendix A.

3.2. Identifying subspaces spanned by eigenfunctions

We are now looking at the cases where $c^2 \le c_0^2(1+4g) + \eta_g$.

Let Z be the subspace of $H^1_{k,0}$ spanned by eigenfunctions of L with positive eigenvalues, and Y the subspace of $H^1_{k,0}$ spanned by eigenfunctions of L with non-positive eigenvalues.

Then $H^1_{k,0} = Y \oplus Z$ and $0 < \dim Y < \infty$ for k sufficiently large.

Let $Q_k(u)$ be the quadratic part of $J_k(u)$, i.e.,

$$Q_k(u) = \frac{1}{2}\int_{-k}^{k} \left[c^2(u'(t))^2 - c_0^2(Au(t))^2 - c_0^2 g(Bu(t))^2\right] \,\mathrm{d}t \ .$$

Further, let x be an eigenfunction of L in $H^1_{k,0}$ with eigenvalue λ_x. Then

$$\begin{aligned}
Q_k(x) &= \frac{1}{2}\int_{-k}^{k}\left[-c^2x(t)x''(t) - c_0^2(Ax(t))^2 - c_0^2 g(Bx(t))^2\right] \mathrm{d}t \\
&= \frac{1}{2}\int_{-k}^{k}\{x(t)\left[\lambda_x x(t) - c_0^2(x(t+1) - 2x(t) + x(t-1))\right. \\
&\qquad \left. -c_0^2 g(x(t+2) - 2x(t) + x(t-2))\right] \\
&\qquad -c_0^2(x(t+1) - x(t))^2 - c_0^2 g(x(t+2) - x(t))^2\} \,\mathrm{d}t \ .
\end{aligned}$$

Using the $2k$ periodicity of x, for $j = 1, 2$, we can define

$$\begin{aligned}
I_1^j &:= \int_{-k}^{k} x(t+j)x(t)\,\mathrm{d}t = \int_{-k}^{k} x(t)x(t-j)\,\mathrm{d}t \ , \\
I_2 &:= \int_{-k}^{k} x^2(t+j)\,\mathrm{d}t = \int_{-k}^{k} x^2(t)\,\mathrm{d}t \ .
\end{aligned}$$

So

$$\begin{aligned}
Q_k(x) &= \frac{1}{2}\int_{-k}^{k}\lambda_x x^2(t)\,\mathrm{d}t - c_0^2\left[2I_1^1 - 2I_2 + g(2I_1^2 - 2I_2)\right] \\
&\qquad - c_0^2\left[2I_2 - 2I_1^1 + g(2I_2 - 2I_1^2)\right] \\
&= \frac{1}{2}\int_{-k}^{k}\lambda_x x^2(t)\,\mathrm{d}t \\
&\begin{cases} > 0 & \text{for } x \in Z \\ \leq 0 & \text{for } x \in Y \end{cases} .
\end{aligned}$$

If x_1 and x_2 are two distinct eigenfunctions of L, a similar argument and the orthogonality of the eigenfunctions gives that

$$Q_k(x_1 + x_2) = Q_k(x_1) + Q_k(x_2) \ .$$

More generally, if $y \in Y$ and $z \in Z$, then

$$Q_k(y + z) = Q_k(y) + Q_k(z) \ . \tag{12}$$

Also notice that if x is an eigenfunction of L in $H^1_{k,0}$, say $x = \sin(n\pi t/k)$, then

$$\|x\|_k^2 = \left(\frac{n\pi}{k}\right)^2 \|x\|_{L^2}^2$$

and

$$Q_k(x) = \frac{1}{2}\lambda_x \left(\frac{k}{n\pi}\right)^2 \|x\|_k^2$$

with

$$\lambda_x = c^2 \left(\frac{n\pi}{k}\right)^2 + 2c_0^2 \left(\cos\left(\frac{n\pi}{k}\right) - 1\right) + 2c_0^2 \left(\cos\left(\frac{2n\pi}{k}\right) - 1\right) ,$$

so

$$Q_k(x) = \frac{1}{2}c^2 \|x\|_k^2 + O\left(\frac{1}{n^2}\right) .$$

The only limit point for the positive eigenvalues for L is at ∞, so Q_k is positive definite on Z and there exists an $\alpha > 0$ such that

$$Q_k(z) > \alpha \|z\|_k^2 \qquad \text{for every } z \in Z . \tag{13}$$

3.3. Linking geometry

We now show that J_k possesses the linking geometry on $H^1_{k,0}$. Several formulations for linking exist and we refer the reader to the literature [14, 16]. Here we use the version of [11, Appendix C.3]. Namely, we say that J_k possesses the *linking geometry* on $H^1_{k,0}$ if there is a radius $r > 0$ such that

$$J_k(z) \geq \delta > 0 \tag{14}$$

on $\{z \mid z \in Z \text{ and } \|z\|_k^2 = r\}$, as well as

$$J_k(u) \leq 0 \tag{15}$$

on the surface, ∂M, of the set

$$M := \{u = y + \lambda z \mid y \in Y, \quad \|u\|_k \leq \rho, \quad \lambda \geq 0\} . \tag{16}$$

with suitable $\rho > 0$ and a fixed $z \in Z$.

Step 1. We first establish (14). Given $\epsilon > 0$, Assumptions (1) and (3) give that

$$|V'(r)| \leq \epsilon r \text{ and } |W'(r)| \leq \epsilon r \qquad \text{if } |r| \text{ is sufficiently small} ,$$

and since $V(0) = W(0) = 0$, it holds that

$$|V(r)| \leq \epsilon \frac{1}{2} r^2 \quad \text{and} \quad |W(r)| \leq \frac{1}{2}\epsilon r^2 .$$

We now use this fact in the first step and Lemma 2.2 in the last step,

$$\begin{aligned}\left|\int_k^k [V(Au) + gW(Bu)]\,\mathrm{d}t\right| &\le \frac{1}{2}\epsilon \int_k^k \left[|Au|^2 + \frac{1}{4}|Bu|^2\right] \mathrm{d}t \\ &= \frac{1}{2}\epsilon\left(\|Au\|_{L^2}^2 + \frac{1}{4}\|Bu\|_{L^2}^2\right) \\ &\le \epsilon\,\|u\|_k^2 \ .\end{aligned}$$

Thus, for $z \in Z$ such that $\|z\|_k^2 = r$ where r is small, using (13),

$$J_k(z) \ge \alpha\,\|z\|_k^2 - \epsilon\,\|z\|_k^2 \ .$$

So we can choose ϵ, and hence r, sufficiently small that there exists δ such that

$$J_k(z) \ge \delta > 0 \qquad \text{on } \|z\|_k^2 = r \ .$$

This establishes (14).

Step 2. We now turn to (15). Let us fix $z = a\sin(n\pi t/k) \in Z$ such that $\|z\|_k = 1$ and n is not a multiple of $2k$; the existence of such a z is trivial.

Let M be the set defined in (16) (ρ is to be chosen later),

$$M := \{u = y + \lambda z \mid y \in Y, \quad \|u\|_k \le \rho, \quad \lambda \ge 0\} \ .$$

Then

$$\partial M = \{u = y + \lambda z \mid y \in Y, \quad \|u\|_k = \rho \text{ and } \lambda \ge 0 \text{ or } \|u\|_k \le \rho \text{ and } \lambda = 0\} \ .$$

Using the orthogonality relation (12), we have

$$J_k(y+\lambda z) = Q_k(y) + \lambda^2 Q_k(z) - \int_{-k}^{k} [V(A(y+\lambda z)) + gW(B(y+\lambda z))]\ \mathrm{d}t \ . \tag{17}$$

From (9), it follows that

$$J_k(y+\lambda z) \le Q_k(y) + \lambda^2 Q_k(z) - C_\theta(1+4g)\,\|A(y+\lambda z)\|_{L^\theta}^\theta \ . \tag{18}$$

The geometry of ∂M makes it natural to consider two cases separately. We first consider the part where $\|y+\lambda z\|_k = \rho$ and $\lambda \ge 0$.

Since $\|z\|_k = 1$ and z and y are orthogonal, $\rho^2 = \|y+\lambda z\|_k^2 = \|y\|_k^2 + \lambda^2$, so $\lambda^2 \le \rho^2$.

Also M is contained in a space of dimension $\dim Y + 1 < \infty$, so $y + \lambda z \in M$ is mapped by A to a finite dimensional space (of dimension $\le 2(\dim Y + 1)$). Norms on finite dimensional spaces are equivalent, hence there exist $\tilde{c}$ and $\tilde{k}$ such that

$$\|A(y+\lambda z)\|_{L^\theta}^\theta \ge \tilde{c}\,\|A(y+\lambda z)\|_{L^2}^\theta$$

and

$$\|y + \lambda z\|_{L^2}^{\theta} \geq \tilde{k} \, \|y + \lambda z\|_k^{\theta} \ .$$

Using the first of these bounds and (18) in the first line, the bound from Lemma A.1 in Appendix A in the second line and then the fact that $Q_k(z) > 0$ together with the second bound in the third line, we obtain

$$\begin{aligned} J_k(y+\lambda z) &\leq \lambda^2 Q_k(z) - \tilde{c} C_\theta (1+4g) \, \|A(y+\lambda z)\|_{L^2}^{\theta} \\ &\leq \lambda^2 Q_k(z) - C_1 \, \|y+\lambda z\|_{L^2}^{\theta} \\ &\leq \rho^2 Q_k(z) - C_1 \tilde{k} \, \|y+\lambda z\|_k^{\theta} \\ &= \rho^2 Q_k(z) - C_1 \tilde{k} \rho^{\theta} \ , \qquad \text{where } C_1 > 0 \ . \end{aligned}$$

(The bound of $\|A(y+\lambda z)\|_{L^2}^{\theta}$ from below by $\|y+\lambda z\|_k^{\theta}$ uses Lemma A.1 and hence depends on the special structure of the eigenfunctions of L.)

Since $\theta > 2$ the right hand side of this inequality will be negative for ρ sufficiently large and then

$$J_k(y+\lambda z) < 0$$

for this part of ∂M.

For the rest of ∂M, that is, the "bottom part" $\|y\|_k \leq \rho$ and $\lambda = 0$, we use (18) and the argument above to find

$$J_k(y) \leq Q_k(y) - C_1 \tilde{k} \, \|y\|^{\theta} \leq 0$$

as $Q_K(y) \leq 0$, and (15) is established.

In summary, $J_k(u)$ possesses the linking geometry in $H^1_{k,0}$.

To conclude the proof of the existence of a periodic solution, we need to show that J_k satisfies the Palais-Smale condition in $H^1_{k,0}$. i.e. if $\{u_n\}_{n\in\mathbb{N}}$ is a sequence such that $J_k(u_n)$ is bounded and $J_k'(u_n) \to 0$ as $n \to \infty$, then $\{u_n\}_{n\in\mathbb{N}}$ has a convergent subsequence.

The argument resembles that for the NN interaction case [11, Theorem 3.3] but differs in detail as estimates on the competing effects of the NN and the NNN interaction are needed. We thus sketch the argument.

Let $\{u_n\}_{n\in\mathbb{N}}$ be a sequence such that $J_k(u_n) \leq K$ for some $K \in \mathbb{R}$ and $J_k'(u_n) \to 0$ as $n \to \infty$. Choose β such that $\frac{1}{\theta} < \beta < \frac{1}{2}$ and choose n sufficiently large that $|\langle J_k'(u_n), u_n\rangle| \leq \|u_n\|_k$.

The first estimates that follow are standard, but the assumptions on the growth of W, see (7), are used in the second inequality. The third inequality uses Lemma 2.2 and that

$-1/4 < g < 0$. The last inequality uses (9) of Lemma 2.5. We have

$$
\begin{aligned}
K+\beta\|u_n\|_k &\ge J_k(u_n)-\beta\left\langle J_k'(u_n),u_n\right\rangle \\
&= \int_{-k}^{k}\left[\frac{c^2}{2}\left|u_n'\right|^2-\frac{c_0^2}{2}\left(|Au_n|^2+g\,|Bu_n|^2\right)-V(Au_n)-gW(Bu_n)\right. \\
&\quad -\beta\bigg(c^2\left|u_n'\right|^2-c_0^2\left(|Au_n|^2+g\,|Bu_n|^2\right) \\
&\quad \left. -V'(Au_n)Au_n-gW'(Bu_n)B(u_n)\bigg)\right]\mathrm{d}t \\
&\ge \int_{-k}^{k}\left[c^2\left(\frac{1}{2}-\beta\right)(u_n')^2-c_0^2\left(\frac{1}{2}-\beta\right)(|Au_n|^2+g\,|Bu_n|^2)\right. \\
&\quad \left. +(\beta\theta-1)\left(V(Au_n)+gW(Bu_n)\right)\right]\mathrm{d}t \\
&\ge c^2\left(\frac{1}{2}-\beta\right)\|u_n\|_k^2-c_0^2\left(\frac{1}{2}-\beta\right)\|Au_n\|_{L^2}^2 \\
&\quad +(\beta\theta-1)\int_{-k}^{k}\left[V(Au_n)+gW(Bu_n)\right]\mathrm{d}t \\
&\ge \left(\frac{1}{2}-\beta\right)(c^2\|u_n\|_k^2-c_0^2\|Au_n\|_{L^2}^2)+(\beta\theta-1)C_\theta(1+4g)\|Au_n\|_{L^\theta}^\theta\ .
\end{aligned}
$$

Since $\theta > 2$, we can write $\mu = 2/(\theta-2) > 0$, and, see Lemma A.2 in Appendix A,

$$
\|Au_n\|_{L^2}^2 \le C_2\|Au_n\|_{L^\theta}^2 \le C_2\left(\frac{1}{\epsilon^\mu}+\epsilon\|Au_n\|_{L^\theta}^\theta\right),
$$

for any $\epsilon > 0$.

Thus the previous inequality yields

$$
\begin{aligned}
K+\beta\|u_n\|_k \ge \left(\frac{1}{2}-\beta\right)c^2\|u_n\|_k^2 \\
+\left[-\epsilon c_0^2C_2\left(\frac{1}{2}-\beta\right)+C_\theta(\beta\theta-1)(1+4g)\right]\|Au_n\|_{L^\theta}^\theta-C_3\frac{1}{\epsilon^\mu}\ .
\end{aligned}
$$

We fix ϵ sufficiently small that the expression in the brackets is positive, then

$$
K+\beta\|u_n\|_k \ge \left(\frac{1}{2}-\beta\right)c^2\|u_n\|_k^2-C_3\frac{1}{\epsilon^\mu}
$$

and $\|u_n\|_k$ is bounded in $H_{k,0}^1$.

The rest of the argument is well-established (see, e.g., [15]) but reproduced here for completeness. The boundedness of u_n implies that u_n has a weakly convergent subsequence $u_{n_j} \rightharpoonup u$ for some u in $H_{k,0}^1$ and hence $Au_{n_j} \rightharpoonup Au$ and $Bu_{n_j} \rightharpoonup Bu$ in $\widehat{H}_{k,0}^1$ and, by the compactness of the Sobolev embedding, in $L^2(-k,k)$.

$$
\begin{aligned}
c^2 \left\|u_{n_j} - u\right\|_k^2 &= \int_{-k}^{k} c^2 \left(u'_{n_j} - u'\right)^2 \mathrm{d}t \\
&= \left\langle J'_k(u_{n_j}) - J'_k(u), u_{n_j} - u\right\rangle + c_0^2 \left\|Au_{n_j} - Au\right\|_{L^2}^2 + c_0^2 g \left\|Bu_{n_j} - Bu\right\|_{L^2}^2 \\
&\quad + \int_{-k}^{k} [V'(Au_{n_j}) - V'(u)](Au_{n_j} - Au)\,\mathrm{d}t \\
&\quad + g \int_{-k}^{k} \left[W'(Bu_{n_j}) - W'(u)\right](Bu_{n_j} - Bu)\,\mathrm{d}t.
\end{aligned}
$$

The first, second and third terms on the right converge to zero. By Lemma 2.2, Au_{n_j} and Bu_{n_j} are bounded in $L^\infty(-k,k)$ and hence, $[V'(Au_{n_j}) - V'(Au)]$ and $[W'(Bu_{n_j}) - W'(Bu)]$ are bounded in $L^\infty(-k,k)$. Since $Au_{n_j} \to Au$ and $Bu_{n_j} \to Bu$ strongly in $L^2(-k,k)$, the two last terms on the right also tend to zero. So $\left\|u_{n_j} - u\right\|_k \to 0$ and J_k satisfies the Palais Smale condition. Hence we have satisfied the conditions for Theorem A.3 in Appendix A with $\alpha = 0$ and $\beta = \delta > 0$.

Since the critical value, b, given by the theorem satisfies $b \geq \beta > 0$, the critical point is non-trivial.

Appendix A. Appendix

Lemma A.1 *In the notation of Subsection 3.3, there exists a constant $C > 0$ such that*

$$
\int_{-k}^{k} (A(y + \lambda z))^2 \,\mathrm{d}t > C \left\|y + \lambda z\right\|_{L^2}^2 \ .
$$

Proof: Remember that

$$
y = c_1 y_1 + c_2 y_2 + \cdots + c_s y_s, \qquad \text{with } y_n = \sin\left(\frac{n\pi t}{k}\right) \ ,
$$

where none of $1, 2, ...s$ are multiples of $2k$. Choose $z = \sin\left(\frac{m\pi t}{k}\right)$ with m not being a multiple of $2k$. Then the following basic integral identities hold.

$$
\|y_n\|_{L^2}^2 = \|y_n(t+1)\|_{L^2}^2 = \|z\|_{L^2}^2 = \|z(t+1)\|_{L^2}^2 = \int_{-k}^{k} \sin^2\left(\frac{n\pi t}{k}\right) \mathrm{d}t = k \ ;
$$

$$
\begin{aligned}
\int_{-k}^{k} y_n(t+1) y_n(t)\,\mathrm{d}t &= \frac{1}{2}\int_{-k}^{k} \cos\left(\frac{n\pi}{k}\right) - \cos\left(\frac{n\pi(2t+1)}{k}\right) \mathrm{d}t \\
&= k\cos\left(\frac{n\pi}{k}\right) = \|y_n\|_{L^2}^2 \cos\left(\frac{n\pi}{k}\right) \ ,
\end{aligned}
$$

$$\int_{-k}^{k} y_n(t+1)y_r(t)\,\mathrm{d}t$$
$$= \frac{1}{2}\int_{-k}^{k} \cos\left(\frac{((n-r)t+n)\pi}{k}\right) - \cos\left(\frac{((n+r)t+n\pi(2t+1)}{k}\right)\,\mathrm{d}t$$
$$= 0 \text{ for } n \neq r\ .$$

So

$$\int_{-k}^{k} (A(y+\lambda z))^2\,\mathrm{d}t = 2c_1^2\,\|y_1\|_{L^2}^2\left(1-\cos\frac{\pi}{k}\right)+\dots$$
$$+\,2c_s^2\,\|y_s\|_{L^2}^2\left(1-\cos\frac{s\pi}{k}\right)+\lambda^2\,\|z\|_{L^2}^2\left(1-\cos\frac{m\pi}{k}\right)\ .$$

By the choice of z and the restrictions on n for the y_n, there exists a δ such that

$$\max\left\{\cos\frac{\pi}{k},\dots,\cos\frac{s\pi}{k},\cos\frac{m\pi}{k}\right\}\le\delta<1$$

and

$$\int_{-k}^{k} (A(y+\lambda z))^2\,\mathrm{d}t > 2(1-\delta)\left(c_1^2\,\|y_1\|_{L^2}^2+\dots+c_s^2\,\|y_s\|_{L^2}^2+\lambda^2\,\|z\|_{L^2}^2\right)$$
$$= 2(1-\delta)\,\|y+\lambda z\|_{L^2}^2\ .$$

□

Lemma A.2 *Let* $\mu = 2/(\theta-2)$ *then, for all* $\epsilon > 0$,

$$\|f\|_{L^\theta}^2 < \frac{1}{\epsilon^\mu}+\epsilon\,\|f\|_{L^\theta}^\theta\ .$$

Proof: Consider the function

$$F(\epsilon) = \frac{1}{\epsilon^\mu}+\epsilon\,\|f\|_{L^\theta}^\theta\ .$$

Then

$$F'(\epsilon) = \frac{-\mu}{\epsilon^{\mu+1}}+\|f\|_{L^\theta}^\theta \qquad \text{and} \qquad F''(\epsilon) = \frac{\mu(\mu+1)}{\epsilon^{\mu+2}}\ ,$$

i.e., $F(\epsilon)$ has a minimum at $\epsilon = \left(\frac{\mu}{\|f\|_{L^\theta}^\theta}\right)^{\frac{1}{\mu+1}}$ and the value of the minimum is

$$\left(\frac{\|f\|_{L^\theta}^\theta}{\mu}\right)^{\frac{\mu}{\mu+1}}+\left(\frac{\mu}{\|f\|_{L^\theta}^\theta}\right)^{\frac{1}{\mu+1}}\|f\|_{L^\theta}^\theta = \left(\frac{1}{\mu^{\frac{\mu}{\mu+1}}}+\mu^{\frac{1}{\mu+1}}\right)\|f\|_{L^\theta}^{\frac{\mu\theta}{\mu+1}}\ .$$

One or other of the terms in the bracket on the right hand side must be greater than one, so their sum is greater than one. Also,

$$\frac{\mu\theta}{\mu+1} = \frac{2\theta/(\theta-2)}{2/(\theta-2)+1} = 2 \ .$$

Hence we have that the minimum of $F(\epsilon) > \|f\|^2_{L^\theta}$. □

We now give, for reference, the specific linking theorem used in the main text. Let H be a Hilbert space expressed as the orthogonal sum $H = Y \oplus Z$ where Y is finite dimensional. Fix z in Z and let $\rho > 0$. Define

$$M := \{u = y + \lambda z : y \in Y, \|u\| \le \rho, \lambda \ge 0\} \ .$$

The boundary of M is the set

$$\partial M = \{u = y + \lambda z : \|u\| = \rho \text{ and } \lambda \ge 0 \ \text{ or } \ \|u\| \le \rho \text{ and } \lambda = 0\} \ .$$

Let

$$N := \{u \in Z : \|u\| = r\} \ .$$

If ϕ is a functional on H, ϕ is said to have the *linking geometry* if we can find $\rho > r > 0$ such that

$$\beta := \inf_{u \in N} \phi(u) > \alpha := \sup_{u \in \partial M} \phi(u) \ .$$

The following statement is taken from [11, Appendix C.3].

THEOREM A.3 *Let ϕ be a functional of class C^1 that satisfies the Palais-Smale condition and possesses the linking geometry. Then if*

$$b := \left\{ \inf_{\gamma \in \Gamma} \sup_{u \in M} \phi(\gamma(u)) \right\} \ ,$$

where

$$\Gamma := \{\gamma \in C(M; H) : \gamma = id \ on \ \partial M\} \ .$$

Then b is a critical value of ϕ and

$$\beta \le b \le \sup_{u \in M} \phi(u) \ .$$

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