Existence and numerical approximation of periodic motions of an infinite lattice of particles *

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Abstract

We prove the existence of periodic motions of an infinite lattice of particles; the proof involves the study of periodic motions for finite lattices by a linking technique and the passage to the limit by means of Lions' concentration-compactness principle. We also give a numerical picture of the motion of some finite lattices and of the way the solutions for finite lattices approach the solution for the infinite lattice by a technique developed by Choi and McKenna [6].

1 Introduction and variational setting

In this paper we prove that an autonomous dynamical system with infinite degrees of freedom consisting of a 1-dimensional lattice of particles, each interacting with its nearest neighbors by means of a force belonging to a certain class, admits a nontrivial periodic motion of finite energy for any assigned period T.

The state of the lattice at time t is represented by a sequence $q(t) = \{q_i(t)\}$, $i \in \mathbb{Z}$, where $q_i(t)$ is the state of the i-th particle; the equation governing $q_i(t)$ reads

$$\ddot{q}_i = \Phi'_{i-1}(q_{i-1} - q_i) - \Phi'_i(q_i - q_{i+1}) \ . \tag{1}$$

We define the potential Φ of the system by

$$\Phi : \mathbb{R}^{\mathbf{Z}} \to \mathbb{R} \qquad \Phi(q) := \sum_{i\in\mathbf{Z}} \Phi_i(q_i - q_{i+1}) \ ,$$

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so that the infinite equations (1) can be written in vectorial form:

$$\ddot{q} = -\Phi'(q) \ . \tag{2}$$

For all $i \in \mathbb{Z}$ we assume the potential Φ_i to satisfy

$$\Phi_i(x) = -\alpha_i x^2 + V_i(x)$$

where $\alpha_i \geq 0$ and

$$(P) \begin{cases} \exists \delta > 0 \text{ such that } V_i'(x)x \geq (2+\delta)V_i(x) \geq 0, \ \forall x \in \mathbb{R} \\ V_i(x) = 0 \Longleftrightarrow x = 0 \\ V_i \in C^{1,1}_{loc} \\ \exists m \in \mathbb{N} \text{ such that } \Phi_{i+m} \equiv \Phi_i \ . \end{cases}$$

Note that the above conditions imply that $\forall i \in \mathbb{Z}$ $\Phi_i(0) = 0$, V_i is superquadratic both at the origin and at infinity and that Φ_i has either a strict local maximum (if $\alpha_i > 0$) or a strict global minimum (if $\alpha_i = 0$) in 0.

In a previous paper [2] the authors proved that if α_i is strictly positive for all $i \in \mathbb{Z}$ and the period T is large, then the system admits a nontrivial solution, which is obtained as a critical point of mountain pass type (see [1]) for a suitable functional; the hypothesis $\alpha_i > 0$ implies that the interparticle forces are repulsive-attractive, i.e. repulsive for small displacements and attractive for large displacements.

By allowing the parameters α_i to be 0, we consider here purely attractive forces as well. The existence of a nontrivial periodic solution of finite energy for this system may be surprising, indeed one could expect that an infinite lattice of particles interacting with strongly nonlinear conservative forces is highly ergodic, i.e. it tends to distribute the energy among the particles, while the existence of a periodic motion of finite energy suggests lack of ergodicity. This physical interpretation would be much more interesting and meaningful if some kind of stability results were available, but the only results of such type known to the authors (see [4]) cannot be applied to this problem. For further physical interpretation of the problem see [10, 12].

From the analytical point of view the problem we study here is quite different to the one in [2], indeed the mountain pass geometry is replaced by a linking [9]; such linking is infinite dimensional and the technique developed by Benci and Rabinowitz in [5] to handle this kind of problems cannot be applied, due to the lack of compactness of the functional. Therefore we address the problem by proving the existence of solutions for finite lattices and taking the limit. Another example of a strongly indefinite variational problem with lack of compactness is studied in [11].

The approximation of the periodic motion in the infinite lattice by motions of finite lattices is also interesting for numerical applications, indeed even if the procedure adopted in [2] leads more directly to the result of existence when compared to the method adopted here, it cannot be used for the numerical study of the problem.

The following theorem summarizes our results:

Theorem 1 *Assume (P); then* $\forall T > 0$ *system (2) admits a nonzero T-periodic solution of finite energy.*

Furthermore if $\alpha_i = 0$ $\forall i$ *this solution is nonconstant* $\forall T > 0$*, otherwise* $\exists \bar{T} > 0$ *such that if* $T > \bar{T}$ *the solution is nonconstant.*

Let $S^1 = [0,T]/\{0,T\}$; our framework is the following Hilbert space:

$$H := \left\{ q \in H^1(S^1, \mathbb{R})^{\mathbf{Z}};\ \int_0^T q_0(t)dt = 0,\ \sum_{i\in\mathbf{Z}} \int_0^T \left[(\dot{q}_i(t))^2 + (q_i(t) - q_{i+1}(t))^2 \right] dt < \infty \right\}$$

endowed with the scalar product

$$(q,p) := \sum_{i\in\mathbf{Z}} \int_0^T \dot{q}_i(t)\dot{p}_i(t)dt + \sum_{i\in\mathbf{Z}} \int_0^T (q_i(t) - q_{i+1}(t))(p_i(t) - p_{i+1}(t))dt \ . \tag{3}$$

It is necessary to impose $\int_0^T q_0(t)dt = 0$ or an equivalent condition in order to have (3) defining a scalar product; it can be checked that such a condition does not affect the nature of the critical points of the functional we consider, that is $J : H \to \mathbb{R}$ defined by

$$J(q) := \frac{1}{2}\int_0^T |\dot{q}(t)|^2 dt - \int_0^T \Phi(q(t))dt \ .$$

The properties of the potential imply that J is well defined on H and that $J \in C^1(H, \mathbb{R})$ (see Proposition 1 in [2]). We prove Theorem 1 by showing that the functional J admits a critical point; note that due to its translation invariance, the functional does not satisfy the Palais-Smale condition.

This paper is organized as follows: in section 2 we prove the existence of critical points $q^{(n)}$ for the functional corresponding to periodic finite lattices and we give uniform estimates of the critical levels and of the norms of $q^{(n)}$ when suitably embedded in the infinite system. In section

3 we use Lions' concentration-compactness technique [8] and the results of section 2 to take the limit and prove the existence of a critical point for J. In sections 4 and 5 we describe the application of an algorithm developed by Choi and McKenna [6] to compute the solutions for finite lattices in the case of repulsive-attractive interactions; the numerical results we obtain describe the process of approximation of the solution for the infinite lattices adopted in our proof.

2 Periodic motions of the finite system

We first consider for all $n = km$ (m as in (P), $k \in \mathbb{N}$) the system (S_n) consisting in a periodic lattice of $2n$ particles, whose motion is described by (1) for $i \in \{-n, \ldots, n-1\}$ (and to simplify the notation we will consider $q_n \equiv q_{-n}$). To study this finite problem we use the set of functions

$$H_n := \left\{ q \in H^1(S^1, \mathbb{R})^{2n};\ \int_0^T q_0 = 0 \right\}$$

which is a Hilbert space when endowed by the scalar product

$$(q,p) := \sum_{i=-n}^{n-1} \int_0^T \left[\dot{q}_i(t)\dot{p}_i(t) + (q_i(t) - q_{i+1}(t))(p_i(t) - p_{i+1}(t))\right] dt \ ;$$

define also $L^2_n := L^2(S^1; \mathbb{R})^{2n}$. We can continuously embed H_n into H by means of the following operator

$$\Upsilon_n : \begin{array}{l} H_n \to H \\ q \mapsto Q \end{array} \qquad \text{where} \qquad Q_i(t) = \begin{cases} \frac{1}{T}\int_0^T q_{n-1}(t)dt & \text{if } i > n-1 \\ q_i(t) & \text{if } i \in [-n, n-1] \\ \frac{1}{T}\int_0^T q_{-n}(t)dt & \text{if } i < -n \ . \end{cases}$$

Consider the functional

$$J_n(q) := \sum_{i=-n}^{n-1} \int_0^T \left[\frac{1}{2}(\dot{q}_i(t))^2 - \Phi_i(q_i(t) - q_{i+1}(t))\right] dt \ ;$$

a periodic solution of system (S_n) is a critical point of J_n. Note that the functionals J_n corresponding to finite lattices do satisfy the Palais-Smale condition:

Lemma 1 *Assume (P); then J_n satisfies the Palais-Smale condition for all $n \in \mathbb{N}$.*

Proof. Let $q^{(k)}$ be a Palais-Smale sequence, then (c_i denote positive constants and $\varepsilon_k \to 0$)

$$\begin{aligned} c_1(1 + \varepsilon_k \|q^{(k)}\|) &\geq 2J_n(q^{(k)}) - J_n'(q^{(k)})[q^{(k)}] \\ &\geq \delta \textstyle\int_0^T \sum_i V_i(q_i^{(k)} - q_{i+1}^{(k)})dt \geq c_2\delta \sum_i \int_0^T (q_i^{(k)} - q_{i+1}^{(k)})^{2+\delta} dt - c_3 \ , \end{aligned}$$

hence

$$\sum_i \int_0^T (q_i^{(k)} - q_{i+1}^{(k)})^2 dt \le c_4(1 + \varepsilon_k \|q^{(k)}\|),$$

$$\int_0^T |\dot{q}^{(k)}|^2 dt \le c_5(1 + \varepsilon_k \|q^{(k)}\|)$$

as $J_n(q^{(k)})$ is bounded, and $\|q^{(k)}\|$ is bounded as well.

By the compact embedding $H_n \subset L^2_n$ we infer that there exists $q \in H_n$ such that, up to a subsequence, $q^{(k)} \rightharpoonup q$ in H_n and $q^{(k)} \to q$ in L^2_n; since $\|J_n'(q^{(k)})\| \to 0$ we also have $\dot{q}^{(k)} \to \dot{q}$ in L^2_n and the assertion follows. □

Next we prove that the geometrical requirements of the linking theorem are satisfied:

Lemma 2 *Assume (P); then for all $n \in \mathbb{N}$ there exists a finite dimensional subspace V_n of H_n and a subspace W_n such that:*

(i) $V_n \oplus W_n = H_n$.

(ii) $\exists \alpha, r > 0$ such that $J_n \ge \alpha$ on $\partial B_r \cap W_n$.

(iii) $\exists R_n > r$, $\exists w \in W_n$ such that $\|w\| > r$ and if $D_{R_n} = (\bar{B}_{R_n} \cap V_n) \oplus [0, w]$ then $J_n \le 0$ on ∂D_{R_n}.

Moreover the constants α, r and the vector w are independent of n.

Proof. We first consider the case where $\alpha_i = 0 \quad \forall i$.

(i) Let V_n be the subspace of the constant functions and $W_n = V_n^\perp$; then $\dim V_n = 2n$.

(ii) Let V be the infinite dimensional subspace of H spanned by the constants and let $W = V^\perp$. There exist two constants $\alpha, r > 0$ such that $J(q) \ge \alpha$ for all q such that $q \in \partial B_r \cap W$, because $\sum_i \|q_i - q_{i+1}\|_\infty^2 \le c\|q\|^2$ (see [2]) and V_i is superquadratic in 0; the assertion follows since $W_n \subset W$ by the operator Υ_n.

(iii) The superquadratic behaviour of V_i at infinity implies that for all $q \in H_n$ there exists $\gamma > 0$ such that $J_n(\gamma q) < 0$, hence we can choose $w \in W_1$ such that the assertion holds $\forall n$.

If $\alpha_i > 0$ for some i the proof is similar: in this case V_n can be taken to be a subspace of the space of constants; if $\alpha_i > 0 \; \forall i$ we have $V_n = \{0\}$ and the linking is in fact a mountain pass. □

Now we can prove the existence of critical points for J_n and we can uniformly estimate their norms and critical levels; we need such estimates when we take the limit for $n \to \infty$.

Theorem 2 *Assume (P) and let α, R_n and D_{R_n} be as in Lemma 2, then the functional J_n has a positive critical value*

$$b_n = \inf_{h\in\Gamma_n} \max_{q\in D_{R_n}} J_n(h(q)) \ ,$$

where $\Gamma_n = \{h \in C(D_{R_n}, H_n);\ h(q) = q\ \forall q \in \partial D_{R_n}\}$.
Furthermore $\exists b, \rho_1, \rho_2 > 0$ (independent of n) such that the following estimates hold:

$$0 < \alpha \le b_n \le b \ , \qquad\qquad 0 < \rho_1 \le \|q^{(n)}\| \le \rho_2 \tag{4}$$

where $q^{(n)}$ is a critical point at level b_n.

Proof. By Lemma 1 J_n satisfies the Palais-Smale condition; the fact that b_n is a critical level follows from Lemma 2 and from the linking theorem (see [9]).
The estimate $b_n \ge \alpha > 0$ follows from Lemma 2 (ii); let $q^{(n)}$ be a critical point at level b_n, the estimate $\|q^{(n)}\| \ge \rho_1 > 0$ follows from the inequality $c\|q^{(n)}\|^2 \ge J_n(q^{(n)}) \ge \alpha$.
Next, notice that for all integers n the identity is in Γ_n and therefore

$$b_n \le \max\{J_n(q);\ q \in D_{R_n}\} \ ;$$

it can be easily seen that there exists $b > 0$ such that $\max\{J_n(q);\ q \in D_{R_n}\} \le b$, $\forall n$.
Let $I := \{i \in \mathbb{Z};\ \alpha_i = 0\}$, for each n let $I_n := I \cap \{-n, \dots, n-1\}$ and denote by $d_i^{(n)} = q_i^{(n)} - q_{i+1}^{(n)}$; the estimate $\|q^{(n)}\| \le \rho_2$ follows if we prove that there exist three positive constants c_i $(i = 1, 2, 3)$ such that

$$c_1 \ge \sum_{i\in\mathbf{Z}} \|\dot{q}_i^{(n)}\|_2^2 \qquad c_2 \ge \sum_{i\notin I_n} \|d_i^{(n)}\|_2^2 \qquad c_3 \ge \sum_{i\in I_n} \|d_i^{(n)}\|_2^2 \ .$$

Note that

$$\begin{aligned} 2b &\ge 2b_n = 2J_n(q^{(n)}) - J_n'(q^{(n)})[q^{(n)}] \\ &= \sum_{i=-n}^{n-1} \int_0^T \left[V_i'(d_i^{(n)})(d_i^{(n)}) - 2V_i(d_i^{(n)})\right] \ge \delta \sum_{i=-n}^{n-1} \int_0^T V_i(d_i^{(n)}) \ , \end{aligned}$$

and since $J_n(q^{(n)}) \le b$ we get

$$\exists c_1, c_2 > 0 \text{ such that } c_1 \ge \sum_{i\in\mathbf{Z}} \|\dot{q}_i^{(n)}\|_2^2 \text{ and } c_2 \ge \sum_{i\notin I} \|d_i^{(n)}\|_2^2 \ ; \tag{5}$$

by the embedding $H^1 \subset L^\infty$ we also get

$$c_4 \ge \sum_{i\notin I} \|d_i^{(n)}\|_\infty^2 \ .$$

If $\alpha_i > 0$ for all i the proof is complete, otherwise note that by integrating equations (1) we infer that there exists $\tilde{k}^{(n)}$ such that

$$\frac{1}{T}\int_0^T \Phi_i'(d_i^{(n)}) = \tilde{k}^{(n)} \quad \forall i \in \{-n, \dots, n-1\} \text{ and therefore } \frac{1}{T}\int_0^T V_i'(d_i^{(n)}) = \tilde{k}^{(n)} \quad \forall i \in I_n \,. \tag{6}$$

Note that $\tilde{k}^{(n)} \to 0$ for $n \to +\infty$: indeed if $|\tilde{k}^{(n)}| \geq \xi > 0$ (assume e.g. that $\tilde{k}^{(n)} \geq \xi > 0$), then there exists $\xi' > 0$ such that the sets $K_i^{(n)} := \{t \in [0,T];\ d_i^{(n)}(t) \geq \xi'\}$ have strictly positive measure uniformly with respect to i, n; as $\sum_{i\in I_n} \int_0^T V_i(d_i^{(n)})$ is bounded, we get a contradiction. By assumption (P) we can choose n so large that for all $i \in I_n$ there exists a unique $k_i^{(n)}$ such that $V_i'(k_i^{(n)}) = \tilde{k}^{(n)}$ and moreover for a given n the numbers $k_i^{(n)}$ all have the same sign (assume with no restriction that they are all positive, otherwise the proof holds with minor changes) and $k_{i+m}^{(n)} = k_i^{(n)}$. By (6) and the continuity of V_i', for all $i \in I_n$ there exists $t_i \in [0,T]$ such that $d_i^{(n)}(t_i) = k_i^{(n)}$; furthermore, by Sobolev embedding $\|\dot{d}_i^{(n)}\|_2 \geq c|d_i^{(n)}(t) - \bar{d}_i^{(n)}|$ for all $t \in [0,T]$, where $\bar{d}_i^{(n)} = \frac{1}{T}\int_0^T d_i^{(n)}(t)$, hence $\|\dot{d}_i^{(n)}\|_2 \geq 2c|d_i^{(n)}(t) - k_i^{(n)}|$, that is

$$k_i^{(n)} - c\|\dot{d}_i^{(n)}\|_2 \leq d_i^{(n)}(t) \leq k_i^{(n)} + c\|\dot{d}_i^{(n)}\|_2 \,. \tag{7}$$

Adding the previous inequalities (recall that $n = km$) we get

$$\sum_{i\in I_n} k_i^{(n)} = \frac{n}{m} \sum_{i\in I_n\cap[1,m]} k_i^{(n)} \leq \sum_{i\in I_n} \left[c\|\dot{d}_i^{(n)}\|_2 + d_i^{(n)}(t)\right] \tag{8}$$

and for all $t \in [0,T]$, as $\sum_{i=-n}^{n-1} d_i^{(n)}(t) = 0$, we have

$$\left|\sum_{i\in I_n} d_i^{(n)}(t)\right| = \left|\sum_{i\notin I_n} d_i^{(n)}(t)\right| \leq \sum_{i\notin I_n} \|d_i^{(n)}\|_\infty \,.$$

Taking the square of (8) we obtain

$$\begin{aligned} \tfrac{n^2}{m^2}\left[\textstyle\sum_{i\in I_n\cap[1,m]} k_i^{(n)}\right]^2 &\leq \left[c\textstyle\sum_{i\in I_n} \|\dot{d}_i^{(n)}\|_2 + \sum_{i\notin I_n} \|d_i^{(n)}\|_\infty\right]^2 \\ &\leq nc'\left(\textstyle\sum_{i\in I_n} \|\dot{d}_i^{(n)}\|_2^2 + \sum_{i\notin I_n} \|d_i^{(n)}\|_\infty^2\right) \leq nc'' \,; \end{aligned}$$

finally (7) gives $|d_i^{(n)}(t)| \leq k_i^{(n)} + c\|\dot{d}_i^{(n)}\|_2$, hence

$$\sum_{i\in I_n} \|d_i^{(n)}\|_\infty^2 \leq c\left[\sum_{i\in\mathbf{Z}} \|\dot{d}_i^{(n)}\|_2^2 + n\sum_{i\in I_n\cap[1,m]} (k_i^{(n)})^2\right] \leq c'$$

and $\sum_{i\in I_n} \|d_i^{(n)}\|_2^2$ is bounded. □

3 Periodic motions of the infinite system

In section 2 we proved the existence of periodic motions in periodic finite lattices with $2n$ particles satisfying estimates (4); we will obtain a periodic motion for the infinite lattice by considering the limit for $n \to \infty$.

By the operators Υ_n we build a bounded Palais-Smale sequence for J; as already mentioned the Palais-Smale condition does not hold for J due to its translation invariance. To manage this lack of compactness, we make use of Lions' concentration-compactness Lemma [8] in a version adapted to our needs (see [2] for the proof).

Lemma 3 *(concentration-compactness)*

Let $\{u^{(n)}\}_{n\in\mathbf{N}}$ be a sequence of sequences, $u^{(n)} = \{u_i^{(n)}\}_{i\in\mathbf{Z}}$, $u_i^{(n)} \geq 0$, $\forall i \in \mathbb{Z}$ and $\forall n \in \mathbb{N}$, such that $\sum_i u_i^{(n)} = \lambda$, $\lambda > 0$, $\forall n \in \mathbb{N}$. Then there exists a subsequence (still denoted by $\{u^{(n)}\}$) such that one of the following properties occurs:

a) Concentration.

There exists a sequence $\{M_n\}_{n\in\mathbf{N}}$ of integers (which can be chosen to be multiples of m) such that $\forall\varepsilon > 0$ there exists $N_\varepsilon \in \mathbb{N}$ such that $\forall n \in \mathbb{N}$ we have

$$\sum_{i=M_n-N_\varepsilon}^{M_n+N_\varepsilon} u_i^{(n)} \geq \lambda - \varepsilon$$

b) Vanishing.

$$\lim_{n\to\infty}\left[\sup_{i\in\mathbf{Z}} u_i^{(n)}\right] = 0$$

c) Dichotomy.

There exist $\alpha \in (0, \lambda)$ and a sequence $\{M_n\}_{n\in\mathbf{N}}$ of integers (which can be chosen to be multiples of m) such that $\forall\varepsilon > 0$ there exist two integers N_ε and N'_ε such that $\forall n \in \mathbb{N}$ we have:

$$\left|\sum_{|i-M_n|\leq N_\varepsilon} u_i^{(n)} - \alpha\right| < \varepsilon \ , \quad \left|\sum_{|i-M_n|>N'_\varepsilon} u_i^{(n)} - (\lambda-\alpha)\right| < \varepsilon$$

and $N'_\varepsilon - N_\varepsilon \to +\infty$ when $\varepsilon \to 0$.

We apply Lemma 3 to the sequence of sequences $\{u_i^{(n)}\}_{n\in\mathbf{N}}$, where

$$u_i^{(n)} = \begin{cases} \int_0^T (\dot{q}_i^{(n)}(t))^2 dt + \int_0^T (q_i^{(n)}(t) - q_{i+1}^{(n)}(t))^2 dt & \text{if } |i| \leq n \\ 0 & \text{if } |i| > n \end{cases} \tag{9}$$

and $q^{(n)} \in H_n$ is the critical point obtained by Theorem 2.

1) Vanishing cannot occur.

Lemma 4 *Let $q^{(n)} \in H_n$ be the critical point obtained by Theorem 2, then the sequence $\{u_i^{(n)}\}$ defined by (9) does not admit a vanishing subsequence.*

Proof. Suppose the converse; then on the vanishing subsequence we know that $\forall \varepsilon > 0\ \exists n \in \mathbb{N}$ such that $\forall i \in \{-n, \dots, n\}$ we have

$$\|q_i^{(n)} - q_{i+1}^{(n)}\|_\infty < \varepsilon \tag{10}$$

and by the superquadraticity of V_i we have

$$|V_i'(q_i^{(n)} - q_{i+1}^{(n)})| \leq \eta_\varepsilon |q_i^{(n)} - q_{i+1}^{(n)}| \text{ with } \eta_\varepsilon \to 0 \text{ as } \varepsilon \to 0\ .$$

Then, by Theorem 2 we have

$$\begin{aligned} 0 < 2\alpha \leq 2J_n(q^{(n)}) &\leq J_n'(q^{(n)})[q^{(n)}] + \textstyle\sum_i \int_0^T V_i'(q_i^{(n)} - q_{i+1}^{(n)})(q_i^{(n)} - q_{i+1}^{(n)}) \\ &= \textstyle\sum_i \int_0^T V_i'(q_i^{(n)} - q_{i+1}^{(n)})(q_i^{(n)} - q_{i+1}^{(n)}) \leq \eta_\varepsilon \sum_i \int_0^T (q_i^{(n)} - q_{i+1}^{(n)})^2 \leq \eta_\varepsilon \cdot \rho_2 \end{aligned}$$

and for ε small enough (i.e. η_ε small enough) we get a contradiction. □

2) Existence of bumps for the dichotomy and concentration cases.

As we excluded the vanishing case, either compactness or dichotomy holds; this means that for all n most of the norm of $q^{(n)}$ (in case of concentration) or a fixed part of it (in case of dichotomy) is "concentrated" around the particle labeled by M_n (M_n is as in Lemma 3). We call "bump" this concentrated part. In both cases we achieve a sequence of functions $q^{(n)}$ whose bump is in a finite part of the lattice. Due to the translation invariance of the functional, with no restriction we can assume that $M_n \equiv 0$ in Lemma 3. Our aim now is to build a Palais-Smale sequence for both the concentration and the dichotomy case.

3) Concentration implies strong convergence.

We consider the case where the sequence $q^{(n)}$ admits a concentrated subsequence (which we still denote by $q^{(n)}$).

Lemma 5 *Suppose that concentration holds for the sequence $\{u_i^{(n)}\}$ defined in (9). Then $\{\Upsilon_n q^{(n)}\}$ is a bounded Palais-Smale sequence for J in H.*

Proof. First note that

$$J(\Upsilon_n q^{(n)}) = J_n(q^{(n)}) - \int_0^T \Phi_{-n-1}(\bar{q}_{-n}^{(n)} - q_{-n}^{(n)}) - \int_0^T \Phi_n(q_n^{(n)} - \bar{q}_n^{(n)}) + \int_0^T \Phi_{n-1}(q_{n-1}^{(n)} - q_{-n}^{(n)}) \quad (11)$$

and for all $p \in H$, $\|p\| = 1$,

$$\begin{aligned} J'(\Upsilon_n q^{(n)})[p] &= \sum_{i=-n}^{n-1} \int_0^T \dot{q}_i^{(n)} \dot{p}_i - \sum_{i=-n}^{n-2} \int_0^T \Phi_i'(q_i^{(n)} - q_{i+1}^{(n)})(p_i - p_{i+1}) \\ &- \int_0^T \Phi_{-n-1}'(\bar{q}_{-n}^{(n)} - q_{-n}^{(n)})(p_{-n-1} - p_{-n}) - \int_0^T \Phi_{n-1}'(q_{n-1}^{(n)} - \bar{q}_{n-1}^{(n)})(p_{n-1} - p_n) \end{aligned} \quad (12)$$

where $\bar{q}_i^{(n)} = \frac{1}{T}\int_0^T q_i^{(n)}(t)dt$. The last two terms vanish for $n \to \infty$ because $\|\bar{q}_{-n}^{(n)} - q_{-n}^{(n)}\|_\infty \to 0$, $\|p_{-n-1} - p_{-n}\|_2 \leq 1$ and similarly the other term.
The sequence $\{\Upsilon_n q^{(n)}\}$ is bounded in H by Theorem 2. As we are in the concentration case, by (11) it follows that $\exists \alpha', b' > 0$ such that $\alpha' \leq J(\Upsilon_n q^{(n)}) \leq b'$.
For all $p \in H_n$ such that $\|p\| = 1$ we have

$$\begin{aligned} 0 = J_n'(q^{(n)})[p] &= \textstyle\sum_{i=-n}^{n-1} \int_0^T \dot{q}_i^{(n)} \dot{p}_i - \sum_{i=-n}^{n-2} \int_0^T \Phi_i'(q_i^{(n)} - q_{i+1}^{(n)})(p_i - p_{i+1}) \\ &- \textstyle\int_0^T \Phi_{n-1}'(q_{n-1}^{(n)} - q_{-n}^{(n)})(p_{n-1} - p_{-n}) \end{aligned}$$

and using again the fact that concentration holds, the last term goes to zero as n increases, by the same reason of the last step. Finally using (12) we infer $\sup_{\|p\|=1} J'(\Upsilon_n q^{(n)})[p] \to 0$, that is $\Upsilon_n q^{(n)}$ is a Palais-Smale sequence. □

As the sequence $\Upsilon_n q^{(n)}$ is bounded in H, up to a subsequence it converges weakly to a function $q \in H$: the convergence is in fact strong, as stated by the following Lemma whose proof follows the same lines as Lemma 3 in [2].

Lemma 6 *If concentration holds for* $\{u_i^{(n)}\}$*, then* $\Upsilon_n q^{(n)} \to q$ *strongly in* H*, hence* q *is a nontrivial critical point of* J *in* H*.*

The previous result states that if the sequence $\Upsilon_n q^{(n)}$ is concentrated (i.e. $\{u_i^{(n)}\}$ is concentrated) we obtain a nonzero solution q of problem (2); if $\exists i$ such that $\alpha_i > 0$ the potential Φ_i has nonzero stationary points, therefore the solution we find could be an equilibrium point for the potential Φ; we can exclude this for large period T by proving that under such condition the critical level of the functional J is lower than the minimum level of a nonzero equilibrium point (see Proposition 2 in [2]).

4) Dichotomy and truncation imply strong convergence.

Finally we consider the dichotomy case for the sequence $\{u_i^{(n)}\}$: by Lemma 3 we know that $\exists \alpha \in (0, \lambda)$ such that, up to a suitable translation, $\forall \varepsilon > 0 \quad \exists N_\varepsilon, N'_\varepsilon \in \mathbb{N}$ such that

$$\left| \sum_{|i| \leq N_\varepsilon} u_i^{(n)} - \alpha \right| < \varepsilon \text{ and } \left| \sum_{N_\varepsilon < |i| < N'_\varepsilon} u_i^{(n)} \right| < \varepsilon \ .$$

Let ε_n be any positive sequence converging to 0 and $\forall n \in \mathbb{N}$ consider $Q^{(n)} \in H$ defined by

$$Q_i^{(n)}(t) = \begin{cases} \frac{1}{T} \int_0^T q_{N_{\varepsilon_n}}^{(n)}(t)dt & \text{if } i > N_{\varepsilon_n} \\ q_i^{(n)}(t) & \text{if } |i| \leq N_{\varepsilon_n} \\ \frac{1}{T} \int_0^T q_{-N_{\varepsilon_n}}^{(n)}(t)dt & \text{if } i < -N_{\varepsilon_n} \ . \end{cases} \tag{13}$$

By similar arguments to those of Lemma 5 we infer that $\{Q^{(n)}\}$ is a bounded Palais-Smale sequence for J in H and therefore $\exists q \in H$ such that $Q^{(n)} \rightharpoonup q$, up to a subsequence; proceeding as in Lemma 4 in [2] one can prove

Lemma 7 *If dichotomy occurs for* $\{u_i^{(n)}\}$ *and if* $Q^{(n)}$ *is as in (13) then:*

a) $\|Q^{(n)}\| \to \alpha$

b) $Q^{(n)} \to q$ *in* H *(therefore* $\|q\| = \alpha$*)*

c) $J'(q) = 0$ *(therefore* q *is a nontrivial solution of (2))*

The proof of Theorem 1 now follows as in [2].

Remark. The concentration-compactness lemma has been used for homogeneity with our previous paper [2], where this technique is used to prove a representation theorem for Palais-Smale sequences; such result is used in [3] as a starting point to build multibump solutions. Disregarding such possible applications one could achieve the proof of Theorem 1 more directly.

4 The numerical algorithm

In this section we describe the algorithm that we have used to obtain numerical approximations of the periodic motions in finite lattices; we only consider the case when $\alpha_i > 0$ i.e. when the linking geometry actually reduces to a mountain pass, although the authors feel that an extension to the general case should not be too difficult to achieve.

Theorem 2 states that a nonzero solution for the system of $2n$ particles can be obtained as a mountain pass point for the functional J_n; we use an algorithm developed by Choi and McKenna

[6] to approximate numerically such mountain pass point for different values of n, and we show how the limit for an increasing number of particles seems to appear.

We give a brief description of the algorithm, and we refer to [6] for an exhaustive treatment.

Let us first recall the geometric layout of the mountain pass theorem: one has two points in a functional space which are divided by a mountain chain whose lowest "pass-point" is at a higher level than the two points; then, under suitable compactness conditions (the Palais-Smale condition or, for instance, the concentration case of Lemma 3), there exists a path whose highest point is minimal, among all the paths connecting the two points. It can be proved that this point is a critical point of the functional.

We cannot consider all possible paths, but we can choose a path, for instance the linear one, and then pull it down along the steepest descent direction until this is not possible anymore.

Suppose that the following constants are chosen:

I, the number of particles

M, the number of steps to discretize the path

L, the number of mesh points to discretize each function q_i.

The steps of the algorithm are the following:

a) We choose 0, which is a local minimum for J as starting point of the paths, while the ending point will be w (see Lemma 2). The numerical procedure starts by defining an $M \times I \times L$ array $\{q_{il}^m\}$ $(m = 0, \ldots, M-1;\ \ l = 0, \ldots, L-1;\ \ i = 0, \ldots, I-1)$ which represents the path we are dealing with; m is the discretized path parametrization, n is the particle number and l is the discretized time. The first path is set to be the segment connecting 0 with w.

b) We look for the maximum of the functional along this path: by construction, if the path mesh is fine enough, this is achieved for $m = \bar{m}$ with $0 < \bar{m} < M$.

c) We improve the approximation of this maximum by a further subdivision of the path between $\bar{m} - 1$ and $\bar{m} + 1$.

d) We compute the steepest descent direction at point $q^{\bar{m}}$. As we are dealing with an infinite dimensional functional space where different norms are not equivalent, a definition of such a direction must be given: we call steepest descent direction at point q the direction pointed by the vector $p \in H$, $\|p\| = 1$, for which $J'(q)[p]$ achieves its minimum. In order to compute p, define the functional

$$I_q(p) = J'(q)[p] + \lambda \|p\|^2$$

where λ is a Lagrange multiplier. We require $I'_q(p) = 0$, i.e. we require the components of p to be $T-$periodic solutions of the equations

$$2\lambda[\ddot{p}_i + p_{i+1} - 2p_i + p_{i-1}] = -\ddot{q}_i - \Phi'_i(q_i - q_{i+1}) + \Phi'_{i-1}(q_{i-1} - q_i) \qquad i = 0, \ldots, I-1 \ . \quad (14)$$

Equations (14) can be discretized and written in the form

$$\lambda Ap = f(q) \ ,$$

where A is a matrix which only depends on the number of particles I, the number of mesh points L and the period T; $f(q)$ is a $I \times L$ array which depends on q and p is the unknown $I \times L$ array. The Lagrange multiplier λ can be computed a posteriori in order to choose the appropriate value for $\|p\|$.

Notice that for a large number of particles and for a sufficiently fine discretization we have to solve a linear system of a remarkable number of equations (ca. 150 in our case), but this does not slow down too much the algorithm because the matrix A^{-1} can be computed once for all, and then used to check different potentials or different starting paths.

e) Once the steepest descent direction has been found, we move the maximum point along it, thus lowering the functional. Attention must be paid in order not to go too far away from the pass point; to this purpose we set a limit for both the maximum norm of the displacement and the maximum decrease of the functional.

f) We repeat steps b) and c) and we estimate $\|J'(q)\|$, where q is the new maximum point: if we are below a selected threshold we are done; otherwise we come back to point d).

The convergence of this algorithm is quite delicate; indeed if the displacement along the steepest descent direction is too small it can happen that steps b) and c) have the opposite effect of steps d) and e) and the algorithm enters a loop. On the other hand, if the displacement is too large it is possible to miss the mountain pass point and in this case the algorithm converges to the zero solution.

To improve the performance of the algorithm, we check at each step the distance (in the H-norm) between the point of maximum and its nearest neighbors, and if such a distance becomes too large we accumulate some mesh point around the maximum.

We insist on remarking that our description of the algorithm is purely made to let the reader taste it: indeed the choice of the various thresholds is very delicate and further attention must be paid to avoid the procedure to fail (see [6] for more details).

5 Some numerical results

We tried various configurations with different number of particles and potentials; to simplify the structure of the program we chose all the interparticle potentials to be equal ($\Phi_i \equiv \Phi$). Figures 1 and 2 represent our results for systems of respectively 8 and 14 particles with the following choice of the potentials:

$$\Phi(x) = -x^2 + x^4 \ .$$

As a matter of fact we did not show the motion of particles -7, -6 and 6 in the second system, as it is negligible.

We remark the following facts:

1) In both cases the particle in the middle of the lattice undergoes the oscillation of maximum amplitude.

2) In both cases only the nearest and second nearest neighbor particles undergo an oscillation of wide amplitude; the amplitude decreases quickly when getting farther away from the middle particle.

3) The results for the systems are quite similar, which permits to conjecture that for an increasing number of particles it would not change.

4) This algorithm produces in fact a Palais-Smale sequence which remains concentrated around the particle in the middle of the lattice.

We also tested other kinds of potentials satisfying our assumptions and we obtained similar results, although some choices of potential raised some difficulties of convergence of the algorithm. We can therefore guess the shape of the motion of an infinite lattice; it seems reasonable to think that such a motion is well represented by motions of finite lattices, the other particles' motion being negligible.

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