PERIODIC MOTIONS IN LATTICES OF PARTICLES

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ABSTRACT: We study an autonomous Hamiltonian system consisting of a lattice of particles each interacting with the adjacent ones; both the cases of a finite number and of an infinite number of particles are considered. For different choices of the forces we establish, by variational methods, the existence of periodic motions.

AMS (MOS) subject classification: 34C35, 58F05, 34C25, 58E05

1. INTRODUCTION

We consider an autonomous Hamiltonian system consisting of a lattice of particles with nearest neighbor interaction: the state of the lattice at time t is represented by a vector function $q(t) = \{q_i(t)\}\ (i \in \mathbf{I}, \mathbf{I} = \{1, ..., N\}$ for finite lattices and $\mathbf{I} = \mathbb{Z}$ for infinite lattices), where $q_i(t)$ is the state of the i-th particle; if $\Phi_i : \mathbb{R} \to \mathbb{R}$ denotes the potential of the interaction between the i-th and the (i+1)-th particle (the assumptions on Φ_i are given below), then the equation governing the state of $q_i(t)$ reads

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

We define the global potential Φ of the system by $\Phi(q) := \sum_{i \in \mathbf{I}} \Phi_i(q_i - q_{i+1})$ so that equations (1) can be written in the vectorial form

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

The starting point of studies of motions in lattices of particles is the celebrated numerical experiment of Fermi et al [10]: they tried to test numerically the conjecture that, even if in a chain of particles with nearest neighbor interactions of linear type the energy of each normal mode is constant, it is enough to introduce a small perturbation in order to destroy such stability and spread the energy among all the modes. Surprisingly, they obtained the opposite result, i.e. they saw that if the perturbation is small enough, the energy does not spread; this is the first step to show that the system is not ergodic. Years later, Toda [18] proved that a chain of particles with exponential interaction potential is integrable, and therefore it does not spread the energy at all: the physical model considered is that of a chain of disks which are allowed to rotate around their axes, the variables $q_i(t)$ being the values of the angle of rotation; the nearest neighbor disks are connected with a spring which rises a force. An alternative model is that of a one-dimensional system of atoms, see [7]. More recently, Ruf & Srikanth [16] proved with variational techniques that a finite lattice of particles with a Toda type potential admits periodic motions of assigned period T. Different kinds of results about lattices of particles can be found in [11, 19].

The results of section 3 have been obtained in collaboration with G. Arioli and Theorem 5 with G. Arioli and S. Terracini; for the proofs of the results stated here we refer to the original papers [1, 2, 3, 12].

2. FINITE LATTICES

In this section we consider finite lattices of N particles $(N \ge 2)$; the state of the lattice at time t is here represented by a vector $q(t) \in \mathbb{R}^N$. We study lattices with one fixed

endpoint, i.e. $q_0 \equiv 0$, in the case where the interparticle potentials Φ_i have repulsive barriers at the endpoints of their (bounded) intervals of definition; (1) become

$$\ddot{q}_i(t) = \Phi'_{i-1}[q_{i-1}(t) - q_i(t)] - \Phi'_i[q_i(t) - q_{i+1}(t)] \qquad i = 1, ..., N - 1$$

$$\ddot{q}_N(t) = \Phi'_{N-1}[q_{N-1}(t) - q_N(t)] . \tag{3}$$

We can figure the model where the disks are free to rotate until a given position from which they are "bounced back" in an elastic way; obviously, (3) may not be satisfied in classical sense and a suitable definition of generalized solution is needed. We establish that (3) admits a periodic generalized solution of assigned energy E or period T: these results are obtained by means of a sequence of approximated problems having a strong force term [13] and by taking the limit when the strong force term tends to vanish; this technique has already been used in [4].

Let us now turn to the mathematical setting of the problem: for all i = 0, ..., N-1 let $a_i, b_i \in \mathbb{R}$, with $a_i < b_i$ and assume that the potentials Φ_i satisfy

$$\Phi_i \in C^2[a_i, b_i] \ . \tag{C}$$

Define $\Omega_T := \{q = (q_1, ..., q_N) \in H_T; q_i(t) - q_{i+1}(t) \in (a_i, b_i) \ \forall i = 0, ..., N-1, \ \forall t \in [0, T]\}$, where H_T is the Hilbert space of absolutely continuous T-periodic functions $q : [0, T] \to \mathbb{R}^N$ with square integrable derivative, endowed with the scalar product

$$\forall q, p \in H_T$$
 $(q, p) = \int_0^T \dot{q}(t) \cdot \dot{p}(t) \ dt + \left(\int_0^T q(t) \ dt\right) \cdot \left(\int_0^T p(t) \ dt\right) \ .$

Let us explain what we mean by generalized periodic solution:

Definition 1 A generalized T-periodic solution of energy E of equation (3) is a function $q \in \bar{\Omega}_T$ such that:

(i) there exist N finite Borel measures $\mu_i(q_i - q_{i+1})$ on [0,T] (i=0,...,N-1) such that

$$B_i(q) := \operatorname{supp} \mu_i \subset \{t \in [0, T]; \ q_i(t) - q_{i+1}(t) \in \{a_i, b_i\}\}$$

(ii) there exists $i \in \{0,...,N-1\}$ such that $B_i(q) \neq \emptyset$

(iii) if $\mu(q) := \sum_i \mu_i(q_i - q_{i+1})$ and $B(q) := \bigcup_i B_i(q)$ then |B(q)| = 0, $q \in C^2[0,T] \setminus B(q)$ and the equation $\ddot{q} = -\Phi'(q) - \mu(q)$ is satisfied in distributional sense i.e.

$$\int_0^T \dot{q}\dot{p} \ dt - \int_0^T \Phi'(q)p \ dt = \int_{B(q)} p \ d\mu(q) \qquad \forall p \in C_T^{\infty}$$

where C_T^{∞} is the space of smooth T-periodic functions with values in \mathbb{R}^N (iv) if $t \in B_i(q)$ then $\dot{q}_i - \dot{q}_{i+1}$ has right and left limit in t and

$$\lim_{s \to t^{-}} [\dot{q}_{i}(s) - \dot{q}_{i+1}(s)] = \lim_{s \to t^{+}} [\dot{q}_{i+1}(s) - \dot{q}_{i}(s)]$$

$$(v) \frac{1}{2} \sum_{i=1}^{N} \dot{q}_i^2(t) + \sum_{i=0}^{N-1} \Phi_i[q_i(t) - q_{i+1}(t)] = E \text{ for all } t \in [0, T] \setminus B(q).$$

If no bounces occur then $\mu_i(q_i - q_{i+1}) \equiv 0$ for all i and a generalized solution of (3) is in fact a classical (C^2) solution.

For the prescribed energy case we have (see [12]):

Theorem 1 Assume (C) and let \mathcal{E} be the set of positive noncritical levels of Φ ; then for all $E \in \mathcal{E}$ there exists T > 0 such that system (3) admits a (possibly) generalized T-periodic solution of energy E. Moreover, there exists $E_0 = E_0(\Phi_i) \geq 0$ such that if $E > E_0$ the generalized solution has at least one bounce; in particular, if $\Phi_i \equiv 0$ for all i, then $E_0 = 0$.

Sketch of the proof. First we add a smooth strong force term $\varepsilon \Psi'_i(q_i - q_{i+1})$ ($\varepsilon > 0$) to the forces Φ'_i in (3): we define $\Psi(q) := \sum_i \Psi_i(q_i - q_{i+1})$, $\Phi_{\varepsilon} = \Phi + \varepsilon \Psi$, and for all $\varepsilon > 0$, the action functional $I_{\varepsilon} : \Omega_1 \to \mathbb{R}$ by

$$I_{arepsilon}(q) = rac{1}{2} \int_0^1 |\dot{q}|^2 dt \cdot \left[E - \int_0^1 [\Phi_{arepsilon}(q)] dt
ight] \; ;$$

we have $I_{\varepsilon} \in C^2(\Omega_1, \mathbb{R})$ and its critical points q at positive level correspond to classical T_{ε} -periodic solutions of energy E of the equation $\ddot{q} = -\Phi'_{\varepsilon}(q)$, after a time scaling. Next, we prove by a suitable linking technique [15], that $\exists q^{\varepsilon}$ such that $I'_{\varepsilon}(q^{\varepsilon}) = 0$; hence, q^{ε} is a classical T_{ε} -periodic motion of energy $E = \frac{1}{2}|\dot{q}^{\varepsilon}(t)|^2 + \Phi_{\varepsilon}[q^{\varepsilon}(t)]$ of the above equation: the assumption $E \in \mathcal{E}$ is used to prove the Palais-Smale condition (PS condition). Finally, we let $\varepsilon \to 0$: we obtain uniform estimates of the norm $||q^{\varepsilon}||$, of the critical level $I_{\varepsilon}(q^{\varepsilon})$ and of the period T_{ε} . These estimates allow to prove that all the requirements of Definition 1 are satisfied: the measures μ_i are the limits (in the weak* measure topology) of the sequences $\{\varepsilon \Psi'_i\}$. To prove that if E is large enough the solution has at least one bounce, we prove that (2) cannot be satisfied in classical sense. A Morse index argument can be used to prove that |B(q)| = 0.

For the prescribed period case we have (see [12]):

Theorem 2 Assume (C); then for all T > 0 there exists E > 0 such that system (3) admits a generalized T-periodic solution of energy E.

Sketch of the proof. This proof is similar to the previous one: we add smooth strong forces $\varepsilon \Psi_i'$, we denote $\Phi_\varepsilon = \Phi + \varepsilon \Psi$ and we consider for all $\varepsilon > 0$, the action functional $J_\varepsilon \in C^2(\Omega_T, \mathbb{R})$ defined by

$$J_{\varepsilon}(q) = \frac{1}{2} \int_0^T |\dot{q}|^2 dt - \int_0^T [\Phi_{\varepsilon}(q)] dt ;$$

its critical points correspond to classical T-periodic solutions of the equation $\ddot{q} = -\Phi'_{\varepsilon}(q)$. To prove the PS condition for J_{ε} we prove that a PS sequence $\{q^n\}$ cannot be unbounded by the comparison between the rates of growth at infinity of $\int_0^T \Phi_{\varepsilon}(q^n)$ and $\int_0^T \Phi'_{\varepsilon}(q^n)q^n$; by means of a suitable linking we obtain the existence of $q^{\varepsilon} \in \Omega_T$ such that $J'_{\varepsilon}(q^{\varepsilon}) = 0$. If we let $\varepsilon \to 0$ we obtain uniform estimates of the norm $\|q^{\varepsilon}\|$, of the critical level $J_{\varepsilon}(q^{\varepsilon})$ and of the energy E_{ε} which allow to conclude as above. Here the existence of at least one bounce is obtained for all T > 0.

3. INFINITE LATTICES

In this section we deal with infinite lattices: the state of the lattice at time t is now represented by a sequence $q(t) = \{q_i(t)\}\ (i \in \mathbb{Z})$ and the potential of the system $\Phi : \mathbb{R}^{\mathbb{Z}} \to \mathbb{R}$ is the series $\Phi(q) := \sum_{i \in \mathbb{Z}} \Phi_i(q_i - q_{i+1})$. For all $i \in \mathbb{Z}$ we assume the

potential Φ_i to satisfy

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

When $\alpha_i > 0$ the force is repulsive-attractive (RA), i.e. repulsive for small displacements and attractive for large displacements, while if $\alpha_i = 0$ the force is purely attractive (PA). Think to an infinite chain of parallel disks: the nearest neighbor disks are connected with a superlinear attractive spring if $\alpha_i = 0$ and also with a linear repulsive spring if $\alpha_i > 0$; in the latter case the disks achieve at least an unstable equilibrium position, when the angles are equal, and two stable equilibrium positions, one in each direction of rotation. For all T>0, we prove the existence of a T-periodic solution of (1): the solution we obtain has finite energy, that is, all the couples (except a finite number) of adjacent disks interacting with RA forces move in a neighborhood of their unstable equilibrium position, i.e. they never fall in the stable position where the potential attains its minimum; for the same reason, almost all the couples of adjacent disks interacting with PA forces move in a neighborhood of the stable equilibrium. Therefore almost all the energy remains contained in a finite region of the space; this fact is also be supported by numerical results. The existence of a nontrivial periodic solution of finite energy for this system may be surprising: 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

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

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

which is a Hilbert space when endowed with the scalar product

$$(q,p) := \sum_{i \in \mathbf{Z}} \int_0^T \left[(\dot{q}_i)(\dot{p}_i) + (q_i - q_{i+1})(p_i - p_{i+1}) \right] \qquad \forall p, q \in H ;$$

we consider the functional $J: H \to \mathbb{R}$ defined by

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

the functional J is well defined on H and $J \in C^1(H, \mathbb{R})$, see [1]. We prove the existence of a T-periodic motion of (2) by showing that the functional J admits a critical point; note that due to its translation invariance, the functional does not satisfy the PS condition. To manage this lack of compactness we use Lions' concentration-compactness Lemma (C-C Lemma) [14] in a discrete version, see [1] for the proof.

The following theorem summarizes our results, see [2]:

Theorem 3 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.

Sketch of the proof. For all n = km (m as in (P), $k \in \mathbb{N}$) consider the system (S_n) consisting in a periodic lattice of 2n particles (i.e. $\mathbf{I} = \{-n, ..., n-1\}$ and $q_n \equiv q_{-n}$): to study this problem we use the Hilbert space $H_n := \{q \in H^1(S^1, \mathbb{R})^{2n}; \int_0^T q_0 = 0\}$ which can be imbedded continuously into H by means of a suitable operator Υ_n . 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 . For all $n \in \mathbb{N}$ the functional J_n satisfies the PS condition and the geometrical requirements of the linking theorem: if $\alpha_i > 0 \ \forall i$ the linking is in fact a mountain pass [15]. The existence of critical points $q^{(n)}$ for J_n follows and we obtain uniform estimates of their norms and critical levels. We prove that $\{\Upsilon_n q^{(n)}\}$ is a bounded PS sequence for J in H, hence $\exists q \in H$ such that $\Upsilon_n q^{(n)} \to q$; as the PS condition does not hold for J, we make use of the discrete C-C Lemma. We apply it to the sequence of sequences $\{u_i^{(n)}\}_{n \in \mathbb{N}}$, where

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

and $q^{(n)} \in H_n$ is the critical point previously obtained. We first exclude the vanishing case of the C-C Lemma. Next we establish the existence of bumps for the dichotomy and concentration cases; 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 a certain particle: 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; we "cut" the periodic lattice between the two particles opposite to the bump. 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. If dichotomy holds for $\{u_i^{(n)}\}$, by a suitable truncation procedure we build another PS sequence $\{Q^{(n)}\}$ and determine $\alpha > 0$ such that $\|Q^{(n)}\| \to \alpha < \liminf_{n \to \infty} \|q^{(n)}\|$ and $Q^{(n)} \to q$ in H: therefore $||q|| = \alpha$ and q is a nonzero periodic solution of (2); hence, the strong limit of the truncated sequence $\{Q^{(n)}\}$ equals the weak limit q of the untruncated sequence $\{q^{(n)}\}$. If $\alpha_i > 0$ for some i, the potential Φ_i has nonzero stationary points and the solution we find could be an equilibrium point for the potential Φ ; we can exclude this for large period T (say T > T) by proving that in such case, the critical level of the functional J is lower than the minimum level of a nonzero equilibrium point, see [1]. Finally, it is easy to see that the energy of the solution is finite.

Remark. If the infinite lattice we consider only has RA forces, i.e. $\alpha_i > 0$ for all $i \in \mathbb{Z}$, we can give a more direct proof of Theorem 3, see [1]: we prove that the functional J admits a PS sequence $\{q^{(n)}\}\subset H$ such that

$$\exists c_1, c_2 > 0$$
 such that $0 < c_1 \le ||q^{(n)}|| \le c_2$ (4)

and we use the same concentration-compactness arguments as above. From the analytical point of view the problem with only RA forces is quite different from the one where at least one force (and hence an infinity of forces by (P)) is PA, indeed in the latter case the mountain pass geometry is replaced by an infinite dimensional linking and the technique developed in [5] to handle this kind of problems cannot be applied, due to the lack of compactness of the functional.

From now on we deal with lattices having only RA forces and we assume the condition $T > \overline{T}$ to be satisfied so that the critical points of J are nonconstant. We can give a detailed picture of the structure of a PS sequence by the same device as in [8, 9]: the functional J is invariant under both a representation of \mathbb{Z} which we denote *, and a representation of S^1 which we denote Ω ; these representations are defined by

$$*: \mathbb{Z} \times H \to H$$
, $(k,q) \mapsto k * q$ where $(k*q(t))_i = q_{i+km}(t) - \frac{1}{T} \int_0^T q_{km}$
 $\Omega: S^1 \times H \to H$, where $[\Omega(\tau,q(t))]_i = q_i(t+\tau)$.

For all $a,b \in \mathbb{R}$ such that $b \leq a$ we denote $J^a = J^{-1}((-\infty,a]), \ J^a_b = J^{-1}([b,a]), \ K = \{q \in H \setminus \{0\}; \ J'(q) = 0\} \text{ and } K^a = J^a \cap K.$ For all $l \in \mathbb{N}, \ \bar{k} = (k^1,...,k^l) \in \mathbb{Z}^l$ and $\bar{q} = (q^1,...,q^l) \in H^l$, we define $\bar{k}*\bar{q}:=\sum_{j=1}^l k^j*q^j;$ for all sequences of l-tuples of integers $\bar{k}_n = (k_n^1,...,k_n^l)$, by $\bar{k}_n \to \infty$ we mean that $|k_n^i - k_n^j| \to \infty$ as $n \to \infty$ for $i \neq j$. The following representation theorem holds, see [1]:

Theorem 4 Assume (P) and let $\{q^{(n)}\}\subset H$ be a PS sequence for J at level b>0 satisfying (4). Then there exist a subsequence still denoted by $\{q^{(n)}\}, \mu \geq 1, l$ points $(1 \leq l \leq \mu) \ q^j \in K \ (j=1,...,l), \ and \ l$ sequences of integers $k_n^j \ (n \in \mathbb{N}), \ such that if <math>\bar{q} = (q^1,...,q^l)$ and $\bar{k}_n = (k_n^1,...,k_n^l), \ then$

$$\left\|q^{(n)} - \bar{k}_n * \bar{q}\right\| \to 0 , \qquad \sum_{j=1}^l J(q^j) = b , \qquad \bar{k}_n \to \infty .$$

This result states that the variational structure of our problem possesses some analogies with that of the problem of homoclinic orbits for non-autonomous Hamiltonian systems with periodic potentials. In both cases, the functional is invariant under the action of a non-compact group \mathbb{Z} and the PS condition does not hold at any critical level; on the other hand, the same action may allow to prove the existence of multibump solutions by a "sticking procedure". This structure was discovered by Séré [17] for the problem of homoclinics studied in [8]. Our problem is invariant under an S^1 -action as well and we can prove the existence of multibump solutions by assuming (\bullet) instead of the more stringent (H) in [17] and (*) in [9], see Theorem 5 below. Let us first explain what we mean by multibump solutions:

Definition 2 A critical point q is a multibump solution of kind $(l, \rho) \in \mathbb{N} \times \mathbb{R}^+$ if $\exists \bar{k} = (k^1, ..., k^l) \in \mathbb{Z}^l$ and $\bar{q} = (q^1, ..., q^l)$, $q^j \in K$, such that $q \in B_{\rho}(\bar{k} * \bar{q})$.

With this notion we can state the following multiplicity result, see [3]:

Theorem 5 Assume (P); then $K/(S^1 \times \mathbb{Z})$ is infinite. More precisely if

(•)
$$\begin{cases} \exists \bar{\alpha} > 0 \text{ and a compact set } \mathcal{K} \subset H \text{ such that} \\ K^{b+\bar{\alpha}} = \bigcup_{k \in \mathbf{Z}} k * \mathcal{K} \text{ with } k_1 * \mathcal{K} \cap k_2 * \mathcal{K} = \emptyset \text{ when } k_1 \neq k_2 \end{cases},$$

then $\forall n \in \mathbb{N}$ and $\forall a, \rho > 0$ system (2) admits infinitely many multibump solutions of kind (n, ρ) in $J_{nb-a}^{nb+a}/(S^1 \times \mathbb{Z})$.

By applying an algorithm developed by Choi & McKenna [6] we computed the solutions for finite lattices in the case of RA forces; the numerical results we obtain describe the process of approximation of the solution for the infinite lattices adopted in the proof of Theorem 3: for a detailed description of our procedure we refer to [2]. In our experiments 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 $(\Phi_i \equiv \Phi)$. In the following table we quote our results for systems of respectively 8 and 14 particles with potentials $\Phi(x) = -x^2 + x^4$: the particle labeled with 0 is the one undergoing the oscillation of maximum amplitude and is in opposition of phase with all the others; we do not show the amplitude of oscillation of particles ± 5 , ± 6 in the second system, as it results to be negligible.

particle number	0	±1	±2	±3	±4
amplitude of oscillation (8)	3	1.2	$3 \cdot 10^{-2}$	$1.2\cdot 10^{-3}$	$4\cdot 10^{-5}$
amplitude of oscillation (14)	4	$8 \cdot 10^{-1}$	$3 \cdot 10^{-2}$	$8 \cdot 10^{-4}$	$3\cdot 10^{-5}$

We remark that 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. The results for the systems are quite similar, which permits to conjecture that for an increasing number of particles it would not change: this algorithm produces in fact a PS sequence which remains concentrated around the particle in the middle of the lattice. We also tested other kinds of potentials satisfying assumptions (P) and we obtained similar results; 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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