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Time Evolution of Infinite Anharmonic Systems

Oscar E. Lanford III,[1] Joel L. Lebowitz,[2,3] and Elliott H. Lieb[4]

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We prove the existence of a time evolution for infinite anharmonic crystals for a large class of initial configurations. When there are strong forces tying particles to their equilibrium positions then the class of permissible initial conditions can be specified explicitly; otherwise it can only be shown to have full measure with respect to the appropriate Gibbs state. Uniqueness of the time evolution is also proven under suitable assumptions on the solutions of the equations of motion.

KEY WORDS: Existence of time evolution; uniqueness; strong restoring forces.

1. INTRODUCTION

The time evolution of classical (or quantum) Hamiltonian dynamical systems containing an infinite number of particles is of great interest in statistical mechanics, being an essential ingredient in the study of nonequilibrium phenomena in macroscopic systems. There are many difficulties, however, in dealing with the dynamics of infinite systems and the available results on the existence of the time evolution of such systems are not entirely satisfactory. It is only for one-dimensional classical systems[(1)] or harmonic crystals[(2)] that we have a strong evolution theorem, i.e., we can specify explicitly a class of initial conditions for which a time evolution exists. This set of initial conditions is furthermore appropriate for a large class of interactions between the particles and has full equilibrium measure for all these interactions. In contrast, all that has been proven so far for higher dimensions[(3–5)] is the

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[1] University of California at Berkeley, Berkeley, California.
[2] Institut des Hautes Etudes Scientifiques, Bures-sur-Yvette, France.
[3] Permanent address: Belfer Graduate School of Science, Yeshiva University, New York, New York.
[4] Princeton University, Princeton, New Jersey.

existence of a time evolution for a given interaction on some unspecified set of initial configurations which has full measure with respect to the equilibrium state for that interaction. It is the purpose of this paper to prove the existence of a strong time evolution for a certain class (where condition A_3 of Section 2 holds) of anharmonic crystals[6] in arbitrary dimensions and a weaker time evolution for very general anharmonic systems (Section 4).

2. EXISTENCE OF TIME EVOLUTION

The setting is the lattice $\mathbb{Z}^\nu$. At each point $i \in \mathbb{Z}^\nu$ we have an oscillator with coordinate $q_i \in \mathbb{R}$ and momentum $p_i \in \mathbb{R}$. Really, we should take q_i and p_i in $\mathbb{R}^k$ for some k; with $k = \nu$ this would represent, physically, the fact that each point of $\mathbb{Z}^\nu$ is the equilibrium position of a particle. To avoid complicating the notation, we take $k = 1$, but our results obviously go through for general k. By $\mathbf{q}$ (resp. $\mathbf{p}$) we denote the collection of oscillator coordinates (resp. momenta).

The oscillator variables are regarded as functions of time t, $\{q_i(t), p_i(t)\}$, and are represented collectively by $\mathbf{q}(t)$ and $\mathbf{p}(t)$. They satisfy the following infinite set of coupled differential equations:

$$dq_i(t)/dt = p_i(t) \tag{1a}$$

$$dp_i(t)/dt = F_i = -\partial U_i(q_i(t))/\partial q_i + R_i(\mathbf{q}(t)) \tag{1b}$$

In Eq. (1b) we wrote F_i, the force acting on the ith particle, as a sum of two terms: a gradient of a "self-energy" term $U_i(q_i)$ and a force R_i, which we shall take (but need not have) to be the gradient of some interaction energy

$$R_i = -\sum_j \partial V_j(\mathbf{q})/\partial q_i \tag{1c}$$

Our basic assumption in this part is that the self-energy $U_i(q_i)$ is such a steeply increasing function of q_i that it "dominates" the motion of the particles when they are far from their equilibrium positions. We also assume that the interactions have a finite range D (this is convenient but not essential). Stated precisely, we assume:

A_1. $V_i(q)$ depends only on those q_j for which the Euclidean distance $|i - j| \leqslant D$.

A_2. Each $U_j(q_j)$ and $V_j(\mathbf{q})$ is a twice continuously differentiable function of its arguments.

A_3. $|q_j| \leqslant C_1 U_j(q_j) + C_2$, C_1 and C_2 nonnegative constants.

A_4. There exist nonnegative bounded constants $A_{ij} < C$, $A_{ij} = 0$ for $|i - j| > D$, such that

$$|p_i R_i(\mathbf{q})| \leqslant \sum_j A_{ij} \mathscr{L}_j \tag{2a}$$

where

$$\mathscr{L}_i(p_i, q_i) = \tfrac{1}{2}p_i^2 + U_i(q_i) + K \geqslant 0, \qquad K \text{ a constant} \tag{2b}$$

Example. Conditions A will be satisfied if $U_i(q_i)$ is a polynomial of degree $2n$ whose leading coefficient λ_i is strictly positive, $\lambda_i \geqslant \lambda > 0$, and $R_i(q)$ is a multinomial of degree at most n.

The nonnegative functions $\mathscr{L}_i$ will play an important role in establishing the existence and uniqueness of solutions to the equations of motion (1). They are similar to self-energy or Lyapunov functions.

The problem posed by Eqs. (1a)–(1c) is the following: Given suitable initial data $\mathbf{q}(0)$, $\mathbf{p}(0)$, find $\mathbf{q}(t)$, $\mathbf{p}(t)$ that agree with the initial data at $t = 0$ and satisfy (1a)–(1c). This problem is equivalent to another one: Find $\mathbf{q}(t)$ such that

$$q_i(t) = q_i(0) + p_i(0)t + \int_0^t (t - s)F_i(\mathbf{q}(s))\, ds \tag{3}$$

Any solution to (3) will satisfy the initial condition and will be differentiable. One can then define $p_i(t) = dq_i(t)/dt$ and (1a)–(1c) will be satisfied. Conversely, any solution to (1a)–(1c) satisfies (3).

Definition. We denote by B_r the real Banach space of sequences $\xi = \{\xi_j\}$, $j \in \mathbb{Z}^\nu$, such that the norm

$$\|\xi\|_r = \sup_{j \in \mathbb{Z}^\nu} \{[\exp(-|j|r)]|\xi_j|\} \tag{4}$$

is finite.

Lemma 1. Let $\mathbf{q}(t)$, $\mathbf{p}(t)$ be solutions of (1a)–(1c) defined for $0 \leqslant t \leqslant T$, with initial data $\mathbf{q}(0)$ such that $\mathscr{L}(0) = \{\mathscr{L}_i(0)\} \in B_r$, where we have written $\mathscr{L}_i(t)$ for $\mathscr{L}_i(p_i(t), q_i(t))$. Then there is a constant a, independent of the initial condition but depending on r, such that

$$\|\mathscr{L}(t)\|_r \leqslant [\exp(at)]\|\mathscr{L}(0)\|_r \tag{5}$$

Proof. Using the equations of motion (1a)–(1c), we have

$$d\mathscr{L}_i(t)/dt = p_i(t)R_i(\mathbf{q}(t)) \tag{6}$$

By conditions A_3 and A_4

$$(d/dt)\mathscr{L}_i(t) \leqslant |d\mathscr{L}_i(t)/dt| \leqslant \sum_j A_{ij}\mathscr{L}_j(t) \tag{7}$$

where the A_{ij} are constants, independent of t; $0 \leqslant A_{ij} \leqslant C$; and $A_{ij} = 0$ for $|i - j| > D$, the range of the potential. If $\mathbf{A}$ denotes the matrix with elements A_{ij}, then[(2)] $\boldsymbol{\Psi}(t) = [\exp(\mathbf{A}t)]|\mathscr{L}(0)|$ is a solution of the equations

$$d\Psi_i/dt = \sum A_{ij}\Psi_j(t), \qquad \Psi_j(0) = |\mathscr{L}_j(0)| \tag{8}$$

Standard arguments show that $|\mathscr{L}_i(t)| \leqslant \Psi_i(t)$, so Eq. (5) follows from (7) with a equal to the r-norm of the bounded operator $\mathbf{A}$ on B_r.

Theorem 1. Let $\mathbf{q}(0)$, $\mathbf{p}(0)$ be such that $\mathscr{L}(0)$ (defined in Lemma 1) belongs to B_r. There then exists a $\in B_r$ solution of Eqs. (1a)–(1c) defined for all t.

Proof. We shall first consider the case of a finite system in a bounded region $\Lambda_\alpha \subset \mathbb{Z}^\nu$. Let $q_i^\alpha(t)$, $p_i^\alpha(t)$ be the solutions of the equations

$$\left.\begin{aligned} dq_i^\alpha/dt &= p_i^\alpha(t) \\ dp_i^\alpha/dt &= F_i(\mathbf{q}^\alpha(t)) \end{aligned}\right\} \quad \text{for} \quad i \in \Lambda_\alpha \tag{9a, 9b}$$

$$dq_i^\alpha/dt = dp_i^\alpha/dt = 0 \quad \text{for} \quad i \notin \Lambda_\alpha \tag{9c}$$

with the initial conditions $q_i^\alpha(0) = q_i(0)$, $p_i^\alpha(0) = p_i(0)$, i.e., Eqs. (9a)–(9c) are time evolution equations for $\mathbf{q}^\alpha(t)$, $\mathbf{p}^\alpha(t)$ with *all* the particles outside Λ_α "tied down" to their initial positions.[2,3] Solutions of (9a)–(9c) are prevented from going to infinity in finite time by Lemma 1; they therefore exist for all time. The time evolution mappings T_t^α generated by (9a)–(9c) leave invariant the energy in Λ_α,

$$H_\alpha(\mathbf{q}, \mathbf{p}) = \sum_{i \in \Lambda_\alpha} [\tfrac{1}{2} p_i^2 + U_i(q_i)] + \sum_j{}' V_j(\mathbf{q})$$

where $\sum'$ is the sum over all j such that $\operatorname{dist}(j, \Lambda_\alpha) \leqslant D$. The solutions of (9a)–(9c) will satisfy the equations

$$\left.\begin{aligned} q_i^\alpha(t) &= q_i^\alpha(0) + p_i^\alpha(0)t + \int_0^t (t - s) F_i(\mathbf{q}^\alpha(s))\, ds \\ p_i^\alpha(t) &= p_i^\alpha(0) + \int_0^t F_i(\mathbf{q}^\alpha(s))\, ds \end{aligned}\right\} \quad \text{for} \quad i \in \Lambda_\alpha \tag{10a, 10b}$$

$$q_i^\alpha(t) = q_i^\alpha(0), \qquad p_i^\alpha(t) = p_i^\alpha(0) \qquad \text{for} \quad i \notin \Lambda_\alpha \tag{10c}$$

Using now the bound (5) for the time evolution T_t^α, we have, by condition A_3, that $|F_i(\mathbf{q}^\alpha(t))| < K_i$ for $t \in [0, T]$ with $K_i < \infty$ independent of Λ_α. Hence by the Arzela–Ascoli theorem we can choose sequences $\Lambda_\alpha \to \mathbb{Z}^\nu$ such that $q_i^\alpha(t)$, $p_i^\alpha(t) \to q_i(t)$, $p_i(t)$ uniformly on $[0, T]$. This is true for all finite T, so the sequence can be further refined to get uniform convergence on *every* bounded interval. The $q_i(t)$ will satisfy Eq. (3), so the $(\mathbf{q}(t), \mathbf{p}(t))$ satisfy (1a)–(1c), the equations of motion for the infinite system, with the initial conditions $(\mathbf{q}(0), \mathbf{p}(0))$.

By our assumption, $\mathscr{L}(0) \in B_r$. Hence, by (5), we also have an estimate of the form

$$\mathscr{L}_j(t) = \tfrac{1}{2} p_i^2(t) + U_j(q_j(t)) + K < K' \exp(r|j|), \qquad |t| \leqslant T$$

for each T (but where K' grows with T). By A_3 this implies

$$|q_j(t)| < C' \exp(r|j|), \qquad |p_j(t)| < C'' \exp(\tfrac{1}{2}r|j|) \tag{11}$$

This gives us rather good control over the time evolution, e.g., if the initial values are bounded, $|q_i(0)| < C$ and $|p_i(0)| < C$, then $q_i(t)$ and $p_i(t)$ will also be bounded for all finite t.

3. UNIQUENESS OF TIME EVOLUTION

Having established the existence of solutions of Eqs. (1a)–(1c) for a large class of initial conditions, we now consider their uniqueness. As is generally the case, e.g., for harmonic systems[2] we can obtain uniqueness only if we impose some conditions on how the solution $\{q_j(t), p_j(t)\}$ grows with $|j|$.

Definition. For any family $\mathbf{B} = \{B_i\}$ of positive constants, define $\Delta(\mathbf{B}) = \{\mathbf{q}: |q_i| \leqslant B_i \text{ for all } i\}$ and define $\bar{B}_k = \sup\{B_i: |i| \leqslant k\}$, $k = 1, 2, \ldots$. We will say $\mathbf{B}$ is a *sequence of uniqueness* if (a) the following holds:

$$\limsup_{k\to\infty} \bar{B}_k^{1/k} < \infty \tag{12a}$$

and (b) there exists a constant c such that

$$\sup_{\mathbf{q}\in\Delta(\mathbf{B})} \sum_j |\partial F_i(\mathbf{q})/\partial q_j| \leqslant ci^2 \qquad \text{for all } i \tag{12b}$$

Theorem 2. Let $\mathbf{B}$ be a sequence of uniqueness. Then two solutions $\mathbf{q}^{(1)}(t)$ and $\mathbf{q}^{(2)}(t)$ of (3), both defined on $[0, T]$ and both taking values in $\Delta(\mathbf{B})$, are identical on $[0, T]$.

Proof. Assume the contrary. Then we can assume that there are arbitrarily small, positive t's for which $\mathbf{q}^{(1)}(t) \neq \mathbf{q}^{(2)}(t)$. We will show that this leads to a contradiction. Writing out (3) for $\{q^{(1)}(t)\}$ and $\{q^{(2)}(t)\}$ and subtracting the two gives

$$q_i^{(1)}(t) - q_i^{(2)}(t) = \int_0^t dt_1\,(t - t_1)[F_i(\mathbf{q}^{(1)}(t_1)) - F_i(\mathbf{q}^{(2)}(t_1))]$$

Let

$$\delta_n(t) = \sup\{|q_i^{(1)}(t) - q_i^{(2)}(t)|: \quad |i| \leqslant nD\}$$

where D is the range of the potential, as defined in A_1. We then get, using (12b),

$$\delta_n(t) \leqslant \left[\int_0^t dt_1\,(t - t_1)\delta_{n+1}(t_1)\right] cn^2$$

Iterating this k times, then using the bound $\delta_{n+k}(t) \leqslant 2\bar{B}_{(n+k)D}$, we obtain

$$\delta_n(t) \leqslant \left[\int_0^t dt\,(t - t_1)^{2k-1}\delta_{n+k}(t)\right] c^k[n(n+1)\cdots(n+k-1)]^2$$

$$\leqslant \frac{t^{2k}}{(2k)!}(2\bar{B}_{(n+k)D})c^k[n(n+1)\cdots(n+k-1)]^2$$

Thus, letting $k \to \infty$, we find that $\delta_n(t) = 0$ for

$$0 < t < \left\{\limsup_{k\to\infty}\left[\frac{2\bar{B}_{(n+k)D}c^k[n(n+1)\cdots(n+k-1)]^2}{(2k)!}\right]^{1/2k}\right\}^{-1}$$

$$= 2(\tfrac{1}{2}\sqrt{c}\limsup_{k\to\infty}\bar{B}_k^{D/2k})^{-1}$$

This is true for all n, so

$$q_i^{(1)}(t) = q_i^{(2)}(t)$$

for all i, provided

$$t < 4[c \limsup_{k\to\infty}(B_k^{D/k})]^{-1/2}$$

which proves the theorem.

Example. If (as in the example of Section 2) there exists a constant c_1 such that

$$|\partial F_i/\partial q_j| \leqslant c_1(\sup\{|q_j|:\ |i-j| \leqslant D\})^{2n-2} \tag{13}$$

then any sequence of the form $B_j = b|j|^{1/(n-1)}$ is a sequence of uniqueness if $n \geqslant 2$.

This means that we have uniqueness in the class of solutions such that

$$\sup_{|t|\leq\tau}\sup\{|q_j(t)|/(|j|^{1/(n-1)}+1)\} < \infty \qquad \text{for all } \tau$$

Arguments similar to those leading to Eq. (11) show that if $\mathscr{L}_j(0)$ grows no faster than $|j|^{1/(n-1)}$, then there does exist a solution in this class.

In the harmonic case ($n = 1$), condition (12b) is vacuous and any sequence (B_j) such that

$$\sup_k\{\bar{B}_k^{1/k}\} < \infty$$

is a sequence of uniqueness (compare Ref. 2).

4. WEAK TIME EVOLUTION FOR GENERAL INTERACTIONS

In this section we sketch a proof that, under very general assumptions, solutions to the equations of motion exist for almost all initial conditions with respect to any Gibbs state. We do not assume here that conditions A_3 and A_4 hold. The proof is very simple and almost nothing needs to be assumed about the interaction, but it should be noted that very reasonable interactions —such as the one-dimensional harmonic chain with formal interaction energy $\frac{1}{2}\sum_i (q_{i+1} - q_i)^2$—do not have any Gibbs states at all.[2] About such interactions our theorem evidently says nothing. We refer the reader to recent work for an analysis of Gibbs states for the kind of system considered here.[7–9]

We will assume as before that our interaction is of Hamiltonian form with range D, i.e., we assume that A_1 and A_2 hold. In addition, we assume that:

B_1. For each finite subset Λ_α of $\mathbb{Z}^\nu$, the equations of motion (9a)–(9c) admit solutions for all time for all initial points.

B_2. For each Λ_α, each $\beta > 0$, and each specification of the q_i for $i \notin \Lambda_\alpha$, the measure

$$\exp[-\beta H_\alpha(\mathbf{q}, \mathbf{p})] \prod_{j\in\Lambda_\alpha} dq_j\, dp_j \tag{14}$$

with H_α given in (10) is finite (normalizable) on $(R \times R)^{\Lambda_\alpha}$.

Condition B_2 makes it possible to define Gibbs states by an obvious adaptation of the definitions used in other cases, but it does not imply the *existence* of nontrivial Gibbs states.

We note that (i) by conservation of energy and Liouville's theorem, any Gibbs state is invariant under T_t^α for all α, t; (ii) with respect to any Gibbs state, the p_i are independent, identically distributed, Gaussian random variables of mean zero.

Theorem 3. Let μ be a Gibbs state for the interaction under consideration. For μ-almost all initial points $\{q_i, p_i\}$, there exists a solution $\{q_i(t)\}$ of Eq. (3) defined for all t and satisfying

$$\sup_t \sup_i \frac{|q_i(t) - q_i|}{(1 + t^2)[\log_+(i)]^{1/2}} < \infty \tag{15}$$

where $\log_+(j) = \sup[\log|j|, 1]$

Proof. (The argument here is similar to that used in Ref. 3.) For any $x = \{q_i, p_i\}$ define

$$B(x) = \sup_i \frac{|p_i|}{[\log_+(q_i)]^{1/2}}$$

$$\bar{B}_\alpha(x) = \int_{-\infty}^{\infty} \frac{dt}{1 + t^2} B(T_t^\alpha x), \qquad \bar{B}_\infty(x) = \liminf_{\alpha\to\infty} \bar{B}_\alpha(x)$$

It follows from (ii) that $\int B\, d\mu < \infty$; hence, from (i) and Fubini's theorem, $\int \bar{B}_\alpha\, d\mu$ is finite and independent of α. By Fatou's lemma, $\int \bar{B}_\alpha\, d\mu < \infty$. We will show: If $\bar{B}_\infty(x) < \infty$, then there exists a solution to (3) satisfying (15).

To see this, note first that there must then exist a sequence $\alpha_n \to \infty$ and a constant C such that

$$\bar{B}_{\alpha_n}(x) \leqslant C \qquad \text{for all } n$$

Hence,

$$\begin{aligned} |q_i^{\alpha_n}(t) - q_i| &\leqslant \left| \int_0^t dt_1\, p_i^{\alpha_n}(t_1) \right| \leqslant (1 + t^2) \int_{-\infty}^{\infty} \frac{dt_1}{1 + t_1^2} |p_i^{\alpha_n}(t_1)| \\ &\leqslant (1 + t^2)[\log_+(i)]^{1/2} \bar{B}_{\alpha_n}(x) \\ &\leqslant (1 + t^2)[\log_+(i)]^{1/2} C \qquad \text{for all } i, n, t \end{aligned} \tag{16}$$

Since F_i depends only on a finite number of the q_j, and since each V_j is continuously differentiable, this bound implies a family of bounds of the form

$$|dp_i^{\alpha_n}(t)/dt| \leqslant K_i(|t|)$$

where each K_i is a nondecreasing function of t (which does not depend on n). The proof of the existence of solutions is now completed in the same way as in Theorem 1; (15) follows from (16) by passage to the limit.

There remains the question of uniqueness. Suppose that (13) holds with some $n > 1$. If $\{q_i, p_i\}$ satisfies

$$\sup_{i \in \mathbb{Z}^\nu} (|q_i|/|i|^{1/(n-1)}) < \infty \tag{17}$$

and if there exists a solution to (3) satisfying (15), then

$$\sup_{|t| \leq \tau} \sup_i [|q_i(t)|/|i|^{1/(n-1)}] \quad \text{is finite for all } \tau$$

Theorem 2 asserts that the solution is unique in this class. We would therefore like to know whether the condition (17) holds μ almost everywhere. A sufficient condition is given by the following:

Proposition. If there exists $\gamma > \nu(n - 1)$ and C such that

$$\int |q_i|^\gamma\, d\mu < C \qquad \text{for all } i \tag{18}$$

then

$$\sup_{i \in \mathbb{Z}^\nu} (|q_i|/|i|^{1/(n-1)}) < \infty \qquad \mu \text{ almost everywhere}$$

Proof.

$$\mu\{|q_i| > |i|^{1/(n-1)}\} = \mu\{|q_i|^\gamma > |i|^{\gamma/(n-1)}\}$$
$$\leqslant \left(\int |q_i|^\gamma \, d\mu\right)/i^{\gamma/(n-1)}$$

Since $\gamma(n-1) > \nu$,

$$\sum_{i\in\mathbb{Z}^\nu} \mu\{|q_i| > |i|^{1/(n-1)}\} < \infty$$

so by the Borel–Cantelli lemma[10]

$$\lim_i \sup(|q_i|/|i|^{1/(n-1)}) \leqslant 1 \qquad \mu \text{ almost everywhere}$$

Collecting the above results, we have the following:

Theorem 4. Let the interactions satisfy conditions A_1, A_2, B_1, and B_2 and also (13) with $n > 1$. Let μ be a Gibbs state for this interaction such that, for some $\gamma > \nu(n-1)$, (18) is satisfied. Then for μ-almost all $\{q_i, p_i\}$ there exists a solution to (3) such that

$$\sup_{|t|\leq\tau} \sup_{i\in\mathbb{Z}^\nu}[|q_i(t)|/|i|^{1/(n-1)}] < \infty \qquad \text{for all } \tau$$

and this solution is unique.

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