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TIME EVOLUTION AND ERGODIC PROPERTIES OF HARMONIC SYSTEMS *

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Abstract

We prove the existence of a time evolution and of a stationary equilibrium measure for the infinite harmonic crystal. The ergodic properties of the system are shown to be related in a simple way to the spectrum of the force matrix; when the spectrum is absolutely continuous, as in the translation invariant crystal, the flow is Bernoulli. The quantum crystal is also discussed.

1. Introduction

The ergodic properties of infinite systems are of considerable interest. They yield information about the expected (average) time dependent behavior of physical observables when the system is in or near equilibrium. Unfortunately very little is known at the present time about such properties for realistic systems. It seems therefore valuable to study the behavior of model systems. These may shed some light on which properties of the interactions are relevant to ergodic behavior. Previous studies along these lines have dealt with the ideal gas, the one dimensional hard rod system and the general noninteracting system in an external field produced by fixed scatterers (e.g. the Lorentz model). (For a review see the article by Goldstein, Lebowitz and Aizenman in this volume.)

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In this note we investigate the time evolution and ergodic properties of the infinite harmonic crystal. The harmonic crystal is commonly used by physicists as a model of an ideal solid and is quite successful in describing many features of real solids.* Explicit calculations of the time evolution of specified phase functions have been carried out for a variety of harmonic systems beginning with the work of Newton and Bernoulli on one dimensional lattices with nearest neighbor interactions† (example (a) below). The deay of time dependent correlations in these systems (which is directly related to ergodic properties) has also been studied by various authors.‡ More recently Titular [3] has studied the harmonic crystal from the general point of view of ergodic theory and has arrived at some of the same conclusions that we arrive at by somewhat different methods.

The outline of this paper is as follows: in Section 2 we prove the existence of the time evolution of the infinite harmonic system for a very large class of initial conditions with only very mild restrictions on the force matrix. This time evolution is the natural limit of the finite system time evolution. In Section 3 we prove the existence of an invariant equilibrium (Gaussian) measure for the infinite system which is the limit of the finite system canonical measure. (For this we require some conditions on the force matrix which fail for translation invariant forces in one and two dimension where the measure space has to be modified.)

In Section 4 we investigate the ergodic-theoretic properties of this dynamical system, and reduce the determination of these

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* For a general reference see Maradudin, Montroll and Weiss [1].

† See Section 4 of Chapter II of [1] for historical background.

‡ See Sections 7 and 8 of Chapter VII of [1] and Section III of [2] for discussion and references to the works of Hemmer, Mazur, Montroll, Rubin and others.

properties to an analysis of the spectrum of the matrix of inter-particle force constants. We also show how to modify our general formalism to apply in one and two dimensions. In Section 5, we extend the analysis of Section 4 by investigating the consequences of translation invariance, and we show that the time evolution flow T^t for a translation-invariant crystal with finite-range interactions is a Bernoulli flow except in special pathological cases. If, however, the crystal is not translation-invariant then the flow may not be ergodic, e.g. if there is a particle with a small mass giving rise to a local mode. In Section 6, we sketch the extension of our analysis to quantum harmonic crystals.

2. Time Evolution

We begin by investigating the time evolution of an infinite harmonic crystal. Our discussion will apply to arbitrary lattices and allows for rather general "defects", but at the expense of a slightly complicated notation.

We can describe a general lattice in the ν-dimensional space $\mathbb{R}^\nu$ by specifying the group Γ of translations carrying the lattice onto itself. Γ is a discrete subgroup of the additive group $\mathbb{R}^\nu$; as an abstract group it is isomorphic to $\mathbb{Z}^\nu$. It need not act transitively on the lattice, i.e., given two lattice sites, there need not be a lattice translation carrying one to the other. If we take the quotient space of $\mathbb{R}^\nu$ under the action of Γ, we obtain a ν-dimensional torus which is called the <u>unit cell</u> (for Γ). If we choose representatives for the elements of the unit cell in a straightforward way, we obtain a parallelepiped Δ_0 in $\mathbb{R}^\nu$; the translates of this parallelepiped under Γ are disjoint and cover all of $\mathbb{R}^\nu$. Labelling these parallelepipeds by elements of Γ, (i.e. $\Delta_\alpha = \Delta_0 + \alpha$), we obtain "coordinates" for $\mathbb{R}^\nu$ in which a point q is described by giving an element α of Γ and a point ξ of Δ_0 ; the point q may be expressed in terms of its "coordinates" by $q = \alpha + \xi$. To complete the description of a regular lattice, we need to specify the set of lattice sites in the unit cell Δ_0 , i.e. we must specify a finite subset $X_0=\{\xi_1,\ldots\xi_J\}$ of Δ_0; then the lattice is precisely the set of points of the form $\alpha + \xi_i$, where α is an arbitrary element of Γ and ξ_i an arbitrary element of X_0.

To allow for defects (e.g., for the absence of some of the particles), we loosen the definition a bit by allowing a different finite subset X_α of Δ_0 for each α, so the points of the "lattice" are then all points of the form $\alpha + \xi_i$; $\alpha \in \Gamma$, $\xi_i \in X_\alpha$. (For most applications, one will want to impose some restrictions on the X_α's, e.g., that they should all be subsets of some fixed finite set $\bar{X}$, but we seem to gain nothing by imposing these restrictions explicitly at this point. Some of them will appear implicitly in the assumptions we make later about the forces.)

The points of our (generalized) lattice are supposed to represent the equilibrium positions of the particles making up our crystal. To describe the dynamics, we introduce a position variable $q_{\alpha,i} \in \mathbb{R}^\nu$ for each lattice site giving the displacement of the particle in question from its equilibrium position and a conjugate momentum variable $p_{\alpha,i}$. Thus, the position of the particle with label (α,i) is $\alpha + \xi_i + q_{\alpha,i}$. The equations of motion read:

$$(2.1) \qquad m_{\alpha,i} \frac{dq_{\alpha,i}}{dt} = p_{\alpha,i} , \qquad \frac{dp_{\alpha,i}}{dt} = F_{\alpha,i}$$

where $m_{\alpha,i}$ is the mass of the (α,i) particle and the force $F_{\alpha,i}$ depends on the $q_{\beta,j}$'s. We now assume that the $F_{\alpha,i}$ are linear functions of the q's, and that $q_{\alpha,i} = 0$ for all α,i represents an equilibrium position. (Note that this last assumption places, implicitly, very strong restrictions on the sort of defects we can allow if we are deriving our equations from a realistic model of a crystal.) Thus, we can write

$$F_{\alpha,i} = - \sum_{\beta,j} V_{\alpha,i;\beta,j}\, q_{\beta,j}$$

where each $V_{\alpha,i;\beta,j}$ is a $\nu \times \nu$ (real) matrix.

The above may be formally simplified if we think of the sequence $(q_{\alpha,i})$ as a vector $\underline{q}$ in an infinite-dimensional vector space. Then the equations of motion can be written schematically as

$$\underline{M}\,\frac{d^2\underline{q}}{dt^2} = -\,\underline{V}\,\underline{q}$$

where $\underline{M}$ is the diagonal matrix with entries $m_{\alpha,i}$ and $\underline{V}$ is the force matrix. Let us look at two simple examples of the above.

(a) The perfect harmonic chain with nearest neighbor interactions: In this case, we take $\nu = 1$, $\Gamma = \mathbb{Z}$, and only one particle in each unit cell. (We may therefore dispense with the subscript i.) The potential energy is then given formally by

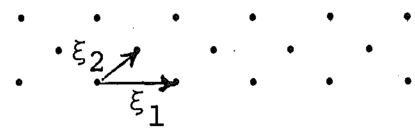
$$\frac{\gamma}{2} \sum_{\alpha} (q_{\alpha+1} - q_{\alpha})^2 , \quad \gamma \text{ a positive constant.}$$

(The q 's are now just numbers, since $\nu = 1$.) We may rewrite this expression as $\frac{1}{2}(\underline{V}\underline{q},\underline{q})$, where $\underline{V}$ is a tridiagonal matrix whose rows and columns are labelled by $\mathbb{Z}$, $V_{\alpha\alpha} = 2\gamma$, $V_{\alpha\beta} = -\gamma$, for $\beta = \alpha \pm 1$ and is zero otherwise.

From the original formula for $\underline{V}$ it is clearly positive semi-definite but not positive definite in the strict sense (If all the q_α's are equal, $(\underline{V}\underline{q},\underline{q}) = 0$. If, however, $\underline{q} \neq 0$ but only finitely many q_α's are different from zero, then $(\underline{V}\underline{q},\underline{q}) > 0$.). The equations of motion may be written simply as

$$m_\alpha \frac{d^2 q_\alpha}{dt^2} = - \sum_\beta V_{\alpha,\beta}\, q_\beta = \gamma\, (q_{\alpha+1} - 2q_\alpha + q_{\alpha-1})$$

(b) The two dimensional triangular lattice. Here we take $\nu = 2$; we again take only one lattice site in each unit cell, and we take the lattice to look like



is generated by ξ_1 and ξ_2. If we choose the unit length so that $|\xi_1| = |\xi_2| = 1$, we have $\xi_1 = (1,0)$; $\xi_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$, and

$$\Gamma = \{(n_1 + \tfrac{1}{2} n_2, \tfrac{\sqrt{3}}{2} n_2) : n_1, n_2 \in \mathbb{Z}\} .$$

We now associate a particle with each lattice site, and let the particles interact by a pair potential $\phi(r)$ which is repulsive for $r < 1$, has a minimum at $r = 1$ and vanishes for $r > r_0$, $r_0 < \sqrt{3}$, (the distance between second neighbor sites on the lattice). The configuration $q_\alpha = 0$ for all α is an equilibrium configuration, and the potential energy near this equilibrium configuration is approximated by

$$\frac{\gamma}{4} \sum_\alpha \sum_\xi \left[((q_{\alpha+\xi} - q_\alpha), \xi) \right]^2 + \text{constant} ,$$

where the sum ξ is taken over the six "nearest neighbors of 0",

$$\pm\xi_1,\ \pm\xi_2,\ \pm(\xi_1 - \xi_2) , \quad \text{and where } \gamma = \phi''(1) .$$

We now return to our general formalism. To specify the initial conditions, for the solution of (2.1) it is necessary to specify a momentum $p_{\alpha,i}$ as well as a position $q_{\alpha,i}$ for each α, i. If $\underline{x}$ denotes a sequence $(q_{\alpha,i}, p_{\alpha,i})$, we define

$$\|\underline{x}\|_k = \sup_{\alpha,i} \frac{|q_{\alpha,i}| \vee |p_{\alpha,i}|}{(1+|\alpha|^2)^k}$$

for any positive integer k. We let χ_k denote the set of sequences $\underline{x}$ such that

$$\lim_{\alpha\to\infty} \sup_i \frac{|q_{\alpha,i}| \vee |p_{\alpha,i}|}{(1+|\alpha|^2)^k} = 0 \ ;$$

χ_k is a Banach space with the norm $\| \ \|_k$. (Note that we have not taken χ_k to be the set of all $\underline{x}$ with $\|\underline{x}\|_k < \infty$. Our choice turns out to be convenient later on; note, however, that if $\|\underline{x}\|_k < \infty$ then $\underline{x} \in \chi_{k+1}$.)

The equation of motion can be written formally as

$$\frac{d}{dt}\, \underline{x}(t) = \underline{A}\; \underline{x}(t) \ ,$$

where

$$(\underline{A}\underline{x})_{\alpha,i} = \Big(\frac{1}{m_{\alpha,i}}\, p_{\alpha,i}\, ,\ - \sum_{\beta,j} V_{\alpha,i;\beta,j}\, q_{\beta,j}\Big) \ .$$

We now assume

(1) $\inf_{\alpha,i} m_{\alpha,i} > 0$.

(2) For each positive integer k, $\sup_{\alpha,i} \sum_{\beta,j} \|V_{\alpha,i;\beta,j}\| \left(1+|\alpha-\beta|^2\right)^k < \infty$.

The second assumption means that the forces between the unit cells Δ_α and Δ_β drop off rapidly as $|\alpha-\beta| \to \infty$. In the case where there is full translation invariance, so

$$V_{\alpha,i;\beta,j} = V_{i,j}(\alpha-\beta)$$

our assumption amounts to the requirement that $V_{i,j}(\xi)$ goes to zero more rapidly than any inverse power of $|\xi|$ as ξ goes to infinity.

Under these assumptions on the forces and masses, it is trivial to prove

<u>Proposition 1</u>. For each k, $\underline{A}$ is a bounded linear operator on χ_k. Hence if $\underline{x}_0 \in \chi_k$, there is a unique global solution $\underline{x}(t)$ of the equation

$$\frac{d\underline{x}}{dt} = \underline{A}\,\underline{x} \quad \text{on} \quad \chi_k \ ,$$

with $\underline{x}(0) = \underline{x}_0$; the solution is given by

$$\underline{x}(t) = e^{t\underline{A}}\,\underline{x}_0 \ ; \qquad e^{t\underline{A}} = \sum_{n=0}^{\infty} \frac{t^n}{n!}\,\underline{A}^n \ .$$

In particular, if $(q_{\alpha,i})$ and $(p_{\alpha,i})$ are arbitrary polynomially bounded sequences, there exist solutions $q_{\alpha,i}(t)$, $p_{\alpha,i}(t)$ of the equations

$$(2.2) \qquad \frac{dq_{\alpha,i}(t)}{dt} = \frac{p_{\alpha,i}(t)}{m_{\alpha,i}} \ ; \qquad \frac{dp_{\alpha,i}(t)}{dt} = -\sum_{\beta,j} V_{\alpha,i;\beta,j}\, q_{\beta,j}(t)$$

with $q_{\alpha,i}(0) = q_{\alpha,i}$; $p_{\alpha,i}(0) = p_{\alpha,i}$, and the solutions remain polynomially bounded (in α) for each t.

The uniqueness statement in the above proposition is not as strong as it sounds. The point here is that what is asserted is only that there is no other solution of the equations of motion such that

$$\lim_{\delta t \to 0} \left\| \frac{\underline{x}(t+\delta t) - \underline{x}(t)}{\delta t} - \underline{A}\underline{x}(t) \right\|_k = 0$$

i.e., no other solution in which the convergence of difference quotients to derivatives has the right amount of uniformity in α, i. We can improve this situation somewhat:

<u>Proposition 2</u>. Let $\underline{x}_0 \in \chi_k$ for some k, and let $\underline{x}(t)$ be a solution of (2.2) with $\underline{x}(0) = \underline{x}_0$ such that for some k', $\varepsilon > 0$,

$$\|\underline{x}(t)\|_{k'} \ \text{is bounded on} \ 0 \leq t < \varepsilon \ .$$

Then $\underline{x}(t) \in \chi_k$ and $\underline{x}(t) = e^{\underline{A}t}\,\underline{x}_0$ for $0 \leq t < \varepsilon$.

This follows in an obvious way from the fact that $e^{\underline{A}t}\,\underline{x}_0 \in \chi_k$ if $\underline{x}_0 \in \chi_k \subset \chi_{k'}$ for $k' \geq k$.

We remark here that for finite range interactions the above results extend immediately to the case where the initial values $\underline{x}_0$ are exponentially bounded in α.

Although we have dealt directly with the infinite system, the time evolution we have obtained is the limit of the finite harmonic system in the region Λ with the boundary "tied down", i.e., with $q_{\alpha,i}(t) \equiv 0 \equiv p_{\alpha,i}(t)$ for $\alpha,i \not\in \Lambda$. We can see this as follows. Let Λ be a finite subset of the crystal, and let P_Λ be the operator on the space of sequences $(q_{\alpha,i}, p_{\alpha,i})$ which puts all coordinates belonging to lattice sites α,i outside Λ equal to zero and leaves those belonging to lattice sites inside Λ unchanged. The equation of motion for the system in Λ is then

$$\frac{d}{dt} \underline{x}_\Lambda(t) = P_\Lambda \underline{A} \, P_\Lambda \, \underline{x}_\Lambda(t) ,$$

i.e.

$$\underline{x}_\Lambda(t) = \exp [t(P_\Lambda \underline{A} \, P_\Lambda)] P_\Lambda \, \underline{x}_0$$

But P_Λ converges strongly to 1 on each χ_k, so

$$\lim_{\Lambda \to \infty} \underline{x}_\Lambda(t) = \underline{x}(t)$$

for all t and all $\underline{x}_0 \in \bigcup_k \chi_k$.

To conclude this section, we establish a number of notational conventions to be observed for the remainder of this article.

1. We will assume that there is exactly one particle per unit cell (Bravais lattice), so the lattice may be identified with Γ. We may therefore drop the subscript i. It should be kept in mind, however, that p_α and q_α are elements of $\mathbb{R}^\nu$, not $\mathbb{R}$, and hence that there is another index which we suppress entirely from our notation.

2. We make a canonical transformation

$$q'_\alpha = m_\alpha^{1/2} q_\alpha \; ; \qquad p'_\alpha = m_\alpha^{-1/2} p_\alpha ,$$

and we introduce

$$S_{\alpha\beta} = (m_\alpha m_\beta)^{-1/2} V_{\alpha\beta}$$

Then the equations of motion read

$$\frac{dq'_\alpha}{dt} = p'_\alpha \;; \qquad \frac{dp'_\alpha}{dt} = -\sum_\beta S_{\alpha\beta}\, q'_\beta$$

i.e., in the new variables the system looks like a system of particles of unit mass with force matrix $S_{\alpha\beta}$. We will from now on use only the variables q'_α , p'_α and will drop the primes.

3. We will need names for various spaces of sequences $(\xi_\alpha)_{\alpha\in\Gamma}$. Such sequences will usually be assumed to take values in $\mathbb{R}^\nu$. We write

$$\ell^2(\Gamma) = \{(\xi_\alpha)_{\alpha\in\Gamma}: \sum_\alpha |\xi_\alpha| < \infty\}$$

$$s(\Gamma) = \{(\xi_\alpha)_{\alpha\in\Gamma}: \sup_\alpha |\xi_\alpha| \cdot (1+|\alpha|)^k < \infty \text{ for all } k\}$$

$$s'(\Gamma) = \{(\xi_\alpha)_{\alpha\in\Gamma}: \sup_\alpha \frac{|\xi_\alpha|}{(1+|\alpha|)^k} < \infty \text{ for some } k\}$$

$$d(\Gamma) = \{(\xi_\alpha)_{\alpha\in\Gamma}: \xi_\alpha = 0 \text{ for all but finitely many } \alpha\}.$$

Occasionally, we will want to consider sequences with values in $\mathbb{C}^\nu$ rather than $\mathbb{R}^\nu$; we then use the subscript $\mathbb{C}$, e.g., $\ell^2_{\mathbb{C}}(\Gamma)$.

3. Equilibrium Statistical Mechanics

The existence of the time evolution was proven without any positivity (or even symmetry) assumption on $\underline{V}$. For physical applications the matrix $\underline{V}$ and hence $\underline{S}$ should be, in an appropriate sense, positive (otherwise we would certainly not have a crystal). We shall therefore assume:

(3) The infinite matris $S_{\alpha\beta}$ defines a (bounded) strictly positive operator S on the sequence space $\ell^2(\Gamma)$ i.e. $(\Psi, S\Psi) \geq 0$, for $\Psi \in \ell^2(\Gamma)$ with the equality holding only if $\Psi = 0$.

It follows from (3) that $H_\Lambda(\underline{q},\underline{p}) > 0$ unless $\underline{q} = \underline{p} = 0$. *

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* $H_\Lambda(\underline{q},\underline{p}) = \frac{1}{2}\sum p_\alpha^2 + \frac{1}{2}\sum S_{\alpha\beta} q_\alpha q_\beta$, $\alpha,\beta \in \Lambda$ is the Hamiltonian of the (finite) crystal in the domain Λ with "tied down" boundary

The equilibrium canonical ensemble* for the finite system (with temperature set equal to unity in appropriate units) may now be described economically as the Gaussian measure on the space of finite sequences $(q_\alpha, p_\alpha)_{\alpha\in\Lambda}$ with mean zero and covariance

$$E_\Lambda\{p_\alpha\ p_\beta\} = \delta_{\alpha\beta}\ ; \quad E_\Lambda\{q_\alpha\ q_\beta\} = (S_\Lambda)^{-1}_{\alpha\beta}\ ; \quad E_\Lambda\{q_\alpha\ p_\beta\} = 0.$$

The matrix S_Λ^{-1} is the matrix obtained by restricting $S_{\alpha,\beta}$ to α,β in Λ and inverting the resulting finite matrix. Thus $(S_\Lambda)^{-1}_{\alpha\beta}$ is not at all the same as $(S^{-1})_{\alpha\beta}$ for $\alpha,\beta \in \Lambda$. By assumption (3) zero is not an eigenvalue of the (positive) operator S_Λ and hence S_Λ^{-1} exists.

Assumption (3) also implies that S^{-1} makes sense as a (usually unbounded) densely defined self-adjoint operator on $\ell^2(\Gamma)$. We denote the positive sequre root of this operator by $S^{-1/2}$. We can now pass (formally at least) to the infinite system if we assume

(4) The vector $e^{(\alpha)} \in \ell^2(\Gamma)$ which has 1 in the αth place and zero elsewhere is in the domain of $S^{-1/2}$ for all α, and the sequence of numbers

$$\| S^{-1/2}\ e^{(\alpha)} \|$$

is polynomially bounded.

It seems to be hard to verify (or disprove) assumption (4) in realistic situations, except that it can normally be expected to fail in one and two dimensions and hold in higher dimensions. We will return to this point later, when we investigate the consequences of assuming that the force matrix $\underline{V}$ is translation invariant. It will be seen that (4) can be relaxed.

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* See Lanford's lectures.

It seems natural to define the canonical ensemble for the infinite harmonic crystal to be the Gaussian probability measure P on the space of pairs (q_α, p_α) of polynomially bounded sequences with mean zero and covariance given by

$$E\{p_\alpha\, p_\beta\} = \delta_{\alpha,\beta}\ , \quad E\{q_\alpha\, q_\beta\} = (S^{-1/2}\, e^{(\alpha)},\ S^{-1/2}\, e^{(\beta)}),\ E\{p_\alpha\, q_\beta\}=0.$$

We will shortly justify this definition by showing that this measure is indeed the limit of the finite system canonical ensemble as Λ becomes infinitely large. Two questions now suggest themselves.

(a) Is the measure P invariant under the time evolution defined by solving the equations of motion

$$\frac{dq_\alpha}{dt} = p_\alpha\ , \qquad \frac{dp_\alpha}{dt} = -\sum_\beta S_{\alpha\beta}\, q_\beta \quad ?$$

(b) If so, what are the ergodic properties of the dynamical system thus defined?

We will give an affirmative answer to (a), and show how (b) can be reduced in a certain sense to an analysis of the spectral properties of S acting on $\ell^2(\Gamma)$.

Invariance of the Measure

If $(q_\alpha(t),\ p_\alpha(t))$ denotes the solution of the equations of motion with initial data (q_α, p_α), it follows easily from the proof of Proposition 1 that the solutions can be written in the form

$$(3.1)\qquad \begin{aligned} q_\alpha(t) &= \sum_\beta K^{(1)}_{\alpha,\beta}(t)\ q_\beta + \sum_\beta K^{(2)}_{\alpha,\beta}(t)\ p_\beta \\ p_\alpha(t) &= \sum_\beta K^{(3)}_{\alpha,\beta}(t)\ q_\beta + \sum_\beta K^{(4)}_{\alpha,\beta}(t)\ p_\beta \end{aligned}$$

where the kernels $K^{(i)}_{\alpha,\beta}(t)$ are rapidly decreasing in β for each fixed α. Because the $\{q_\alpha, p_\alpha\}$ are Gaussian, the random variables

$q_\alpha(t)$ and $p_\alpha(t)$ are also Gaussian. Thus, the measure P_t obtained by evolving the initial measure P to time t is Gaussian with mean zero and covariance

$$E\{q_\alpha(t)\ q_\beta(t)\}\ ,\quad \text{etc.}$$

Since a Gaussian measure is uniquely determined by its mean and covariance, in order to prove that $P_t = P$ (i.e. that P is invariant), it suffices to prove that

$$E\{q_\alpha(t)\ q_\beta(t)\} = E\{q_\alpha\ q_\beta\}\ ,\quad \text{etc.}$$

From the fact that the equations of motion are linear and autonomous, we see that the quantities

$$\frac{d}{dt}E\{q_\alpha(t)\ q_\beta(t)\}\ ,\quad \frac{d}{dt}E\{p_\alpha(t)\ p_\beta(t)\}\ ,\quad \frac{d}{dt}E\{q_\alpha(t)\ p_\beta(t)\}\ ,$$

can be expressed as linear combinations of the same derivatives at $t = 0$. Thus to prove that the derivatives are equal to zero at all times, it is enough to prove it at $t = 0$. Now, at $t = 0$

$$\frac{d}{dt}E\{q_\alpha(t)\ q_\beta(t)\}\Big|_{t=0} = E\{p_\alpha\ q_\beta\} + E\{q_\alpha\ p_\beta\} = 0$$

$$\frac{d}{dt}E\{p_\alpha(t)\ p_\beta(t)\}\Big|_{t=0} = E\{-\sum_\gamma S_{\alpha\gamma}\ q_\gamma\ p_\beta\} + E\{-\sum_\gamma S_{\beta\gamma} p_\alpha q_\gamma\} = 0$$

$$\frac{d}{dt}E\{q_\alpha(t)\ p_\beta(t)\}\Big|_{t=0} = E\{p_\alpha\ p_\beta\} - \sum_\gamma S_{\beta\gamma}\ E\{q_\alpha\ q_\gamma\}$$

$$= \delta_{\alpha\beta} - \sum_\gamma S_{\beta\gamma}\big(S^{-1/2}\ e^{(\alpha)}, S^{-1/2}\ e^{(\gamma)}\big).$$

Now, because of the rapid decrease of $S_{\beta\gamma}$ in γ, $\sum_\gamma S_{\beta\gamma}\ S^{-1/2} e^{(\gamma)}$ converges in $\ell^2(\Gamma)$, as does $\sum_\gamma S_{\beta\gamma}\ e^{(\gamma)} = S\ e^{(\beta)}$. Thus, since $S^{-1/2}$ is a closed operator,

$$\sum_\gamma S_{\beta\gamma}\big(S^{-1/2} e^{(\alpha)}, S^{-1/2} e^{(\gamma)}\big) = \big(S^{-1/2} e^{(\alpha)}, S^{-1/2} S\ e^{(\beta)}\big)$$

$$= \big(S^{-1/2}\ e^{(\alpha)},\ S^{1/2}\ e^{(\beta)}\big) = \delta_{\alpha\beta}\ ,$$

so $\frac{d}{dt} E\{q_\alpha(t)\ p_\beta(t)\}_{t=0} = \delta_{\alpha\beta} - \delta_{\alpha\beta} = 0$, which completes the proof that P is invariant under the time-evolution.

The Thermodynamic Limit

We investigate now the sense in which the Gaussian probability measure P on the space of polynomially bounded sequences $\{q_\alpha, p_\alpha\}$ is the limit of the finite-system canonical ensembles.

Proposition 3.1. Assume (1) - (4). Then the joint distribution of any finite set of p's and q's, $p_{\alpha_1}, \ldots, p_{\alpha_n}, q_{\beta_1}, \ldots, q_{\beta_m}$ with respect to the canonical ensemble in Λ converges as $\Lambda \uparrow \infty$ to the joint distribution of the same set of p's and q's with respect to the infinite-system equilibrium measure P.

Proof: Because of the Gaussian character of all the measures involved, it suffices to prove that the covariances converge. Since

$$E_\Lambda(p_\alpha\ p_\beta) = \delta_{\alpha\beta}, \qquad E_\Lambda(p_\alpha\ q_\beta) = 0$$

provided $\alpha, \beta \in \Lambda$, and since the same formulas hold for the infinite system equilibrium measure, it is only necessary to prove that

$$\lim_{\Lambda\to\infty} (S_\Lambda)^{-1}_{\alpha\beta} = \left(S^{-1/2}\, e^{(\alpha)},\ S^{-1/2}\, e^{(\beta)}\right) \tag{3.2}$$

for all α, β. By polarization, it suffices in fact to prove that

$$\lim_{\Lambda\to\infty} \sum_{\alpha,\beta} (S_\Lambda)^{-1}_{\alpha\beta}\, \xi_\alpha\, \xi_\beta = \left(S^{-1/2}\, \xi,\ S^{-1/2}\, \xi\right)$$

for all $\xi \in d(\Gamma)$ (the set of finite sequences).

We now fix $\xi \in d(\Gamma)$, and consider only Λ's such that $\xi_\alpha = 0$ for all $\alpha \notin \Lambda$. We prove (3.2) by proving the following four statements:*

* The argument is similar to that used in ferromagnetic spin systems, cf. Lebowitz and Martin-Löf [4].

(a) If $\Lambda \subset \Lambda_1$, then $(S_\Lambda^{-1}\xi,\xi) \leq (S_{\Lambda_1}^{-1}\xi,\xi)$

(b) If $\kappa > 0$, then

$\big((S_\Lambda+\kappa 1_\Lambda)^{-1}\xi,\xi\big)$ increases to $\big((S+\kappa 1)^{-1}\xi,\xi\big)$ as Λ increases to ∞.

(c) $\big((S+\kappa 1)^{-1}\xi,\xi\big)$ increases to $(S^{-1/2}\xi,\ S^{-1/2}\xi)$ as κ decreases to zero.

(d) $\big((S_\Lambda+\kappa 1_\Lambda)^{-1}\xi,\xi\big)$ increases to $(S_\Lambda^{-1}\xi,\xi)$ as κ decreases to zero.

Here 1_Λ is the unit matrix in Λ, $1_\Lambda \to 1$ as Λ increases to infinity.

Let us first assume these four statements and verify (3.2). Combining (b) and (c) shows that

$$\big((S_\Lambda + \kappa 1_\Lambda)^{-1}\ \xi,\xi\big) \leq \big(S^{-1/2}\ \xi,\ S^{-1/2}\ \xi\big) \quad \text{for all } \kappa,\Lambda.$$

Hence, by (d)

$$(S_\Lambda^{-1}\ \xi,\xi) \leq \big(S^{-1/2}\ \xi,\ S^{-1/2}\ \xi\big) \quad \text{for all } \Lambda.$$

From this bound, and (a), we conclude that

$\lim_{\Lambda\to\infty} (S_\Lambda^{-1}\ \xi,\xi)$ exists and is no larger than $(S^{-1/2}\ \xi,\ S^{-1/2}\ \xi)$.

On the other hand, let $\varepsilon > 0$. By (c) choose κ so that

$$\big((S + \kappa 1)^{-1}\ \xi,\xi\big) \geq \big(S^{-1/2}\ \xi,\ S^{-1/2}\ \xi\big) - \frac{\varepsilon}{2}\ ;$$

then (b) implies that, for sufficiently large Λ,

$$\big((S_\Lambda + \kappa 1_\Lambda)^{-1}\ \xi,\xi\big) \geq \big(S^{-1/2}\ \xi,\ S^{-1/2}\ \xi\big) - \varepsilon.$$

But

$$\big((S_\Lambda + \kappa 1_\Lambda)^{-1}\ \xi,\xi\big) \leq \big(S_\Lambda^{-1}\ \xi,\xi\big) \qquad \text{by (d)},$$

so

$$\big(S_\Lambda^{-1}\ \xi,\xi\big) \geq \big(S^{-1/2}\ \xi,\ S^{-1/2}\xi\big) - \varepsilon$$

for all sufficiently large Λ, i.e.

$$\lim_{\Lambda\to\infty} (S_\Lambda^{-1}\ \xi,\xi) = \big(S^{-1/2}\ \xi, S^{-1/2}\ \xi\big)\ .$$

Thus we have only to prove (a), (b), (c), (d). Statements (c) and (d) are straightforward consequences of the spectral theorem. To prove (a) we consider

$$\left(S_{\Lambda_1}+\kappa\, 1_{\Lambda_1/\Lambda}\right)^{-1}$$

where $1_{\Lambda_1/\Lambda}$ is the projection of $\ell^2(\Lambda_1)$ onto $\ell^2(\Lambda_1/\Lambda)$. For $\kappa = 0$, this is simply $(S_{\Lambda_1})^{-1}$. Moreover, as κ increases

$$\left(\left(S_{\Lambda_1}+\kappa\, 1_{\Lambda_1/\Lambda}\right)^{-1} \xi,\xi\right)$$

decreases (since $A \to A^{-1}$ is operator monotone-decreasing). Finally,

$$\lim_{\kappa\to\infty} \left(\left(S_{\Lambda_1}+\kappa\, 1_{\Lambda_1/\Lambda}\right)^{-1} \xi,\xi\right) = \left(S_\Lambda^{-1}\ \xi,\xi\right) . \tag{3.1}$$

This is true since

$$\left(\left(S_{\Lambda_1}+\kappa\, 1_{\Lambda_1/\Lambda}\right)^{-1} \xi,\xi\right)$$

$$= \frac{\int d\underline{q} \exp\left(-\frac{1}{2}\sum_{\alpha,\beta\in\Lambda_1} S_{\alpha\beta}q_\alpha q_\beta - \frac{1}{2}\kappa \sum_{\alpha\in\Lambda_1/\Lambda} q_\alpha^2\right)\left(\sum_\alpha \xi_\alpha q_\alpha\right)^2}{\int dq \exp\left(-\frac{1}{2}\sum_{\alpha,\beta\in\Lambda_1} S_{\alpha\beta}q_\alpha q_\beta - \frac{1}{2}\kappa \sum_{\alpha\in\Lambda_1/\Lambda} q_\alpha^2\right)}$$

and letting $\kappa \to \infty$ simply has the effect of putting $q_\alpha = 0$ for $\alpha \in \Lambda_1/\Lambda$. This is also intuitively reasonable, since $S_{\Lambda_1} + 1_{\Lambda_1/\Lambda}$ is a force matrix with an interaction differing from the original one by the addition of a restoring force $-\kappa\, q_\alpha$ at each $\alpha \in \Lambda_1/\Lambda$; as $\kappa \to \infty$, the oscillators at these lattice sites become more and more firmly tied to their equilibrium positions, so in the limit they are rigidly fixed. Hence, as κ increases from 0 to ∞,

$$\left(\left(S_{\Lambda_1}+\kappa\, 1_{\Lambda_1/\Lambda}\right)^{-1} \xi,\xi\right)$$

decreases from $(S_{\Lambda_1}^{-1}\xi,\xi)$ to $(S_\Lambda^{-1}\ \xi,\xi)$; in particular,

$$(S_\Lambda^{-1}\ \xi,\xi) \le (S_{\Lambda_1}^{-1}\ \xi,\xi) .$$

To prove (b) we note that (a) implies that

$$((S_\Lambda + \kappa\, 1_\Lambda)^{-1}\, \xi, \xi)$$

increases with Λ, so we want to show

$$\lim_{\Lambda \to \infty} ((S_\Lambda + \kappa\, 1_\Lambda)^{-1}\, \xi, \xi) = ((S + \kappa\, 1)^{-1}\, \xi, \xi) .$$

As a function of (complex) κ,

$$g_\Lambda(\kappa) = ((S_\Lambda + \kappa\, 1_\Lambda)^{-1}\, \xi, \xi)$$

is analytic in the complement of the spectrum of $-S_\Lambda$. Since the spectrum of S_Λ is contained in $[0, \|S\|]$, $g_\Lambda(\kappa)$ is bounded uniformly in Λ on any closed set which does not intersect the interval $[-\|S\|, 0]$ on the real axis. Also, expanding $(S_\Lambda + \kappa\, 1_\Lambda)^{-1}$ in its Neumann series for large κ shows that

$$\lim_{\Lambda \to \infty} g_\Lambda(\kappa) = ((S + \kappa\, 1)^{-1}\, \xi, \xi)$$

for sufficiently large $|\kappa|$. Vitali's theorem then implies

$$\lim_{\Lambda \to \infty} g_\Lambda(\kappa) = ((S + \kappa\, 1)^{-1}\, \xi, \xi)$$

for all strictly positive κ.

This, then, completes the proof of Proposition 3. The argument actually proves more than is included in the statement of the proposition: If we drop Assumption (4) but continue to assume that zero is not an eigenvalue of S, we can still prove that, for any $\xi \in d(\Gamma)$,

$$(S_\Lambda^{-1}\, \xi, \xi) = E_\Lambda((\sum_\alpha \xi_\alpha\, q_\alpha)^2)$$

increases to a limit as Λ increases to ∞, but that the limit is infinite if $\xi \notin \mathcal{D}(S^{-1/2})$. The interpretation in this case is simply that the square fluctuation of $\sum_\alpha \xi_\alpha\, q_\alpha$ becomes infinite with Λ.

4. Ergodic Properties

We have seen that the solution mappings to the equations of motion define a flow T^t on the space $s'(\Gamma) \oplus s'(\Gamma)$ of polynomially bounded sequences of displacements and momenta, and that, subject to assumptions (3), (4) of Section 3, the thermodynamic limit of finite-volume ensembles exists and defines a centered Gaussian probability measure on $s'(\Gamma) \oplus s'(\Gamma)$ invariant under the solution flow. We want next to analyze the ergodic properties of the dynamical system so constructed. The essential step in doing this will be the observation that this problem may be recast into a question about one-parameter groups of orthogonal mappings on Hilbert space.

As in the preceding section, we let P denote the infinite-volume equilibrium state as a probability measure on $s'(\Gamma) \oplus s'(\Gamma)$. We let $h_1 \subset L^2(P)$ denote the subspace of linear real valued random variables, i.e., the closure in $L^2(P)$ of the set of finite linear combinations of p_α's and q_α's. We have seen that the action of T^t on $L^2(P)$ carries h_1 into (hence, onto) itself. Let $U_1(t)$ denote the one-parameter group of orthogonal transformations on h_1 given by the action of T^t. We will proceed by showing first how to determine most of the ergodic-theoretic properties of T^t from Hilbert space properties of the orthogonal group $U_1(t)$; we will then introduce coordinates in h_1 which enable us to reduce the study of $U_1(t)$ to the analysis of the spectral properties of S acting on $\ell^2(\Gamma)$.

To begin, we fit the situation under consideration into a more general context. Let $(X,\mathcal{O}\!\mathcal{L},P)$ denote a probability space. By a generating Gaussian subspace of $(X,\mathcal{O}\!\mathcal{L},P)$ we mean a closed subspace h_1 of $L^2(P)$ such that

(1) Every Ψ in h_1 is a centered Gaussian random variable.
(2) h_1 generates the σ-algebra $\mathfrak{A}$, i.e., $\mathfrak{A}$ is the smallest σ-algebra with respect to which every Ψ in h_1 is measurable.
It follows easily that any finite set of Ψ's in h_1 is jointly Gaussian.

Now let $(X,\mathfrak{A},P)$ and $(\hat{X},\hat{\mathfrak{A}},\hat{P})$ be two probability spaces equipped with generating Gaussian subspaces h_1 and $\hat{h}_1$ respectively, and let U be an orthogonal mapping of h_1 onto $\hat{h}_1$ (i.e., a Hilbert-space isomorphism of h_1 onto $\hat{h}_1$). We claim that there is a unique measure algebra isomorphism T of $(\hat{X},\hat{\mathfrak{A}},\hat{P})$ onto $(X,\mathfrak{A},P)$ such that

$$U\,\Psi = \Psi \circ T$$

for all $\Psi \in h_1$. (If the two measure spaces in question are Lebesgue spaces [5], then T gives rise to an essentially unique measure-preserving transformation). The claim is easy to prove if h_1 and $\hat{h}_1$ are finite-dimensional. In the general case, we may use the finite-dimensional result to construct an isomorphism between the subalgebra of $\hat{\mathfrak{A}}$ generated by $U\mathcal{K}$ and the subalgebra of $\mathfrak{A}$ denerated by $\mathcal{K}$, for any finite-dimensional subspace $\mathcal{K}$ of h_1. By uniqueness, these partial isomorphisms fit together to define an isomorphism of all of $\hat{\mathfrak{A}}$ onto all of $\mathfrak{A}$.

Thus, in particular, any orthogonal transformation U of h_1 onto itself induces a corresponding automorphism T of $(X,\mathfrak{A},P)$, and any group of orthogonal transformations induces an anti-isomorphic group of automorphisms. (Not every automorphism T of $(X,\mathfrak{A},P)$ arises in this way; it is necessary that $\Psi \circ T \in h_1$ if $\Psi \in h_1$.) If U, U' are two orthogonal transformations which are orthogonally equivalent, i.e., if there exists an orthogonal transformation V such that

$$U' = V^{-1}\,U\,V\,,$$

then the induced automorphisms T, T' are isomorphic. A part of the problem of determining the ergodic properties of the time-development of the infinite harmonic crystal is contained in the more general problem of determining the ergodic properties of an automorphism T induced by an orthogonal transformation U in terms of the spectral properties of U. The following results give a fairly complete answer to this general problem.

Proposition 4.1. Let $(X, \mathcal{O}\!\!\mathcal{l}, P)$ be a probability space with a generating Gaussian subspace h_1. Then there is an isomorphism between $L^2(P)$ and $\bigoplus_{n=0}^{\infty} (h_1)^{\otimes n}_{\text{symm}}$ such that, if U is any orthogonal transformation on h_1 and if T is the induced automorphism of $(X, \mathcal{O}\!\!\mathcal{l}, P)$, the action of T on $L^2(P)$ corresponds to

$$\bigoplus_{n=0}^{\infty} \underbrace{U \otimes_s \cdots \otimes_s U}_{n \text{ times}} \quad \text{on} \quad \bigoplus_{n=0}^{\infty} (h_1)^{\otimes n}_{\text{symm}} .$$

Proposition 4.2. Let the notation be as in the preceding proposition. Then

(1) T is ergodic if and only if U, acting on the complexification $(h_1)_{\mathbb{C}}$ of h_1, has no point spectrum.

(2) T is mixing if and only if

$$\operatorname*{weak\,lim}_{|n| \to \infty} U^n = 0 .$$

(3) T has Lebesgue spectrum if and only if U, acting on $(h_1)_{\mathbb{C}}$ has Lebesgue spectrum.

Proposition 4.3. T is a Bernoulli automorphism if and only if U has Lebesgue spectrum.

Remarks on terminology:

1. As we have defined them, generating Gaussian subspaces are real Hilbert spaces, not complex Hilbert spaces. To obtain a simple spectral theory for orthogonal transformations, we pass to

a complex Hilbert space, called the complexification of h_1 obtained formally as $h_1 \oplus h_1$. An orthogonal transformation of h_1 extends by complex linearity to a unitary operator on $(h_1)_{\mathbb{C}}$.

2. If U is a unitary operator on a complex Hilbert space, the spectral theorem implies that there is a unique representation

$$U = \int_0^{2\pi} e^{i\theta} E(d\theta)$$

where $E(d\theta)$ is a projection-valued measure. We say that U has Lebesgue spectrum if $E(d\theta)$ is absolutely continuous with respect to Lebesgue measure.

The proof of the first half of Proposition 4.1 is a standard argument about Gaussian random variables; we will only sketch it. Since the Ψ's in h_1 are Gaussian, any polynomial in them is square square-integrable, and the set of all polynomials is dense in $L^2(P)$. Let $h^{\leq n}$ denote the closed subspace generated by the polynomials of degree no greater than n, and let $h_n = h^{\leq n} \ominus h^{\leq (n-1)}$. Then

$$L^2(P) = \bigoplus_{n=0}^{\infty} h_n ,$$

and our two uses of the symbol h_1 are consistent. We will construct for each n an orthogonal mapping of $(h_1)^{\otimes n}_{\text{symm}}$ onto h_n as follows: Let π_n be the projection onto h_n. For $\Psi_1, \ldots, \Psi_n$ in h_1, map

$$\Psi_1 \otimes_s \cdots \otimes_s \Psi_n \longmapsto \Psi_1 \cdot \Psi_2 \cdot \cdots \cdot \Psi_n \longmapsto \pi_n (\Psi_1 \cdot \cdots \cdot \Psi_n)$$

and extend by linearity. A straightforward calculation shows that the resulting mapping, divided by $\sqrt{n!}$ is an isometry. (See, for example, Section 6.3 of [6].) Since π_n applied to the set of all nth degree monomials is a total set in h_n, we have constructed the desired orthogonal mapping of $(h_1)^{\otimes n}_{\text{symm}}$ onto h_n. The statement that $U^{\otimes n}_{\text{symm}}$ goes over to the action of T on h_n is immediate since

$$(U\Psi_1) \otimes_s (U\Psi_2) \otimes_s \cdots \otimes_s (U\Psi_n) \longmapsto (\Psi_1 \cdot \ldots \cdot \Psi_n) \circ T \longmapsto [\pi_n(\Psi_1 \cdot \ldots \cdot \Psi_n)] \circ T$$

where the last identity follows from the fact that composition with T carries over $h^{\leq n}$ onto itself and hence commutes with π_n.

The proofs of statements (2) and (3) of Proposition 4.2 are straightforward from Proposition 4.1 and will be omitted. To prove (1), first assume that U has an eigenvector Ψ in $(h_1)_{\mathbb{C}}$. Since $(h_1)_{\mathbb{C}}$ may be regarded as the space of complex-valued functions on (X, ,P) which are complex linear combinations of elements of h_1, we may regard Ψ as an element of $L^2_{\mathbb{C}}(P)$. Then $|\Psi|$ (the pointwise absolute value) is invariant under T, so, if it is not constant, T is not ergodic. But since the real and imaginary parts of Ψ are Gaussian random variables (and therefore unbounded), $|\Psi|$ cannot be constant.

Conversely, suppose U has no point spectrum. It is then easy to see (using the spectral theorem) that $\underbrace{U \otimes \ldots \otimes U}_{n \text{ times}}$ has no point spectrum for any $n > 0$. Since $U \otimes_s \ldots \otimes_s U$ is the restriction of $U \otimes \ldots \otimes U$ to the symmetric subspace, the symmetric tensor product also has no point spectrum so it follows from Proposition 4.1 that T has no eigenfunctions except the constants. Thus, if U has no point spectrum, T is weakly mixing and hence ergodic. Note that we have shown that an automorphism which arises from an orthogonal transformation on a generating Gaussian subspace is weakly mixing if it is ergodic.

To prove Proposition 4.3, we note first that, since a Bernoulli automorphism has Lebesgue spectrum, statement (3) of Proposition 4.2 implies that T cannot be a Bernoulli automorphism unless U has Lebesgue spectrum. To prove the converse, we consider first the special case in which U has Lebesgue spectrum of uniform multiplicity on the unit circle. There then exists a direct sum decomposition

$$h_1 = \bigoplus_{m=-\infty}^{\infty} g_m \text{ ,}$$

such that $U\, g_m = g_{m+1}$ for all m (i.e., U is equivalent to a shift operator). Let F_m be the smallest σ-algebra with respect to which all Ψ in g_m are measurable. Then

(a) the orthogonality of the subspaces g_m implies that the F_m are independent (orthogonal centered Gaussian random variables are independent);

(b) the fact that the g_m span h_1, together with the fact that h_1 generates $\mathcal{O}\!\mathcal{L}$, implies

$$\bigvee_m F_m = \mathcal{O}\!\mathcal{L} \text{ ;}$$

(c) the equation $U\, g_m = g_{m+1}$ implies

$$T\, F_m = F_{m+1}$$

Hence, F_0 is an independent generator for T, so T is a Bernoulli automorphism. Since the σ-algebra F_0 is non-atomic, the entropy of T must be infinite.

To finish the proof we must eliminate the assumption of uniform multiplicity of the spectrum of U. Thus, let U be any orthogonal transformation with Lebesgue spectrum on a generating Gaussian subspace h_1. It follows easily from the spectral theorem that there exists $\hat{U}$ on h_1 with "complementary spectrum" such that $U \oplus \hat{U}$ on $h_1 \oplus h_1$ has Lebesgue spectrum of uniform multiplicity. We may identify $h_1 \oplus h_1$ with the generating Gaussian subspace

$$h_1 \otimes_{id} \oplus_{id} \otimes h_1$$

on $(X \times X, \mathcal{O}\!\mathcal{L} \otimes \mathcal{O}\!\mathcal{L}, P \otimes P)$. The automorphism of the product space induced by $U \oplus \hat{U}$ is $T \times \hat{T}$, which is a Bernoulli automorphism since $U \oplus \hat{U}$ has uniform Lebesgue spectrum. Thus, T is a factor of a Bernoulli automorphism. But Ornstein has proved that any factor of a Bernoulli automorphism is again a Bernoulli automorphism, so T must be a Bernoulli automorphism, as desired. (For a statement and proof of Ornstein's result, see [7].)

The above Propositions 4.1 - 4.3 give a nearly complete description of the ergodic-theoretic properties of the time-development flow of the infinite harmonic crystal provided we can determine the spectral properties of the one-parameter unitary group $U_1(t)$ on h_1. While we cannot do this explicitly in general, we can by introducing appropriate coordinates reduce it to determining the spectral properties of the operator S on $\ell^2(\Gamma)$. We equip $\mathcal{D}(S^{-1/2}) \subset \ell^2(\Gamma)$ with the norm

$$\|\Psi\|_{-1/2} = \|S^{-1/2}\Psi\| ;$$

this makes $\mathcal{D}(S^{-1/2})$ into a Hilbert space. Now we map $d(\Gamma) \oplus d(\Gamma)$ onto a dense subspace of h_1 by sending $\xi \oplus \eta$ to $\sum_\alpha (\xi_\alpha q_\alpha + \eta_\alpha p_\alpha)$. By a straightforward calculation,

$$\|\sum_\alpha (\xi_\alpha q_\alpha + \eta_\alpha p_\alpha)\|^2 = \|\xi\|^2_{-1/2} + \|\eta\|^2$$

(where the norm on the left means the norm on $L^2(P)$).

Taking into account the following lemma, we may extend this mapping to an orthogonal mapping of $\mathcal{D}(S^{-1/2}) \oplus \ell^2(\Gamma)$ onto h_1.

<u>Lemma 4.4</u>. $d(\Gamma)$ is dense in $\mathcal{D}(S^{-1/2})$.

<u>Proof</u>: Assume not. Then there exists a non-zero vector Ψ in $\mathcal{D}(S^{-1/2})$ such that $(S^{-1/2}\Psi, S^{-1/2}\xi) = 0$ for all ξ in $d(\Gamma)$. By taking limits, using the fact that $S^{-1/2}$ is a closed operator and the assumed polynomial boundedness of $\|S^{-1/2} e^{(\alpha)}\|$, we see that this remains true for all ξ in $s(\Gamma)$. But S maps $d(\Gamma)$ into $s(\Gamma)$, so replacing ξ by $S\,\xi'$ we get

$$0 = (S^{-1/2}\Psi, S^{-1/2} S\,\xi') = (S^{-1/2}\Psi, S^{1/2}\xi') = (\Psi, \xi') ,$$

for all $\xi' \in d(\Gamma)$. This evidently contradicts the assumption that $\Psi \neq 0$. We are thus able to identify h_1 with $\mathcal{D}(S^{-1/2}) \oplus \ell^2(\Gamma)$, and can carry over the orthogonal group $U_1(t)$ under this identification to obtain a one-parameter orthogonal group on $\mathcal{D}(S^{-1/2}) \oplus \ell^2(\Gamma)$. To identify the group so obtained, we compute its infinitesimal generator:

$$\frac{d}{dt} \sum_\alpha \left(\xi_\alpha q_\alpha(t) + \eta_\alpha p_\alpha(t)\right)\Big|_{t=0} = \sum_\alpha \xi_\alpha p_\alpha - \sum_{\alpha,\beta} \eta_\alpha S_{\alpha\beta} q_\beta \ , \ (\xi,\eta) \in d(\Gamma))$$

and hence the infinitesimal generator on $d(\Gamma) \oplus d(\Gamma)$ is given by:

$$\begin{pmatrix} 0 & -S \\ 1 & 0 \end{pmatrix}$$

This operator is easily checked to be skew-adjoint and bounded on $\mathcal{D}(S^{-1/2}) \oplus \ell^2(\Gamma)$ so the transformed orthogonal group must be

$$\exp\left[t\begin{pmatrix} 0 & -S \\ 1 & 0 \end{pmatrix}\right]$$

We can further simplify matters by identifying $\mathcal{D}(S^{-1/2})$ with $\ell^2(\Gamma)$ through the mapping $\xi \mapsto S^{-1/2}\xi$; this sets up an isomorphism between h_1 and $\ell^2(\Gamma) \oplus \ell^2(\Gamma)$ which carries $U_1(t)$ to the group generated by $\begin{pmatrix} 0 & -S^{1/2} \\ S^{1/2} & 0 \end{pmatrix}$.

All these rearrangements were carried out by treating the Hilbert spaces involved as real. Propositions 4.2 and 4.3, however, express the ergodic-theoretic properties of T^t in terms of the spectral properties of the unitary group obtained by complexifying the underlying Hilbert space. If we allow complex changes of coordinates, then the generator $\begin{pmatrix} 0 & -S^{1/2} \\ S^{1/2} & 0 \end{pmatrix}$ may be converted into $\begin{pmatrix} iS^{1/2} & 0 \\ 0 & -iS^{1/2} \end{pmatrix}$. Combining these remarks with Propositions 4.2 and 4.3, we get

<u>Proposition 4.5</u>. The time-evolution flow T^t for the infinite harmonic crystal is

(1) ergodic if and only if S, acting on $\ell^2_{\mathbb{C}}(\Gamma)$, has no point spectrum

(2) a Bernoulli flow if and only if S has Lebesgue spectrum.

Let us now see what happens when assumption (3) of Section 3 holds, but (4) does not. Abstracting from the above results, we may describe the infinite system equilibrium state as an orthogonal mapping from $\mathcal{D}(S^{-1/2})\oplus\ell^2(\Gamma)$ onto a generating Gaussian subspace of a probability space, with the interpretation that the random variable corresponding to $\xi \oplus \eta$ is $\sum_\alpha (\xi_\alpha q_\alpha + \eta_\alpha p_\alpha)$. The time evolution flow is induced by the one-parameter orthogonal group on $\mathcal{D}(S^{-1/2}) \oplus \ell^2(\Gamma)$ with infinitesimal generator $\begin{pmatrix} 0 & -S \\ 1 & 0 \end{pmatrix}$. If (ξ_α) is a sequence which does not belong to $\mathcal{D}(S^{-1/2})$, the series $\sum_\alpha \xi_\alpha q_\alpha$ does not make sense as a random variable.

This description of the equilibrium state and time evolution flow works perfectly well whether or not the coordinate vectors $e^{(\alpha)}$ are in the domain of $S^{-1/2}$. However, if $e^{(\alpha)} \notin \mathcal{D}(S^{-1/2})$, then the position of the αth particle does not make sense as a random variable. Indeed, as we have seen, if $e^{(\alpha)} \notin \mathcal{D}(S^{-1/2})$, then

$$\lim_{\Lambda\to\infty} (S_\Lambda^{-1})_{\alpha\alpha} = \infty ,$$

i.e., the variance of the position of the αth particle goes to infinity with Λ. A typical situation, exemplified by the one-dimensional harmonic chain with nearest neighbor interaction, is that $\xi \in d(\Gamma)$ is in $\mathcal{D}(S^{-1/2})$ if and only if $\sum_\alpha \xi_\alpha = 0$, i.e., if and only if $\sum_\alpha \xi_\alpha q_\alpha$ may be written as a linear combination of difference variables $q_\alpha - q_\beta$. In this case, the variances of difference variables approach finite limits as $\Lambda \to \infty$ even though the variances of individual positions do not. Moreover, the joint distribution of the difference variables for the finite system canonical ensemble converges to the corresponding distributions for the infinite system.

5. Translation Invariance

The preceding section shows how to determine the behavior of the harmonic crystal in the thermodynamic limit provided we know enough about the operator S. Specifically, we need to know

(1) is 0 an eigenvalue of S ;

(2) are the coordinate vectors $e^{(\alpha)}$ in $\mathcal{D}(S^{-1/2})$;

(3) what is the spectral type of S ?

These equations are hard to answer in general. However, if the matrix S is translation-invariant, Fourier transformation can be used to simplify matters somewhat.

We let $\hat{\Gamma}$ denote the "first Brillouin zone", i.e., the compact dual group of the discrete additive group Γ, and let V denote the volume of $\hat{\Gamma}$. Fourier transformation gives a unitary mapping of $\ell^2_{\mathbb{C}}(\Gamma)$ onto $L^2_{\mathbb{C}}(\hat{\Gamma})$ sending ξ to $\tilde{\xi}$, where ξ and $\tilde{\xi}$ are related by [1]

$$\xi_\alpha = \frac{1}{\sqrt{V}} \int_{\hat{\Gamma}} e^{ip\alpha}\, \tilde{\xi}(p)\, dp \ .$$

Translation invariance means simply that $S_{\alpha\beta}$ depends only on $\alpha-\beta$; we write $S(\alpha-\beta)$ for $S_{\alpha\beta}$ in this case. The operator S becomes a convolution operator:

$$(S\xi)_\alpha = \sum_\beta S(\alpha-\beta)\ \xi_\beta$$

which under Fourier transformation becomes a multiplication operator:

$$(S\xi)\ (p) = \tilde{S}(p)\ \tilde{\xi}(p)$$

with

$$\tilde{S}(p) = \sum_\alpha e^{ip\alpha}\ S(\alpha) \ .$$

Recall, however, that $S(\alpha-\beta)$ is a $\nu \times \nu$ matrix, so the same is true for $\tilde{S}(p)$ and we have not yet completely diagonalized S; to do this, we would have to diagonalize each $\tilde{S}(p)$. This can only be done on a case-by-case basis, but there are a number of remarks which clarify the situation without requiring intricate computations:

(i) The symmetry and reality of S imply that $\tilde{S}(p)$ is self-adjoint for each p and that $\tilde{S}(-p) = \tilde{S}(p)$. Since $S(\alpha)$ is assumed to be rapidly decreasing in α, $\tilde{S}(p)$ is an infinitely differentiable function of p.

(ii) In order that S be positive semidefinite it is necessary and sufficient that $\tilde{S}(p)$ be positive semidefinite for all p; similarly, S does not have zero as an eigenvalue if and only if $\tilde{S}(p)$ is strictly positive definite for almost all p.

(iii) Assumption 4 of Section 3 holds if and only if $\int dp \, \|\tilde{S}(p)^{-1}\| < \infty$.

(iv) In most interesting cases $\tilde{S}(0) = 0$. This reflects the fact that a uniform displacement of all the atoms in the crystal costs no energy. Because $\tilde{S}(-p) = \tilde{S}(p)$, this implies that each eigenvalue of $\tilde{S}(p)$ vanishes at least as fast as $|p|^2$ as p approaches zero. Thus, we must expect that

$$\int dp \, \|\tilde{S}(p)^{-1}\| = \infty$$

in one and two dimensions. This argument does not apply in three or more dimensions, and it is not hard to check that the above integral converges at zero for many reasonable interactions. The problem in showing that the overall integral is finite is that some eigenvalues may have "accidental" zeros at non-zero values of p.

The preceding analysis may be applied if the force matrix V is translation invariant even if strict translation invariance is destroyed by variation of the masses. From the definition of S it follows readily that $\| S^{-1/2} e^{(\alpha)} \|^2 = m_\alpha \| V^{-1/2} e^{(\alpha)} \|^2$. Hence, as long as the masses are bounded, and bounded away from zero, assumptions (3) and (4) hold if and only if they hold with S replaced by V.

The spectrum of S is almost arbitrary under our assumptions; we may simply choose any periodic infinitely differentiable matrix-valued function $\tilde{S}(p)$ which is strictly positive definite every where and satisfies the qualitative conditions of (i) and construct $S(\alpha)$ as its inverse Fourier transform. If we take $\tilde{S}(p)$ constant on some non-empty open set, then S has an eigenvalue with infinite multiplicity. On the other hand, if $S(\alpha) = 0$ for all sufficiently large α (or, more generally, if $S(\alpha)$ decreases exponentially with α), then $\tilde{S}(p)$ is a real-analytic function of p. We claim that, in this case, either $\tilde{S}(p)$ has at least one p-independent eigenvalue or else S has Lebesgue spectrum. To see this, we argue as follows: If $\tilde{S}(p)$ is an analytic function of p then, on the complement of a closed nowhere dense set of Lebesgue measure zero, the eigenvalues of $\tilde{S}(p)$ are analytic functions of p. Then if no eigenvalue is constant, the set where some eigenvalue has zero derivative is again a closed set of Lebesgue measure zero. By excluding these closed sets of measure zero, we see that S is unitarily equivalent to multiplication by a smooth function with nowhere vanishing derivative on an open set in Euclidean space; such an operator has Lebesgue spectrum. In concrete cases it is frequently easy (e.g. by looking at behavior near $p = 0$) to show that there is no constant eigenvalue and hence that T^t is a Bernoulli flow.

This is indeed the expected behavior of physically reasonable models of harmonic crystals with strict translation invariance [1,8]. It is true in particular for those systems for which the time dependence of expectations of the type $E(p_\alpha(t)\ p_\beta(0))$ has been calculated explicitly [1], [2] (see footnote ‡ in section 1). Since these systems are Bernoulli (and hence mixing) thexe correlations will go to zero as $|t| \to \infty$. The rate of decay cannot of course be obtained from the general theory; the calculations show it behaves generally as $t^{-(1/2)\nu}$ [1,2,9]. The way this inifnite volume behavior is approached as $\Lambda \to \infty$ (for finite Λ the system is not even ergodic) is also discussed in these studies.

The situation may be quite different however when the system does not have strict translation invariance. In this case the crystal may have localized modes in the neighborhood of the defect (deviation from regularity) giving rise to a point spectrum for S. An example of this is the case where one of the masses, say m_γ , is (sufficiently) smaller than the other masses, $m_\gamma < m_\alpha = m$ for all $\alpha \neq \gamma$, while V is translation invariant. It follows then from Rayleigh's theorems (Chapter V of [1]) that there will be an isolated frequency, or discrete eigenvalue of S. (This remains true if there are a finite number of such mass defects [1], [2].) Hence such a system will not be ergodic (as found also by Cukier and Mazur [10] from explicit calculations in the one dimensional case).

6. Quantum Mechanics of the Harmonic Crystal.

Because the equations of motion are linear the quantum-mechanical time evolution of the infinite harmonic crystal is easily deduced from the classical time evolution. Equation (3.1) gives, in the classical case,

$$q_\alpha(t) = \sum_\beta K^{(1)}_{\alpha\beta}\ q_\beta + K^{(2)}_{\alpha\beta}\ p_\beta\ ,$$

and similarly for $p_\alpha(t)$. To get the quantum theory (in the Heisenberg picture) it is only necessary to substitute a set of operators Q_α , P_α satisfying the canonical commutation relations for the numerical initial data q_α , p_α. This gives the time evolution, formally at least, as a one-parameter group of automorphisms of an algebra of unbounded operators. It is technically preferable to pass to a one-parameter group of automorphisms of an C^* algebra "of bounded operators" associated with representation of the commutation relations. This can be done without difficulty -- the time evolution automorphisms become Bogoliubov transformations -- but we will not give the details [11].

The equilibrium statistical mechanics of the quantum crystal is also simple to obtain. For a finite crystal Λ, a straightforward calculation shows that the canonical ensemble at inverse temperature β is a quasi-free state ρ_Λ (i.e., the truncated expectation values of degree greater than two vanish) with two-point function given by [1]

$$\rho_\Lambda(Q_\alpha\ Q_\beta) = \left[\frac{S_\Lambda^{-1/2}}{2} \coth\left(\frac{\beta S_\Lambda^{1/2}}{2}\right)\right]_{\alpha\beta}$$

$$\rho_\Lambda(P_\alpha\ P_\beta) = \left[\frac{S_\Lambda^{+1/2}}{2} \coth\left(\frac{\beta S_\Lambda^{1/2}}{2}\right)\right]_{\alpha\beta}$$

$$\rho_\Lambda(P_\alpha\ Q_\beta + Q_\beta\ P_\alpha) = 0\ .$$

(Note that $\rho(P_\alpha Q_\beta)$ can be computed from the third equation and the commutation relations.) We have put $\hbar = 1$ in these expressions. To obtain the equilibrium state for the infinite crystal, we must let $\Lambda \to \infty$. Let us look first at the expression for $\rho_\Lambda(P_\alpha P_\beta)$. The function

$$z \longmapsto \frac{z^{1/2}}{2} \coth\left(\frac{\beta z^{1/2}}{2}\right)$$

is analytic in a neighborhood of the real line (including $z = 0$). We may regard S_Λ as a positive operator on $\ell^2(\Gamma)$ which is zero on the orthogonal complement of $\ell^2(\Gamma)$. Then S_Λ converges strongly to S as $\Lambda \to \infty$, and hence

$$\frac{S_\Lambda^{1/2}}{2} \coth\left(\frac{\beta S_\Lambda^{1/2}}{2}\right)$$

converges strongly to

$$\frac{S^{1/2}}{2} \coth\left(\frac{S^{1/2}}{2}\right)$$

Therefore

$$\lim_{\Lambda\to\infty} \rho_\Lambda(P_\alpha P_\beta) = \left(\frac{S^{1/2}}{2} \coth\left(\frac{S^{1/2}}{2}\right)\right)_{\alpha\beta}$$

The limit for $\rho_\Lambda(Q_\alpha Q_\beta)$ involves one more step. The function

$$z \longmapsto \frac{z^{-1/2}}{2} \coth\left(\frac{\beta z^{1/2}}{2}\right)$$

is not analytic on the real axis; it has a pole at the origin. However, the difference between this function and $\beta^{-1}z^{-1}$ is analytic. Hence, by the above argument,

$$\lim_{\Lambda\to\infty} \{\rho_\Lambda(Q_\alpha Q_\beta) - \beta^{-1}(S_\Lambda^{-1})_{\alpha\beta}\}$$

exists. If, in addition, Assumption (4) of Section 3 holds, the results of that section imply that

$$\lim_{\Lambda\to\infty} (S_\Lambda^{-1})_{\alpha\beta} = (S^{-1/2} e^{(\alpha)}, S^{-1/2} e^{(\beta)}) ,$$

so we can conclude that

(1) each $e^{(\alpha)}$ is in the domain of $\left[\frac{S^{-1/2}}{2} \coth\left(\frac{\beta S^{1/2}}{2}\right)\right]^{1/2}$

(2) $$\lim_{\Lambda\to\infty} \rho_\Lambda(Q_\alpha Q_\beta) = \left(\left[\frac{S^{-1/2}}{2} \coth\left(\frac{\beta S^{1/2}}{2}\right)\right]^{1/2} e^{(\alpha)},\right.$$

(*) $$\left.\left[\frac{S^{-1/2}}{2} \coth\left(\frac{\beta S^{1/2}}{2}\right)\right]^{1/2} e^{(\beta)}\right).$$

Thus: the infinite-system equilibrium state is the quasi-free state of the canonical commutation relations with two-point function given by

$$\rho(Q_\alpha Q_\beta) = \left[\frac{S^{-1/2}}{2} \coth\left(\frac{\beta S^{1/2}}{2}\right)\right]_{\alpha\beta} \quad \text{(defined by the right-hand side of (*))}$$

$$\rho(P_\alpha P_\beta) = \left[\frac{S^{1/2}}{2} \coth\left(\frac{\beta S^{1/2}}{2}\right)\right]_{\alpha\beta}$$

$$\rho(P_\alpha Q_\beta + Q_\beta P_\alpha) = 0 .$$

Calculations similar to those used to prove the invariance of the classical equilibrium state show that this state of the quantum system is invariant under the time-development automorphisms.

If Assumption (4) of Section 3 fails, a part of the theory of equilibrium states for the infinite crystal can be salvaged as indicated in Section 4 for the classical system. In the resulting theory, positions of the individual oscillators are not observables, but appropriate linear combinations of the positions are.

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