The Extension of Classical Dynamics for Unstable Hamiltonian Systems

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Abstract—Classical dynamics can be formulated in terms of trajectories or in terms of statistical ensembles whose time evolution is described by the Liouville equation. It is shown that for the class of large nonintegrable Poincaré systems (LPS), the two descriptions are not equivalent. Practically all dynamical systems studied in statistical mechanics belong to this class. The basic step is the extension of the Liouville operator $L_H$ outside the Hilbert space to functions singular in their Fourier transformation. This function space plays an important role in statistical mechanics as functions of the Hamiltonian, and therefore equilibrium distribution functions belong to this class. Physically, these functions correspond to situations characterized by "persistent interactions" as they are realized in macroscopic physics. Persistent interactions are introduced in contrast to "transient interactions" studied in quantum mechanics by the $S$-matrix approach (asymptotically free in and out states). The eigenvalue problem for the Liouville operator $L_H$ is solved in this generalized function space for LPS. We obtain a complex, irreducible spectral representation. Complex means that the eigenvalues are complex numbers, whose imaginary parts refer to the various irreversible processes such as relaxation times, diffusion.... Irreducible means that these representations cannot be implemented by trajectory theory. As the result, the dynamical group of evolution splits into two semigroups. Moreover, the laws of classical dynamics take a new form as they have to be formulated on the statistical level. They express "possibilities" and no more "certitudes". Two examples of typical classical systems, i.e., interacting particles and anharmonic lattices are studied.

Keywords—Irreversibility, Large Poincaré systems, Complex spectral representation, Persistent processes, Delta function singularities.

1. INTRODUCTION

In recent years, a radical change in perspective in science is witnessed. We see in a variety of areas, ranging from elementary particle physics and cosmology to chemistry and biology, the role of irreversibility and instability. How can these findings be incorporated in the basic laws of classical or quantum mechanics?

It is well known since the pioneering work of Gibbs and Einstein, that we can describe dynamics from two points of view. On one hand, we have the individual description in terms of trajectories (or of wave functions); on the other hand, the statistical description in terms of probability distributions $\rho$ (called the density matrix in quantum theory). It was always assumed that the two levels of description were equivalent. In previous papers in our group [1–18], we have shown that this is not so for the classes of systems where we expect irreversible processes to arise.

This paper incorporates a number of previous works obtained notably by C. George, F. Henin, A. Grecos, I. Antoniou and S. Tasaki. This paper has benefited from much constructive criticism and discussion from I. Antoniou and B. Misra. We are grateful to C. George, M. de Haan and E. C. G. Sudarshan for interesting remarks. We also acknowledge the U.S. Department of Energy Grant No. DE-FG03-94ER14465, the Robert A. Welch Foundation Grant No. F-0365, and the European Community Contract No. PSS*0661 for support of this work.
Then the basic description is in terms of the statistical description. We obtain new solutions for the probability distribution which are "irreducible" as they do not apply to single trajectories. Moreover, in this new formulation, symmetry between past and future is broken.

Consider classical dynamics. Our formulation requires essentially two conditions. First, Poincaré nonintegrability and more precisely, so-called "Large Poincaré Systems" (LPS) in which frequencies depend continuously on the wave vector \( \mathbf{k} \). In addition, we need "persistent" interactions. This is in contrast to "transitory" interactions, as studied, e.g., in ordinary scattering experiments. Persistent interactions require singular distribution functions. As the result, we have to go outside the usual Hilbert space. We obtain then new spectral representations of the evolution operators, here the Liouville operator in generalized function space with complex eigenvalues. The dynamical group is broken into two semigroups. We can in this way construct \( \mathcal{H} \)-functions on a purely dynamical basis and unify dynamics and thermodynamics. It is important to stress that irreversibility appears as an emergent property somewhat analogous to phase transitions which can only be defined on the level of ensembles.

Here we shall present an overview of our extension of classical mechanics for LPS. We shall consider two typical classical systems: the one is interacting particles, and the other is anharmonic lattices.

We first consider \( N \) interacting particles whose Hamiltonian is of the form

\[
H(q, p) = H_0(p) + \lambda V(q) = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \lambda \sum_{j>i}^{N} V(|q_i - q_j|),
\]

where \( \lambda \) is the coupling constant, and \( q \) and \( p \) are \( N \)-component vectors, i.e., \( q \equiv (q_1, \ldots, q_N) \) with three-dimensional vectors \( q_j \), and so on. The system is put into a large box with volume \( L^3 \). These are the systems studied in equilibrium and nonequilibrium statistical mechanics. It is well known that these systems are in general nonintegrable in the sense of Poincaré. In the large limit \( L^3 \rightarrow \infty \), we obtain LPS. The number of particles \( N \) may be finite or infinite. We shall be specially interested in the "thermodynamic limit",

\[
N \rightarrow \infty \quad \text{and} \quad L^3 \rightarrow \infty, \quad \text{with} \quad c = \frac{N}{L^3} = \text{finite}.
\]

The statistical description in classical dynamics is expressed by the Liouville equation for the distribution function [19–23],

\[
i \frac{\partial}{\partial t} \rho(t) = \mathcal{L}_H \rho(t).
\]

Here \( \mathcal{L}_H \rho \equiv i\{H, \rho\} \) is the Poisson bracket of \( \rho \) with the Hamiltonian \( H \).

In this paper, we show that we can extend the Liouville operator (or Liouvillian in short) for LPS to a class of functions outside the Hilbert space. This class of functions has a very simple physical meaning as it includes equilibrium distributions which are functions of the Hamiltonian. These functions are characterized by well-defined singularities in their Fourier transforms. It will be useful to distinguish between ensembles localized in space and nonlocal ensembles. A special case of localized ensembles are single trajectories,¹

\[
\rho(q, p, 0) = \frac{1}{L^{3N}} \prod_{j=1}^{N} \sum_{k_j} e^{ik_j (q_j - q_j^0)} \delta (p_j - p_j^0) - \prod_{j=1}^{N} \delta (q_j - q_j^0) \delta (p_j - p_j^0), \quad \text{for} \quad L \rightarrow \infty.
\]

¹In the box normalization formalism which we shall consider in this paper, the delta function in space is replaced by a periodic delta function with the period \( L \), the size of the box. This replacement does not introduce any "width" for the delta function, so that this ensemble corresponds still to single point of phase space.
The Extension of Classical Dynamics

Associated with a finite number of particles, localized distributions $\rho$ describe transient interactions (free in and out states) as studied in quantum $S$-matrix theory. In contrast, nonlocal ensembles describe persistent interactions as studied in statistical mechanics. They are, as just mentioned, characterized by singularities in their Fourier expression (see Section 3).

Our extended spectral representation for $L_H$ is presented in Sections 4 and 5. It has quite remarkable features as it exhibits "non-Newtonian" features. There appear indeed diffusive effects associated with collision operators $\Theta$ of the Fokker-Planck type, familiar from phenomenological theories. The appearance of these contributions is due to the coupling of dynamical "events" through Poincaré resonances. The eigenvalues of $L_H$ in this extended functional space are complex.

The non-Newtonian effects lead to the construction of nonunitary transformation operators $\Lambda$ which intertwine $L_H$ and the collision operators, which are dissipative operators. This generalizes the unitary transformation which leads for integrable systems from $L_H$ to $L_0$, the Liouvillian corresponding to $H_0$ (Section 6). The complex spectral representation also leads to subdynamics which corresponds to an extension of the kinetic theory to all correlation spaces [18,24–35]. In our previous work, subdynamics have been constructed by using an ansatz for the analytic continuation (the so-called $\epsilon$ rule) (see, for example, [35]). We now may derive subdynamics from the complex spectral representation. Using our nonunitary transformation theory, we can transform the Liouville equation for $\rho$ into an infinite set of "kinetic equations" (see Section 6). We also obtain a new formulation of Heisenberg type of equation for the evolution of observables which makes explicit the role of dissipative processes. As the result of the breaking of time-symmetry, we can easily construct Lyapounov functions which are dynamical analogies of the "$H$-functions" derived usually through phenomenological assumptions (Section 7). Our nonunitary transformation theory allows to reformulate the second law of thermodynamics as a "selection principle" for the class of initial conditions which are realized in nature.

The intertwining relations between $L_H$ and $\Theta$ lead to a nonlinear extension of the Lippmann-Schwinger type equations, well known from quantum scattering theory (see Section 8). When dissipative effects can be neglected, the nonlinear terms vanish and we come back to a classical version of the Lippmann-Schwinger equations.

However, our equations differ from the Lippmann-Schwinger equations by our analytic continuation. There appears a degeneracy for LPS. The existence of Poincaré resonances even in the nondissipative limit lead to a new spectral decomposition of the Liouvillian in addition to the usual spectral representations in terms of advanced or retarded solutions. It is this alternative spectral representation which we have extended in Sections 4 and 5 to include dissipation.

In Sections 9–12, we discuss the conditions under which the non-Newtonian effects which appear in our spectral representation of $L_H$ can be observed. This depends essentially on the type of distribution functions (associated with regular or singular Fourier transforms) and on the number of particles ($N$ finite, or $N \to \infty$ as in the thermodynamic limit).

For $N$ finite and localized, regular distribution functions all dissipative effects disappear. These systems while presenting Poincaré resonances are integrable. The situation changes dramatically when we consider persistent interactions associated with distribution functions which are singular in their Fourier representation (Sections 11,12). Of special importance is the thermodynamic limit. When we apply our spectral representation to this class of distribution functions, we recover all results derived in nonequilibrium statistical mechanics [19] (such as Fokker-Planck equations, Boltzmann equations, generalized master equations, ...). This shows that dissipative processes are part of the exact dynamical description when we consider LPS and extend the functional space to include functions which are singular in their Fourier representation.

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2Here, we have in mind the Poincaré resonances expressed by the frequency (or "energy") conservation between the initial and final states such as $\delta(\omega_i - \omega_f)$ in the usual $S$-matrix theory. The Poincaré resonances already appear for repulsive interactions. These resonances are not related to "resonance poles" associated with the so-called resonance scattering.
It is very interesting that the functional form of these distribution functions (see (3.15)) is invariant with respect to time. This form even acts as an attractor (see (6.21)). This brings us to the question: are trajectories also preserved? As mentioned, for \( N \) finite, all dissipative effects disappear. A trajectory remains a trajectory for all times. But what happens in the thermodynamic limit?

This question may sound surprising. Since ever trajectories had been considered as "primitive", undecomposable objects. Still the delta function \( \delta(q - q_0) \), when written as a Fourier integral, can be considered as the coherent superposition of plane waves corresponding to wave vectors \( k \).

Now in the statistical description, the natural variables are precisely the wave vectors (see Section 2). The trajectory becomes a construct. Resonances correspond to nonlocal processes in space-time. They are responsible for the appearance of diffusive processes. Such processes may destroy the coherence of the wave packet in Fourier space and therefore also the trajectory. We have then a "collapse" of trajectories to borrow the terminology from quantum mechanics (see Section 12).

We ask: under which conditions does (1.4) in the limits \( L \rightarrow \infty \) and \( N \rightarrow \infty \) lead to a well-defined "thermodynamic limit"? A necessary condition is that all reduced quantities tend to a finite limit independent of \( N \). This implies strict conditions for LPS as Poincaré resonances lead to long range correlations between the particles (see Section 9).

Our predictions have been verified analytically and by computer simulations in simple situations such as the Lorentz model (see \([5,6,21]\)).

In Sections 13 and 14, we shall consider another typical example in classical mechanics: the problems of anharmonic lattices which are of great interest as it brings us close to nonlinear quantum field theory. We consider the thermodynamic limit for which the number of particles \( N \rightarrow \infty \). Moreover, we require that the distinction between intensive variables and extensive variables be maintained in this limit. For example, the displacement of a single particle has to remain finite as well as the density of energy \( H/N \). Anharmonic lattices have been studied from this point of view since long \([19,36]\). From our point of view, their interest is that they are indeed LPS and that the interactions are automatically persistent (remember that normal modes and angles-action variables are collective variables, see Section 13). The situation is therefore simpler than for interacting particles.

We first consider the case of a harmonic lattice and consider the limit \( N \rightarrow \infty \). The dynamic description can then be performed on the level of trajectories or in terms of distribution functions associated with a Hilbert space (Section 13). We then consider the case of anharmonic lattices (Section 14) and show that the thermodynamic limit destroys the Hilbert space structure. Moreover, due to Poincaré resonances, new diffusive terms appear which destroy trajectories. The trajectory again “collapses”.

The results obtained for the anharmonic lattices are much stronger than for systems of interacting particles. There we considered situations which already at the initial time were outside the Hilbert space. Here the Hilbert space structure is destroyed by anharmonic forces in the thermodynamics limit even if we start with a distribution function with a finite Hilbert norm.

The results described here can be extended easily to quantum theory. There also the equivalence between the individual description (in terms of wave functions) and the statistical description (in terms of density matrices) is broken. This will be reported in a separate paper (see \([37]\)).

2. THE LIouvillian FORMALISM

The evolution of the system is governed by the Liouville equation (1.3) for the distribution function \( \rho(q,p,t) \) in phase space. We assume that the distribution function vanishes quickly enough for large values of momentum,

\[
\lim_{|p| \to \infty} \rho(q,p) \to 0.
\]
However, we shall not generally impose a similar condition for the coordinate dependence, because we are interested not only in single trajectories, but also in nonlocal ensembles in phase space as considered in typical situations in statistical mechanics.

The formal solution of the Liouville equation is

$$\rho(t) = U(t) \rho(0),$$

(2.2)

with

$$U(t) = e^{-iL_H t}.$$  

(2.3)

$U(t)$ is the evolution operator.

For integrable systems, the Liouville equation does not introduce any new features. If we can integrate Hamilton's equations of motion, we can solve the Liouville equation and vice versa. Usually, one equips the phase space with a Hilbert space structure. In this space, the scalar product of the phase functions $f$ and $g$ is defined by (with $\int dq = \int dq_1 \ldots \int dq_N$, and so on)

$$\langle f | g \rangle = \int dq \int dp \langle f | q, p \rangle \langle q, p | g \rangle = \int dq \int dp f^*(q, p) g(q, p),$$

(2.4)

and their Hilbert norms by

$$\|f\| = \sqrt{\langle f | f \rangle}.$$  

(2.5)

We have introduced Dirac's "bra" and "ket" notations, i.e., $\langle f |$ and $| g \rangle$, analogous to quantum mechanics. This permits us to use various representations. The Liouvillian $L_H$ is a Hermitian operator and $U(t)$ unitary. That means that, as long as we remain in Hilbert space, the eigenvalues $\lambda$ of $L_H$ are real, and the eigenvalues $\exp(-i\lambda t)$ of $U(t)$ are of modulo one. In short, the distribution function oscillates in time and there is no place for irreversible processes. To obtain irreversible processes associated with complex eigenvalues of $L_H$, we need to go out of the Hilbert space (this is a necessary condition).

In the statistical description, a single trajectory $|\rho(0)\rangle = |q^0, p^0\rangle$ is represented by Dirac's delta function

$$\rho(q, p, u) = \langle q, p | \rho(u) \rangle = \delta(q - q^0) \delta(p - p^0),$$

(2.6)

where $\delta(p) = \prod_{r=1}^N \delta(p_r)$ with $\delta(p) = \delta(p_x)\delta(p_y)\delta(p_z)$.

To each observable $M(q, p)$, we can associate a bra-state

$$\langle \langle M \rangle | \equiv \langle \langle M \rangle | q, p \rangle.$$  

(2.7)

When acting on a trajectory $|q, p\rangle$, this leads back to a phase function as

$$M(q, p) = \langle \langle M \rangle | q, p \rangle.$$  

(2.8)

The evolution of the observables is given by

$$\langle \langle \dot{M} (t) \rangle | = \langle \langle \dot{M} \rangle | U(t).$$

(2.9)

They satisfy the classical "Heisenberg equations" of motion

$$i \frac{\partial}{\partial t} |\langle M(t) \rangle\rangle = -L_H |\langle M(t) \rangle\rangle.$$  

(2.10)

3Following the tradition for nonequilibrium statistical mechanics [23], we use the convention that the distribution functions are associated with ket-states, while the observables are associated with bra-states.
The Hamilton equations of motion correspond to a special case of the Heisenberg equations for the set of observables \((\hat{q}_j, \hat{p}_j)\) associated with trajectories. Similarly, the Liouville equation (1.3) corresponds to the classical "Schrödinger" picture of the equation of motion.

The expectation value of \(M\) is given by

\[
\langle M \rangle_s = \langle \langle \hat{M}(0) | \rho(t) \rangle \rangle = \langle \langle \hat{M}(t) | \rho(0) \rangle \rangle.
\]  

(2.11)

Let us consider a system described by the Hamiltonian (1.1). For simplicity, we assume short-range repulsive interactions. Corresponding to the decomposition of the Hamiltonian (1.1), we have also (with \(L_0 \equiv L_{H_0}\))

\[
L_H = L_0 + \lambda L\gamma.
\]  

(2.12)

The unperturbed Liouvillian is the derivative operator \(L_0 = -i\nu \cdot \partial / \partial q\), where \(\nu_j \equiv p_j / m_j\) is the velocity of the particle \(j\). Then the eigenstates of \(L_0\) are given by

\[
L_0 |k, p\rangle = (k \cdot \nu) |k, p\rangle.
\]  

(2.13)

Here, \(k \cdot \nu \equiv k_1 \cdot \nu_1 + \cdots + k_N \cdot \nu_N\), and

\[
\langle \langle q, p' | k, p \rangle \rangle = L^{-3N/2} e^{i k \cdot q} \delta (p' - p),
\]  

(2.14)

where \(k_j\) is a real vector. For periodic boundary conditions and using the box normalization, we have (with integer vectors \(n_j\), and with \(\Delta k = 2\pi / L\), where \(L^3\) corresponds to the volume of the box)

\[
k_j = n_j \Delta k.
\]  

(2.15)

In the limit of large volumes \(\Omega \equiv (L/2\pi)^3 \to \infty\),

\[
\Omega^{-1} \sum_k \to \int dk, \quad \delta_{\Omega} (k) \equiv \Omega \delta^{kr} (k) \to \delta (k),
\]  

(2.16)

where \(\delta^{kr} (k) \equiv \delta_{k, 0}\) is Kronecker’s delta.

Note that the eigenfunctions (2.14) of the unperturbed Liouvillian \(L_0\) are plane waves corresponding to "wave vectors" \(k\) as the Fourier indices. They satisfy the orthogonality and completeness relations

\[
\langle \langle k, p | k', p' \rangle \rangle = \delta^{kr} (k - k') \delta (p - p'), \quad \sum_k \int dp |k, p\rangle \langle k, p| = 1.
\]  

(2.17)

As a result, the solution \(\rho(q, p, t)\) for the unperturbed system can also be written as a superposition of plane waves

\[
\rho(q, p, t) = \frac{1}{L^{3N/2}} \sum_k e^{ik \cdot (q - p)} \langle \langle k, p | \rho(0) \rangle \rangle.
\]  

(2.18)

For a trajectory, we have (see (1.4))

\[
\langle \langle k, p | \rho(0) \rangle \rangle = \frac{1}{L^{3N/2}} e^{-ik \cdot q^0} \delta (p - p^0).
\]  

(2.19)

This leads with (2.18) to

\[
\rho(q, p, t) = \delta (q - q^0 - ut) \delta (p - p^0).
\]  

(2.20)

Hence, the delta function remains a delta function. The delta function corresponds to a coherent superposition of plane waves. As we shall see in the thermodynamic limit, Poincaré resonances may destroy this coherent superposition and therefore also the trajectory (see Section 11).
In the Fourier representation, the evolution generated by the unperturbed Liouvillian is diagonal, while the part corresponding to the perturbation $\lambda L_V$ is off-diagonal and leads to transitions from one set of wave vectors to another. We can calculate the matrix elements $(L_V)_{k',p';k,p}$ defined as

$$
(L_V)_{k',p';k,p} = \langle \langle k',p'|L_V|k,p \rangle \rangle = \frac{1}{L^{3N}} \int dq \int dq' \ e^{-i k' \cdot q} \langle \langle q,p'|L_V|q',p \rangle \rangle e^{i k \cdot q}.
$$

(2.21)

In this example, the only nonvanishing matrix elements are \[ \langle \langle k',k',\{k\}^{N-2},p'|L_V|k,j,k,n,\{k\}^{N-2},p \rangle \rangle = \delta_{k',k'} \delta_{j,n} \delta(p-p') \] \[ \times \frac{1}{2} \delta_k^{kr} \delta_{kj} \delta_{kn} \delta(p-p') \],

(2.22)

where

$$
d_{jk} \equiv \frac{\partial}{\partial p_j} - \frac{\partial}{\partial p_n}
$$

(2.23)

and $\{k\}^{N-2}$ is a set of wave vectors excluding the particles $j$ and $n$. The function $V_j$ is the Fourier coefficients of the potential

$$
V(|q|) = \frac{1}{2} \sum_i V_i e^{i q_i}.
$$

(2.24)

We assume $V_0 = 0$, i.e.,

$$
\int dq V(|q|) = 0.
$$

(2.25)

All indices $k$ in (2.22) keep their values, except the two indices $k_j, k_n$; moreover, we have the conservation law of wave vectors,

$$
k_n + k_j = k + k_j.
$$

(2.26)

All these results are direct consequences of the assumption of binary interactions and of invariance in respect to translation.

### 3. SINGULAR FOURIER EXPANSION AND PROJECTION OPERATORS

The statistical description of dynamics in terms of the Liouville equation deals with a wide class of ensembles; this includes ensembles localized in space, as well as nonlocal ensembles. Let us first consider local ensembles. We consider the Fourier expansion of the distribution function

$$
\rho(q,p,t) = \frac{1}{L^{3N}} \sum_k e^{ik \cdot q} \tilde{\rho}_k(p,t),
$$

(3.1)

where (see the volume factor in (2.14))

$$
\tilde{\rho}_k(p,t) \equiv L^{3N/2} \langle \langle k,p | \rho(t) \rangle \rangle.
$$

(3.2)

For local ensembles, the coefficients $\tilde{\rho}_k(p)$ do not depend of the volume in the limit $\Omega \to \infty$. As we shall see later, this is not the case for nonlocal ensembles where $\rho(q,p) \neq 0$ in the limit $|q_j| \to \infty$. In order to emphasize this fact and to distinguish (3.1) from the Fourier coefficients $\rho_k(p)$ for

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If this is not the case, we redefine the unperturbed Hamiltonian by incorporating the element $V_0$ into $H_0$. 

nonlocal ensembles, we put the bar on the coefficients $\bar{p}_k$. The distribution function (3.1) is normalizable as

$$\int dq \int dp \rho(q,p) = \int dp \bar{\rho}_0(p) = 1.$$  

(3.3)

A single trajectory belongs to this class (see (1.4)). The characteristic feature of this class of ensembles is that all Fourier components of the distribution function have the same volume dependence $L^{-3N}$ regardless of the number of nonvanishing elements $k_j$ in the wave vector $k = (k_1, \ldots, k_N)$.

The Hilbert space norm of this class of distributions is given by (for $L \to \infty$)

$$\langle \rho|\rho\rangle = \frac{1}{L^{3N}} \sum_k \int dp |\bar{\rho}_k(p)|^2 \to \frac{1}{(2\pi)^{3N}} \int dk \int dp |\bar{\rho}_k(p)|^2.$$  

(3.4)

Hence, there exists a Hilbert norm for square integrable functions and for $N$ finite.5

On the other hand, statistical mechanics (equilibrium and nonequilibrium) deals mainly with nonlocal distributions, such as canonical distribution function. As in an equilibrium problem, it is useful to introduce reduced distribution functions $f_s$ referring to $s$ particles. From the normalizable distribution function $\rho$, we may deduce the probability $\rho_s(q_1, \ldots, q_s, p_1, \ldots, p_s)$ of finding, at a given time $t$, a set of $s$ specific particles $1, 2, \ldots, s$, with momenta $p_1, \ldots, p_s$, and coordinates $q_1, \ldots, q_s$.

$$\rho_s(q_1, \ldots, q_s, p_1, \ldots, p_s) = \int dq^{N-s} dp^{N-s} \rho(q, p, t).$$  

(3.5)

Distribution functions that refer to specified particles are called specific distribution functions [19]. We shall in general be more interested in the probability of finding $s$ arbitrary particles at positions $q_1, \ldots, q_s, p_1, \ldots, p_s$.

This probability, which we shall call $f_s$, is found by multiplying $\rho_s$ by the factor $N!/(N-s)!$ This is the number of possible ways in which a sequence of $s$ particles can be chosen out of $N$. Therefore,

$$f_s(q_1, \ldots, q_s, p_1, \ldots, p_s) = \frac{N!}{(N-s)!} \rho_s(q_1, \ldots, q_s, p_1, \ldots, p_s)$$

$$= \frac{N!}{(N-s)!} \int dq^{N-s} dp^{N-s} \rho(q, p).$$  

(3.6)

We shall also use distribution function $\varphi_s$ in momentum space and $n_s$ in coordinate space defined by

$$\varphi_s(p_1, \ldots, p_s) = \frac{(N-s)!}{N!} \int dq^s f_s,$$

$$n_s(q_1, \ldots, q_s) = \int dp^s f_s.$$  

(3.7)

The reduced distribution functions $f_s$, $\varphi_s$, and $n_s$ are called generic distribution functions to distinguish them from the specific distribution functions. In the following discussion, we shall use the specific distribution functions whenever it is necessary to specify coordinate and the momentum of each particle, such as the case for a single trajectory, otherwise we shall mainly use the generic distribution functions.

In general, statistical mechanics deals with situations where there are no asymptotic free in and out states. The interactions are persistent. As mentioned, this requires the use of nonlocal distributions. For this case, distribution functions have “delta function singularities” in their Fourier representation [19]. For example, let us consider the reduced number density in space

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5Trajectories are a special case of this class of distributions. They satisfy (3.3) but have no Hilbert space norm.
given by \( n_1(q) = c + h(q) \), where \( c \) is a constant and \( h \) is an absolutely integrable function. In the Fourier representation, we have (see (2.16))

\[
n_1(q) = \frac{1}{\Omega} \sum_k (c\delta_\Omega(k) + h_k) e^{ik\cdot q}.
\]

(3.8)

In the limit of large volume, the uniform part has a delta function singularity at \( k = 0 \).

We note that the Hamiltonian (1.1) is also a nonlocal phase function, which has again a delta function singularity in its Fourier expansion,

\[
H(q, p) = \frac{1}{\Omega} \sum_k \sum_i^N \left[ \frac{p_i^2}{m_i} \delta_\Omega(k) + \lambda \sum_{j>i}^N V_{kj} e^{-ik\cdot q_j} \right] e^{ik\cdot q_i}.
\]

(3.9)

Let us now show that this leads to delta function singularities for equilibrium distributions which are functions of the Hamiltonian

\[
\rho^{eq}(q, p) = \frac{f(H_0 + \lambda V)}{\int dq dp f(H_0 + \lambda V)}.
\]

(3.10)

We assume the normalization

\[
\int dp f(H_0) = 1.
\]

(3.11)

Then, using (2.25) we have the power series expansion in the coupling constant \( \lambda \) for the Hamiltonian (1.1),

\[
\rho^{eq} = \frac{1}{L^{3N}} \left[ 1 + \frac{1}{2!} \sum_{i,j}^N V_{ij} \frac{\partial}{\partial H_0} + \frac{\lambda^2}{2} \left( \frac{1}{2!} \sum_{i,j}^N V_{ij} V_{ij} + \frac{1}{3!} \sum_{i,j,m}^N V_{ij} V_{jm} \right) \\
+ \frac{1}{4!} \sum_{i,j,m,n}^N V_{ij} V_{mn} \right] \frac{\beta^2}{2 L^{3N}} \int dq V^2 \int dp \left( \frac{\partial^2 f(H_0)}{\partial H_0^2} \right) + \lambda^3 \ldots f(H_0),
\]

(3.12)

where we have written explicitly the particle indices, such as \( i \) and \( j \). Different particle indices \( i, j \) denote different particles. Let us consider the canonical distribution function (for systems with the same mass \( m_i = m \) of particles)

\[
f(H) = \left( \frac{\beta}{2\pi m} \right)^{3N/2} e^{-\beta(H_0 + \lambda V)}.
\]

(3.13)

We then obtain (with (3.9))

\[
\rho^{eq}(q, p) = \frac{1}{L^{3N}} \left( \frac{\beta}{2\pi m} \right)^{3N/2} e^{-\beta H_0} \left[ 1 + \lambda^2 \ldots \right. \\
+ \frac{1}{2\Omega} \sum_{i,j}^N \sum_k^\Omega e^{ik\cdot (q_i - q_j)} \left( -\lambda \partial V_{ij} + \lambda^2 \frac{\beta}{2} \sum_{k'} V_{k'j} V_{k'\cdot -k} + \lambda^3 \ldots \right) \\
+ \frac{1}{3!\Omega^2} \sum_{i,j,m}^N \sum_k^\Omega \sum_{k'} e^{i(k+k')\cdot (q_i - q_j - q_m)} \left( \lambda^2 \partial^2 V_{ij} V_{k'\cdot -k} + \lambda^3 \ldots \right) + \ldots \right].
\]

(3.14)

Here, the first term in the bracket does not depend on the coordinates, so that this term is associated with a Fourier coefficient which has only vanishing wave vectors. The second term corresponds to contributions which have nonvanishing wave vectors \( k_i = k \) and \( k_j = -k \) for only
two particles, i and j, and so on. As the Hamiltonian is translational invariant, the equilibrium distribution is “homogeneous” in space (it is invariant when \( q_j = q_j + \mathbf{a} \) for all \( j \), then the total wave vector vanishes \( k_i + k_j + \cdots = 0 \)).

The remarkable feature of the equilibrium distribution is that \( \rho^{eq} \) can be decomposed into the “vacuum of correlations” (i.e., the first term in the bracket of (3.14)), binary correlations (the second term), ternary correlations (the third term), . . . . Moreover, we see the appearance of delta function singularities as in (3.8). The existence of this expansion ensures the existence of reduced variables (i.e., “intensive variables”) depending on a finite number of particles, as well as of the “cluster expansion” of the distribution function \( \rho \) in terms of correlation functions which have a finite range of correlations in the thermodynamics limit [19,22].

In our previous work in nonequilibrium statistical mechanics, we used the class of ensembles which correspond to the natural generalization of the canonical distribution [19,22]:

\[
\rho_{(q_1, p_1)} = \frac{1}{L^{3N}} \sum_k e^{ikq} \left[ \rho_0(p) \delta^{kr}(k) + \frac{1}{\Omega} \sum_{j>i} \rho_{k_i, -k_i}(p_i, p_j \mid p^{N-2}) \delta_{k_i + k_j, 0} \delta^{kr}(k) ight] + \frac{1}{\Omega^2} \sum_{n>2} \rho_{k_i, k_j, k_n}(p_i, p_j, p_n \mid p^{N-3}) \delta_{k_i + k_j + k_n, 0} \delta^{kr}(k) + \cdots 
\]

(3.15)

Here, \( \delta^{kr}(k) \) is a product of \( N \) Kronecker’s delta, \( \delta^{kr}(k) \) a product of \( N - 1 \) Kronecker’s delta which excludes the particle \( j \), and \( \delta^{kr}(k) \) a product of \( N - 2 \) Kronecker’s delta which excludes the particles \( i \) and \( j \), and so on. We have decomposed the Fourier components according to the number of nonvanishing elements \( k_j \) in the wave vector \( k \). In the expression \( \rho_{k_i, k_j, \ldots}(p_i, p_j, \ldots \mid p^{N-r}) \), the momentum arguments on the left side of bar denote the particle \( i \) with a nonvanishing wave vector \( k_i \), the particle \( j \) with \( k_j \), . . . , while the arguments on the right side of the bar denote the remaining particles which have zero wave vectors and are therefore uniformly distributed. We assume that \( \rho_{k_i, k_j, \ldots} \) and \( \rho'_{k_i, k_j, \ldots} \) do not depend on the volume \( \Omega \), and that their dependence on the wave vectors is smooth.

In order to emphasize the difference in the volume dependence from the one for local ensembles such as (3.1), we have introduced the new notations \( \rho_{k_i, k_j, \ldots} \) and \( \rho'_{k_i, k_j, \ldots} \) instead of \( \rho_{k_i, k_j, \ldots} \) for the Fourier coefficients in (3.15). Here, the coefficients \( \rho_{k_i, k_j} \) are associated with the homogeneous components of the distribution function in space (i.e., the component where the total wave vector vanishes \( k_i + k_j + \cdots = 0 \)), while the coefficients \( \rho'_{k_i, k_j} \) are associated with the “inhomogeneous” components (with \( k_i + k_j + \cdots \neq 0 \)). This form of expansion leads to an extension of the cluster expansion in terms of the correlation functions in nonequilibrium statistical mechanics: i.e., the coefficients \( \rho_0(p) \), \( \rho_{k_i, k_j}(p) \), \( \rho_{k_i, k_j, k_n}(p) \), . . . are just the Fourier components of the momentum distribution functions (which corresponds to the “vacuum of correlation”), of the binary correlations, of the ternary correlations, and so on [19,22]. As we have seen, interactions lead to transitions from one set of wave vectors to another. This corresponds to a “dynamics of correlations” [19].

A characteristic feature of the distributions (3.15) is that all reduced quantities are well defined. For example, the expectation value of \( q_1 - q_2 \) is given by (in the thermodynamic limit)

\[
\int dq_1 \int dp_1 \int dq_2 \int dp_2 \rho(q_1, q_2) = -i \left[ \frac{\partial}{\partial k} \int dp \rho_{k, -k}(p) \mid p^{N-2} \right]_{k=0}.
\]

(3.16)

Assuming a finite range of correlation, this quantity is finite.

An important aspect of this class of distribution functions is its stability during the time evolution. Indeed, dynamics of correlation leaves the form (3.15) invariant. For example, let
us assume that the system is initially in the vacuum of correlation. Because of the volume
dependence in (2.14), we first note the relation between the Fourier coefficients \( \rho_k(p) \) and the
\((k,p)\)-components \( \langle k, p | \rho \rangle \) of the distribution function

\[
\langle 0,0 | \rho \rangle = \frac{1}{L^{3N/2}} \rho_0(|p|),
\]

\[
\langle k, -k, \{0\}^{N-2} | \rho \rangle \delta_{ij}(k) = \frac{1}{L^{3N/2}} \frac{1}{\Omega} \rho_{k,-k, \{0\}^{N-2}}(p_i, p_j | p^{N-2}), \tag{3.17}
\]

Also,

\[
\langle k, k, \{0\}^{N-2} | \lambda L | \rho \rangle = \int dp' \langle k, k, \{0\}^{N-2}, p | \lambda L | 0, p' \rangle \langle 0, p' | \rho \rangle

- \frac{1}{L^{3N/2}} \frac{1}{\Omega} \lambda V[\{k_i\}] \cdot d_j n (p) \delta_{ij} + \delta_{ij}.
\]

This gives the same volume dependence as in the second expression in (3.17). One can extend
this result to all orders of \( \lambda \) and to all Fourier components (see [19,22] for more detail). This
is quite remarkable. Indeed, as we shall see later, this is the only class of distribution functions
which is stable in this sense in the thermodynamic limit (see Sections 6 and 11).

We note the distribution function (3.15) satisfies (3.3). In contrast, the Hilbert space norm
of (3.15) vanishes as in the thermodynamic limit

\[
\langle \rho | \rho \rangle = \frac{1}{L^{3N}} \left( \int dp | \rho_0(p)|^2 + \frac{1}{\Omega^2} \sum_j \sum_k \int dp | \rho_k(p_j | p^{N-1})|^2 + \cdots \right) \to 0. \tag{3.19}
\]

Hence, distributions of this class do not belong to the Hilbert space.

Also observables \( M \) which depend on a reduced number \( r < N \) of coordinates have a delta
function singularity in their Fourier expansion as (for \( s \leq N \))

\[
M(q_1, \ldots, q_r, p_1, \ldots, p_s) = \frac{1}{\Omega^N} \sum_k e^{ik \cdot q} M_k(p_1, \ldots, p_s) \delta_\Omega(k_{r+1}) \cdots \delta_\Omega(k_N). \tag{3.20}
\]

To investigate the time evolution of this class of phase functions, it is convenient to introduce
projection operator \( P_{a}^{(v)} \) which extracts single eigenmodes of the unperturbed Liouvillian in the
Fourier expansion of the phase functions

\[
P^{(0)} = \int dp \langle k, p | \langle k, p | \delta_{ij}(k) \rangle, \quad P_{ij}^{(k, k_i, -k_j)} = \int dp \langle k, p | \delta_{k_i, k_j} \rangle, \quad \cdots,

P_{ij}^{(k)} = \int dp \langle k, p | \delta_{ij}^{(k)} \rangle, \quad P_{ij}^{(k, k_j)} = \int dp \langle k, p | \delta_{ij}^{(k)} \rangle, \cdots. \tag{3.21}
\]

The index \( a \) in \( P_{a}^{(v)} \) denotes the particles associated with nonvanishing wave vectors, while the
index \( v \) denotes the value of their wave vectors. The projection operators in the first line in (3.21)
extract the homogeneous components in the Fourier expansion of the phase functions, while the
projection operators in the second line in (3.21) extract the inhomogeneous components of the
phase functions.

Note that the momentum \( \hat{p}_j \) as defined in (2.7) lies in the vacuum of correlation subspace \( P^{(0)} \),

\[
\langle \hat{p}_j \rangle = \int dq \int dp \int dp' \sum_k P_{j} (q, p | k, p') \langle k, p' | = L^{3N/2} \int dp \hat{p}_j \langle 0, p | P^{(0)}. \tag{3.22}
\]
The projection operators $P_a^{(\nu)}$ commute with the unperturbed Liouvillian
\[ L_0 P_a^{(\nu)} = (k \cdot v) P_a^{(\nu)} = P_a^{(\nu)} L_0. \] (3.23)
Moreover,
\[ P_a^{(\nu)} P_b^{(\mu)} = P_a^{(\nu)} \delta_{\nu,\mu} \delta_{a,b}, \quad \sum_\nu \sum_a P_a^{(\nu)} = 1. \] (3.24)

To shorten the notation, we have not written the delta functions for the momenta (cf. (2.17)).

We also introduce the projection operators $Q_a^{(\nu)}$,
\[ Q_a^{(\nu)} = 1 - P_a^{(\nu)}, \] (3.25)
which are orthogonal to $P_a^{(\nu)}$, i.e.,
\[ P_a^{(\nu)} Q_a^{(\nu)} = Q_a^{(\nu)} P_a^{(\nu)} = 0. \] (3.26)

We note that
\[ P_a^{(\nu)} L_0 P_a^{(\nu)} = 0. \] (3.27)

In the following discussion, we shall often use the notation
\[ P^{(\nu)} = |\nu\rangle \langle \nu|, \] (3.28)
as well as $l_\nu$ for the eigenvalue of $L_0$. Then, the spectral decomposition of the $L_0$ is
\[ L_0 = \sum_\nu |\nu\rangle l_\nu \langle \nu|. \] (3.29)

We come now to the main problem, the study of the spectral representation of $L_H$ in the extended function space.

4. COMPLEX SPECTRAL REPRESENTATION OF THE LIOUVILLIAN—THE RIGHT EIGENSTATES

For nonintegrable systems, the spectral decomposition of the Liouvillian corresponding to the Hamiltonian (1.1) in Hilbert space is generally not known. In contrast, we shall give the solution of the eigenvalue problem for the Liouvillian for the class of functions with singularities in their Fourier transforms. As these functions have no Hilbert space norm (3.19), we have to extend the eigenvalue problem outside the Hilbert space. This has already done in the case of deterministic chaos [13–18]. Our extension introduced here is quite natural, as the class of functions we consider includes the equilibrium distributions. As we shall see, in this extended function space, the Liouvillian has "complex" eigenvalues. That means that time-symmetry is broken. We may therefore expect that this complex spectral representation allows us to describe irreversible processes such as the approach to equilibrium. Our spectral representation makes explicit the role of Poincaré resonances which lead to collision operators of the Fokker-Planck type. As a special case with no singular Fourier components, we recover the spectral representation in the Hilbert space.

We consider the eigenvalue problem [5]
\[ L_H |F_\alpha^{(\nu)}(\lambda)\rangle = Z_\alpha^{(\nu)} |F_\alpha^{(\nu)}(\lambda)\rangle, \] (4.1)
with the boundary condition
\[ |F_\alpha^{(\nu)}(\lambda)\rangle \to P^{(\nu)} |F_\alpha^{(\nu)}(0)\rangle, \quad \text{for } \lambda \to 0. \] (4.2)

The indices $\alpha$ (together with $\nu$) are the parameters characterizing the eigenfunctions.
As we shall show, the eigenvalues $Z_\alpha^{(\nu)}$ are generally complex numbers. The time evolution of LPS splits into two semigroups. For the semigroup corresponding to $t > 0$, the eigenstates are associated with the eigenvalues with $\text{Im } Z_\alpha^{(\nu)} \leq 0$ (including the case $\text{Im } Z_\alpha^{(\nu)} < 0$) and equilibrium is reached in our future for $t \to +\infty$, while for the other the eigenvalues are the complex conjugate of $Z_\alpha^{(\nu)}$ and equilibrium is reached in our past. Experience shows that all irreversible processes have the same time orientation. To be self-consistent, we have to choose the semigroup oriented towards our future.

For complex eigenvalues, the left eigenstates of $L_H$ are not the Hermitian conjugate of the right eigenstates. Let us denote the left eigenstates corresponding to the same eigenvalue $Z_\alpha^{(\nu)}$ by $\langle \tilde{\hat{F}}^{(\nu)}_\alpha |$, i.e.,

$$\langle \tilde{\hat{F}}^{(\nu)}_\alpha | L_H = \langle \tilde{\hat{F}}^{(\nu)}_\alpha | Z_\alpha^{(\nu)} ,$$

again with the boundary condition

$$\langle \tilde{\hat{F}}^{(\nu)}_\alpha (\lambda) | \to \langle \tilde{\hat{F}}^{(\nu)}_\alpha (0) | F^{(\nu)} , \quad \text{for } \lambda \to 0 .$$

We assume the biorthogonality and bicompleteness relations

$$\langle \langle \tilde{\hat{F}}^{(\nu)}_\alpha | F^{(\mu)}_\beta \rangle \rangle = \delta_{\nu,\mu} \delta_{\alpha,\beta} , \quad \sum_{\nu} \sum_{\alpha} | F^{(\nu)}_\alpha \rangle \langle F^{(\nu)}_\alpha | = 1 .$$

We assume also that the eigenstates of the Liouvillian are not degenerate for the different indices of $\nu$ and $\alpha$. The biorthogonality relation is the direct consequence of the assumption of nondegeneracy. This assumption, as well as bicompleteness of the eigenstates, should be verified for each specific Hamiltonian.\(^6\)

Moreover, we assume that the Liouvillian is diagonalizable

$$L_H = \sum_{\nu} \sum_{\alpha} | F^{(\nu)}_\alpha \rangle \langle F^{(\nu)}_\alpha | .$$

In this paper, we shall not consider more general situations which would lead to Jordan blocks (see [18,32]).

Let us first consider the eigenvalue problem (4.1) for the right eigenstates. As mentioned, we consider eigenfunctions which have the structure (3.15). We limit ourselves to homogeneous situations where the eigenfunctions are translationally invariant. We shall therefore study the eigenvalue problem for functions characterized by the singular Fourier expansions (abbreviating the argument $\lambda$):

$$\langle \langle q,p | F^{(\nu)}_\alpha \rangle \rangle = \frac{1}{L^{3N/2}} \sum_{k} e^{ikq} \left[ F^{(\nu)}_0 (p,\alpha) \delta^{kr}(k) + \frac{1}{\Omega} \sum_{j>i}^{N} F^{(\nu)}_{k_i,k_j}(p,\alpha) \delta_{k_i+k_j} \delta^{kr}(k) \right. \left. + \frac{1}{\Omega^2} \sum_{n>j>i} F^{(\nu)}_{k_i,k_j,k_n}(p,\alpha) \delta_{k_i+k_j+k_n} \delta^{kr}(k) + \cdots \right] .$$

We assume that the Fourier coefficients $F^{(\nu)}_{k_i,k_j,\cdots}$ do not depend on the volume in the limit of the large volumes $\Omega \to \infty$. $F^{(\nu)}_0$ corresponds to the vacuum of correlation, $F^{(\nu)}_{k_i,-k_i}$ to binary correlations, $\cdots$ as $\rho$ in (3.15).

Note that the eigenstates $| F^{(\nu)}_\alpha \rangle$ for $\lambda \neq 0$ contain components in the range of all projection operators $P^{(\nu)}$. We call $P^{(\nu)} | F^{(\nu)}_\alpha \rangle$ the “privileged” component of $| F^{(\nu)}_\alpha \rangle$.

\(^6\)The proof of the biorthogonality and bicompleteness for the complex spectral representation for the quantum Friedrichs model as well as potential scattering can be found in [5,9,11].
We formulate the eigenvalue problem for an arbitrary number $N$ of particles, including $N \rightarrow \infty$. For this case, special care is necessary, as the perturbed Liouvillian $L_V$ in (2.22) contains $N^2$ terms involving all pairs of particles $j$ and $n$. We therefore take the inner product of the eigenvalue equation (4.1) with observables (3.20) which depend on an arbitrary but finite number of particles:

$$\langle \langle \hat{M} | L_H | F^{(\nu)}_\alpha \rangle \rangle = Z^{(\nu)}_\alpha \langle \langle \hat{M} | F^{(\nu)}_\alpha \rangle \rangle. \quad (4.8)$$

This operation reduces the number of pairs and leads to a finite contribution in the thermodynamic limit (1.2). In our discussion of the eigenvalue problem, we shall always understand our formulae as in (4.8). We shall come back to this problem later in Sections 8 and 10 (see also [19]).

Applying the projection operators $P^{(\nu)}_\alpha$ and $Q^{(\nu)}_\alpha$ in (3.25) to (4.1), we derive the set of equations

$$P^{(\nu)}_\alpha L_H \left( P^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle + Q^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle \right) = Z^{(\nu)}_\alpha P^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle, \quad (4.9a)$$

$$Q^{(\nu)}_\alpha L_H \left( P^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle + Q^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle \right) = Z^{(\nu)}_\alpha Q^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle. \quad (4.9b)$$

Equation (4.9b) leads to

$$\left( Z^{(\nu)}_\alpha - Q^{(\nu)}_\alpha L_H Q^{(\nu)}_\alpha \right) Q^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle = Q^{(\nu)}_\alpha \lambda L_V P^{(\nu)}_\alpha | F^{(\nu)}_\alpha \rangle \rangle. \quad (4.10)$$

Hence, we obtain for $Q^{(\nu)}_\alpha | F^{(\nu)}_\alpha (z) \rangle \rangle$

$$Q^{(\nu)}_\alpha | F^{(\nu)}_\alpha (z) \rangle \rangle = C^{(\nu)}(z) P^{(\nu)}_\alpha | F^{(\nu)}_\alpha (z) \rangle \rangle, \quad (4.11)$$

where

$$C^{(\nu)}(z) = \frac{-1}{Q^{(\nu)}_\alpha L_H Q^{(\nu)}_\alpha - z} Q^{(\nu)}_\alpha \lambda L_V P^{(\nu)}_\alpha. \quad (4.12)$$

If this geometrical series converges, we have

$$C^{(\nu)}(z) = \sum_{n=0}^{\infty} \left( \frac{-1}{L_0 - z} Q^{(\nu)}_\alpha \lambda L_V Q^{(\nu)}_\alpha \right)^n \frac{-1}{L_0 - z} Q^{(\nu)}_\alpha \lambda L_V P^{(\nu)}_\alpha. \quad (4.13)$$

This expansion for $C^{(\nu)}$ corresponds to a sequence of "irreducible transitions", as the intermediate states are orthogonal to the initial state in the space $P^{(\nu)}_\alpha$ (see [19]). The operator $C^{(\nu)}_\alpha$ is called the "creation-of-correlation" operator, or "creation operator" for short. The creation operator describes off-diagonal transitions from $P^{(\nu)}_\alpha$ to orthogonal states in $Q^{(\nu)}_\alpha$ subspace

$$C^{(\nu)}(z) = Q^{(\nu)}_\alpha C^{(\nu)}(z) P^{(\nu)}_\alpha. \quad (4.14)$$

The substitution of $z$ by $Z^{(\nu)}_\alpha$ leads to a solution of (4.10). However, we have to be careful with the analytic continuation of $(z - L_0)^{-1}$ in (4.13) to avoid divergences associated with the Poincaré resonances [12]. This is achieved using the so-called "ic-rule" for the analytic continuation [18,30,35]. For two-body scattering (or potential scattering) considered in our previous article [5], we have proved that the ic-rule follows from the biorthogonality condition of the eigenstates of the Liouvillian. Let us recall the ic-rule for the two-body scattering [5] (see also [35]). In order to specify the analytic continuation in accordance with the ic-rule, we define the index $d_\nu$ of the "degree of correlation" of the unperturbed state $| \nu \rangle$ as the integer which is the minimum number of interactions $\lambda L_V$ required to raise the state $| \nu \rangle$ from the state $| 0, p \rangle$, the "vacuum of correlation". The degree of the correlation for $| 0, p \rangle$ is $d_0 = 0$. The second term of the Fourier component in (4.7) corresponds to $d_\nu = 1$, and the third term to $d_\nu = 2$, and so on.
For the two-body scattering, the maximum order of correlation is $d_{\nu} = 1$. Then the orthogonality condition for the eigenstates of $L_{H}$ uniquely determines the analytic continuation of the propagators for $t > 0$ as [5]

$$\lim_{\Omega \to \infty} \langle \mu | \lambda L_{V} | \nu \rangle = 0. \quad (4.15)$$

Here, $\epsilon_{\mu \nu}$ is defined by

$$\epsilon_{\mu \nu} = \begin{cases} -i \epsilon, & \text{for } d_{\mu} \geq d_{\nu}, \\ +i \epsilon, & \text{for } d_{\mu} < d_{\nu}, \end{cases} \quad (4.16)$$

and $\epsilon$ is a positive infinitesimal $\epsilon \to 0^+$. This limit should be taken after the limit to the continuous spectrum $\Omega \to \infty$. Hereafter, we shall always understand the limit in this sense.

We can generalize this result for the complex eigenvalues $Z_{\alpha}^{(\nu)}$ with finite imaginary parts (instead of $-i \epsilon$) in terms of geometrical series. Corresponding to (4.15), we introduce the notation

$$P^{(\mu)} \frac{-1}{(l_{\mu} - Z_{\alpha}^{(\nu)}) C_{\mu \nu}} \equiv P^{(\mu)} \frac{-1}{[l_{\mu} - Z_{\alpha}^{(\nu)}]^{n+1}}, \quad \text{for } d_{\mu} > d_{\nu}, \quad (4.17a)$$

$$P^{(\mu)} \frac{-1}{(l_{\mu} - Z_{\alpha}^{(\nu)}) C_{\mu \nu}} \equiv P^{(\mu)} \frac{-1}{l_{\mu} - Z_{\alpha}^{(\nu)}}, \quad \text{for } d_{\mu} < d_{\nu}, \quad (4.17b)$$

Here,

$$\int_{\mathbb{R}} dw \frac{f(w)}{[w - z]^{n+1}} = \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \int_{\mathbb{R}} dw \frac{(-i \epsilon)^{n+1}}{(w - w' - i \epsilon)^{n+1}} f(w), \quad (4.18)$$

and

$$\int_{\mathbb{R}} dw \frac{f(w)}{w - Z_{\alpha}^{(\nu)}} = \lim_{\epsilon \to 0^+} \sum_{n=0}^{\infty} \int_{\mathbb{R}} dw \frac{(-i \epsilon)^{n}}{(w - w' + i \epsilon)^{n+1}} f(w), \quad (4.19)$$

where $Z_{\alpha}^{(\nu)} = w' - i \gamma$ with $w'$ and $\gamma \geq 0$ real, and the integrations are performed with a suitable test functions $f(w)$ on the real axis $\mathbb{R}$. We can perform the summation of the geometrical series (4.18) by introducing the “complex distribution” defined by [8]

$$\int_{\mathbb{R}} dw \frac{f(w)}{[w - z]^{n+1}} = \lim_{z \to z_{\alpha}^{(\nu)}} \int_{\mathbb{R}} dw \frac{f(w)}{w - z}. \quad (4.20)$$

Here, $z \downarrow Z_{\alpha}^{(\nu)}$ means that we first evaluate the integration in the upper-half plane of $z$ (i.e., $\text{Im} z > 0$), then take the limit $z \to Z_{\alpha}^{(\nu)}$ in the lower-half plane [2].

There is another branch of the analytic continuation in (4.13), which corresponds to the complex conjugate of (4.17). But we shall not consider this branch, as this leads to the eigenstates belonging to the other semigroup oriented towards our past.

Then, with (4.17) we have the solution of (4.10)

$$Q^{(\nu)} | F_{\alpha}^{(\nu)} \rangle = C^{(\nu)} \left( Z_{\alpha}^{(\nu)} \right) P^{(\nu)} | F_{\alpha}^{(\nu)} \rangle, \quad (4.21)$$

where

$$P^{(\mu)} C^{(\nu)} \left( Z_{\alpha}^{(\nu)} \right) P^{(\nu)} = P^{(\mu)} \frac{-1}{(l_{\mu} - Z_{\alpha}^{(\nu)}) C_{\mu \nu}} T^{(\nu)} \left( Z_{\alpha}^{(\nu)} \right) P^{(\nu)}. \quad (4.22)$$

Here we have introduced the “$T$-matrix” which is defined as the solution of the equation

$$T^{(\nu)}_{\alpha} (z) = \lambda Q^{(\nu)} L_{V} + \sum_{\mu} \lambda Q^{(\nu)} L_{V} P^{(\mu)} \frac{-1}{(l_{\mu} - z) C_{\mu \nu}} T^{(\nu)}_{\alpha} (z). \quad (4.23)$$
Substituting (4.21) into (4.9b), we obtain the nonlinear equation [32]

$$
\psi^{(\nu)} \left( Z^{(\nu)}_\alpha | u^{(\nu)}_\alpha \right) = Z^{(\nu)}_\alpha | u^{(\nu)}_\alpha \right),
$$

(4.24)

where

$$
| u^{(\nu)}_\alpha \rangle = P^{(\nu)} | F^{(\nu)}_\alpha \rangle.
$$

(4.25)

Equation (4.25) implies

$$
L_0 | u^{(\nu)}_\alpha \rangle = \nu | u^{(\nu)}_\alpha \rangle.
$$

(4.26)

Here, $\psi^{(\nu)}$ is the generalization of "collision operator" familiar from nonequilibrium statistical mechanics [19]. This operator is associated with diagonal transitions between two states corresponding to the same projection operator $P^{(\nu)}$. The collision operator is defined through

$$
\psi^{(\nu)} \left( Z^{(\nu)}_\alpha \right) = L_0 P^{(\nu)} + \lambda P^{(\nu)} L_V C^{(\nu)} \left( Z^{(\nu)}_\alpha \right) P^{(\nu)}.
$$

(4.27)

Assuming completeness in the space $P^{(\nu)}$, we may always construct a set of states $\{\langle \tilde{u}^{(\nu)}_\alpha | \rangle\}$ biorthogonal to $\{|u^{(\nu)}_\alpha \rangle\}$, i.e.,

$$
\langle \tilde{u}^{(\nu)}_\alpha | u^{(\nu)}_\beta \rangle = \delta_{\alpha,\beta} \delta_{\nu,\beta}, \quad \sum_\alpha \langle u^{(\nu)}_\alpha | \tilde{u}^{(\nu)}_\alpha \rangle = P^{(\nu)}.
$$

(4.28)

We have

$$
\langle \tilde{u}^{(\nu)}_\alpha | L_0 = \langle \tilde{u}^{(\nu)}_\alpha | \nu.
$$

(4.29)

We note that the states $\langle \tilde{u}^{(\nu)}_\alpha |$ are generally not the left eigenstates of $\psi^{(\nu)} \left( Z^{(\nu)}_\alpha \right)$ (see [31]).

Let us then introduce the "global" collision operator by

$$
\tilde{\theta}^{(\nu)}_C \equiv \sum_\alpha \psi^{(\nu)} \left( Z^{(\nu)}_\alpha \right) | u^{(\nu)}_\alpha \rangle \langle \tilde{u}^{(\nu)}_\alpha | = \sum_\alpha | u^{(\nu)}_\alpha \rangle \langle \tilde{u}^{(\nu)}_\alpha | Z^{(\nu)}_\alpha \langle \tilde{u}^{(\nu)}_\alpha |,
$$

(4.30)

as well as the "global" creation operator,

$$
C^{(\nu)} \equiv \sum_\alpha C^{(\nu)} \left( Z^{(\nu)}_\alpha \right) | u^{(\nu)}_\alpha \rangle \langle \tilde{u}^{(\nu)}_\alpha |.
$$

(4.31)

We shall call also $\tilde{\theta}^{(\nu)}_C$ the collision operator and $C^{(\nu)}$ the creation operator for simplicity, as far as no confusion is possible. Then we have [33]

$$
\tilde{\theta}^{(\nu)}_C = L_0 P^{(\nu)} + \lambda P^{(\nu)} L_V C^{(\nu)} P^{(\nu)},
$$

(4.32)

and

$$
\langle \tilde{u}^{(\nu)}_\alpha | \tilde{\theta}^{(\nu)}_C | u^{(\nu)}_\alpha \rangle = Z^{(\nu)}_\alpha | u^{(\nu)}_\alpha \rangle, \quad \langle \tilde{u}^{(\nu)}_\alpha | \tilde{\theta}^{(\nu)}_C | \tilde{u}^{(\nu)}_\alpha \rangle = \langle \tilde{u}^{(\nu)}_\alpha | Z^{(\nu)}_\alpha | u^{(\nu)}_\alpha \rangle.
$$

(4.33)

Therefore, $| u^{(\nu)}_\alpha \rangle$ and $\langle \tilde{u}^{(\nu)}_\alpha |$ are right and left eigenstates of the global collision operator, respectively.

With the creation operator, we have also

$$
Q^{(\nu)} \left| F^{(\nu)}_\alpha \rightangle = Q^{(\nu)} C^{(\nu)} P^{(\nu)} \left| F^{(\nu)}_\alpha \rightangle.
$$

(4.34)

Formula (4.25) shows that the privileged components $P^{(\nu)} \left| F^{(\nu)}_\alpha \rightangle$ are eigenstates of the collision operator, which has the same eigenvalues $Z^{(\nu)}_\alpha$ as the Liouvillian. The solution of the eigenvalue problem of the Liouvillian for our class of singular functions (4.7) has unique features. The privileged components satisfy closed equations and the $Q^{(\nu)}$ components are "driven" by the
privileged components (see (4.34)). In the previous work on subdynamic theory (for nonequilibrium statistical mechanics as well as for deterministic chaos), this property has been presented as an “ansatz” [18,35]. Here we derive this property through the complex spectral representation of $L_H$ for the singular class of eigenstates (4.7).

The collision operators are dissipative operators, and they are the central objects of nonequilibrium statistical mechanics [19,22]. Of special interest is $\theta_C^{(0)}$ corresponding to the vacuum of correlations, as it leads to well-known kinetic equations for the momentum distribution function in the thermodynamic limit; e.g., for weakly coupling limit, $\theta_C^{(0)}$ reduces to the Fokker-Planck operator

$$\theta_C^{(0)} \approx \lambda^2 \theta_2^{(0)} = \lambda^2 P^{(0)} L_V Q^{(0)} \frac{1}{i \epsilon - L_0} Q^{(0)} L_V P^{(0)},$$

which gives

$$\lambda^2 \langle \langle 0, p | \theta_2^{(0)} | 0, p' \rangle \rangle = \lim_{\alpha \to -\infty} \frac{\lambda^2}{\alpha^2} \sum_{j > n}^N \sum_k |V_k|^2 k \cdot d_{jn} \pi \delta (k \cdot g_{jn}) k \cdot d_{jn} \delta (p - p'),$$

where

$$g_{jn} \equiv v_j - v_n.$$

Also in the low concentration limit, $\theta_C^{(0)}$ reduces to the collision operator of the Boltzmann equation [19].

The Fokker-Planck operator (4.35) is an anti-Hermitian operator and has nonvanishing negative imaginary eigenvalues (i.e., $\text{Im} \, Z^{(0)}_\alpha < 0$) associated with diffusive processes in momentum space (see [19,22]). This illustrates the consistency of our construction of the eigenstates of the Liouvillian with $\text{Im} \, Z^{(0)}_\alpha < 0$. Moreover, the contribution of the Fokker-Planck operator comes from the integration over wave vectors satisfying Poincaré’s resonances condition $k \cdot g_{jn} = 0$. This means that the dissipation has a dynamical origin associated with “nonintegrability” of LPS due to Poincaré’s resonances. The Fokker-Planck operator leads to “Brownian motion”. Instead of separate dynamical events described by each interaction $XL_v$, we have events “coupled” by the resonance condition $\delta (k \cdot g_{jn})$. The diffusion process is “irreducible” to trajectory dynamics. We have “non-Newtonian” processes due to the Poincaré resonances.

In the correlation subspace $P^{(\nu)}$, the collision operators $\theta_C^{(\nu)}$ leads to a natural generalization of the kinetic theory. In general, the denominators in the operators involves both directions of the analytic continuation (4.17). Nevertheless, the analytic continuations of the diagonal operators, such as $\theta_C^{(\nu)}$, are uniquely determined in the thermodynamic limit by the complex distributions (4.17a). This is the result of the so-called Henin’s theorem [26]; i.e., for the diagonal transition between the states in $P^{(\nu)}$, the intermediates states should correspond to higher degree of correlation than $P^{(\nu)}$. Indeed, the diagonal transition restricts the wave vector transfer and leads to extra volume factors $\Omega^{-1}$ through the interaction (see (2.22)). The diagonal transitions give nonvanishing contributions only when the intermediate states involve more particles than the states in $P^{(\nu)}$, as the summation over the particles leads to extra factor $N$ which then compensates the factor $\Omega^{-1}$. We then obtain, for example, to the lowest order contribution of $\theta_C^{(\nu)}$ (i.e., to $\lambda^2$ order),

$$\theta_C^{(\nu)} \approx L_0 P^{(\nu)} + \lambda^2 \theta_2^{(\nu)} = L_0 P^{(\nu)} + \lambda^2 P^{(\nu)} L_V Q^{(\nu)} \frac{1}{L_v + i \epsilon - L_0} Q^{(\nu)} L_V P^{(\nu)}.$$  

Combining (4.34) with (4.25), we obtain the right eigenstates (4.1) of the Liouvillian,

$$|F^{(\nu)}_\alpha \rangle \rangle = N^{(\nu)}_\alpha 1/2 \left( P^{(\nu)} + C^{(\nu)} \left( F^{(\nu)}_\alpha \right) \right) |n^{(\nu)}_\alpha \rangle \rangle = N^{(\nu)}_\alpha 1/2 \left( P^{(\nu)} + C^{(\nu)} \right) |n^{(\nu)}_\alpha \rangle \rangle,$$

where $N^{(\nu)}_\alpha$ is a normalization constant which we shall specify later (see (5.17)).
Let us note that (4.24) is a "nonlinear eigenvalue problem", as the collision operator \( \psi^{(\nu)} \) itself depends on \( Z^{(\nu)}_\alpha \). Unknown eigenvalues \( Z^{(\nu)}_\alpha \) appear in the propagator inside the collision operator. This corresponds to Brillouin-Wigner's formulation of the eigenvalue problem of the Hamiltonian \( H \) for integrable quantum systems when the eigenvalues are real. We can extend this formulation to the eigenvalue problem of \( L_H \) for nonintegrable classical systems [8]. The Brillouin-Wigner theory gives a systematic approximation scheme for the solution of the eigenvalue problem. In Section 8, we shall also construct a nonlinear equation [18] for \( C^{(\nu)} \), through which we can determine the explicit form of the creation operator by a perturbation series in powers of \( \lambda \) (see (8.3)).

Replacing \( P^{(\nu)} \) by the projection operators corresponding to the inhomogeneous components, the construction of eigenstates associated with the inhomogeneous situation is straightforward, and we do not repeat the calculations. We now turn to the left eigenstates of \( L_H \).

5. COMPLEX SPECTRAL REPRESENTATION OF THE LIOUVILLIAN THE LEFT EIGENSTATES

Let us now consider the eigenvalue problem (4.3) for the left eigenstates. As for the right eigenstates, we obtain

\[
\langle \langle \bar{\Phi}^{(\nu)}_\alpha \mid = \langle \langle \bar{\varphi}^{(\nu)}_\alpha \mid \left(P^{(\nu)} + D^{(\nu)} \left(Z^{(\nu)}_\alpha \right)\right)N^{(\nu)}_\alpha \nu^{1/2} = \langle \langle \bar{\varphi}^{(\nu)}_\alpha \mid \left(P^{(\nu)} + D^{(\nu)} \right)N^{(\nu)}_\alpha \nu^{1/2}. \tag{5.1}\]

The operator \( D^{(\nu)}(Z^{(\nu)}_\alpha) \) is called the "destruction-of-correlation" operator, or "destruction operator" for short. This operator is defined by

\[
P^{(\nu)} D^{(\nu)} \left(Z^{(\nu)}_\alpha \right) P^{(\mu)} = P^{(\nu)} T^{(\nu)}_D \left(Z^{(\nu)}_\alpha \right) \frac{1}{\left(Z^{(\nu)}_\alpha - l_\mu \right) D_{\mu \nu}}, \tag{5.2}\]

where we have introduced the "T-matrix" similar to (4.23),

\[
T^{(\nu)}_D(z) = \lambda I_{\nu} Q^{(\nu)} + \sum_\mu T^{(\nu)}_D(z) \frac{1}{(z - l_\mu) D_{\mu \nu}} P^{(\mu)} \lambda L_{\nu} Q^{(\nu)}, \tag{5.3}\]

using the analytic continuation given by (cf. (4.17))

\[
\frac{1}{\left(Z^{(\nu)}_\alpha - l_\mu \right) D_{\mu \nu}} P^{(\mu)} \equiv \frac{1}{[z - l_\mu]^{+} Z^{(\nu)}_\alpha} P^{(\mu)}, \quad \text{for } d_\nu < d_\mu, \tag{5.4a}\]

\[
\frac{1}{\left(Z^{(\nu)}_\alpha - l_\mu \right) D_{\mu \nu}} P^{(\mu)} \equiv \frac{1}{Z^{(\nu)}_\alpha - l_\mu} P^{(\mu)}, \quad \text{for } d_\nu \geq d_\mu. \tag{5.4b}\]

Again \( D^{(\nu)}(z) \) corresponds to the off-diagonal transitions (see (4.14))

\[
D^{(\nu)}(z) = P^{(\nu)} D^{(\nu)}(z) Q^{(\nu)}. \tag{5.5}\]

\( D^{(\nu)} \) is the global destruction operator defined below (see (5.12)). We have

\[
\langle \langle \bar{\varphi}^{(\nu)}_\alpha \mid = \langle \langle \bar{\Phi}^{(\nu)}_\alpha \mid P^{(\nu)}, \tag{5.6}\]

and

\[
\langle \langle \bar{\Phi}^{(\nu)}_\alpha \mid Q^{(\nu)} = \langle \langle \bar{\Phi}^{(\nu)}_\alpha \mid P^{(\nu)} D^{(\nu)} \left(Z^{(\nu)}_\alpha \right) = \langle \langle \bar{\Phi}^{(\nu)}_\alpha \mid P^{(\nu)} D^{(\nu)} \right. \tag{5.7}\]
\[ \langle \tilde{v}_\alpha^{(\nu)} \rangle \text{ are the left eigenstates of the collision operator } \psi^{(\nu)}, \]
\[ \langle \tilde{v}_\alpha^{(\nu)} \rangle \psi^{(\nu)} \left( Z_\alpha^{(\nu)} \right) = \langle \tilde{v}_\alpha^{(\nu)} \rangle Z_\alpha^{(\nu)}, \quad (5.8) \]

where
\[ \psi^{(\nu)} \left( Z_\alpha^{(\nu)} \right) = P^{(\nu)} L_0 + \lambda P^{(\nu)} D^{(\nu)} \left( Z_\alpha^{(\nu)} \right) I_\nu P^{(\nu)} \quad (5.9) \]

We note that the analytic continuations in (5.4) lead to the same collision operator as (4.27).

We denote by \( |v_\alpha^{(\nu)} \rangle \) the functions which are biorthogonal to \( \langle \tilde{v}_\alpha^{(\nu)} \rangle \). Again we assume
\[ \langle \tilde{v}_\alpha^{(\nu)} | v_\beta^{(\nu)} \rangle = \delta_{\nu,\mu} \delta_{\alpha,\beta}, \quad \sum_{\alpha} |v_\alpha^{(\nu)}\rangle \langle \tilde{v}_\alpha^{(\nu)}| = P^{(\nu)}. \quad (5.10) \]

We have
\[ L_0 |v_\alpha^{(\nu)} \rangle = I_\nu |v_\alpha^{(\nu)} \rangle \], \quad \langle \tilde{v}_\alpha^{(\nu)} | L_0 = \langle \tilde{v}_\alpha^{(\nu)} | I_\nu. \quad (5.11) \]

Then the "global" destruction operator is defined by
\[ D^{(\nu)} = \sum_{\alpha} |v_\alpha^{(\nu)}\rangle \langle \tilde{v}_\alpha^{(\nu)}| D^{(\nu)} \left( Z_\alpha^{(\nu)} \right). \quad (5.12) \]

Similarly to \( C^{(\nu)} \), the operator \( D^{(\nu)} \) satisfies a nonlinear equation given later (see (8.3)). We can also introduce the "global" collision operator (see (4.30))
\[ \theta_D^{(\nu)} = \sum_{\alpha} |v_\alpha^{(\nu)}\rangle \langle \tilde{v}_\alpha^{(\nu)}| = L_0 P^{(\nu)} + \lambda P^{(\nu)} D^{(\nu)} I_\nu P^{(\nu)}. \quad (5.13) \]

We have
\[ \theta_D^{(\nu)} |v_\alpha^{(\nu)} \rangle = Z_\alpha^{(\nu)} |v_\alpha^{(\nu)} \rangle, \quad \langle \tilde{v}_\alpha^{(\nu)} | \theta_D^{(\nu)} = \langle \tilde{v}_\alpha^{(\nu)} | Z_\alpha^{(\nu)}. \quad (5.14) \]

We note that
\[ \theta_D^{(\nu)} = \theta_D^{(\nu)}. \quad (5.15) \]

But both operators share the same eigenvalues \( Z_\alpha^{(\nu)}. \)

One can now determine the normalization constant as follows: as the result of the biorthogonal relation (4.5), we have
\[ \delta_{\alpha,\beta} = \langle \tilde{F}_\alpha^{(\nu)} | F_\beta^{(\nu)} \rangle = \left( N_\alpha^{(\nu)} N_\beta^{(\nu)} \right)^{1/2} \langle \tilde{v}_\alpha^{(\nu)} | \left( P^{(\nu)} + D^{(\nu)} C^{(\nu)} \right) | v_\beta^{(\nu)} \rangle. \quad (5.16) \]

This gives us the normalization constant in (4.39) and (5.1) as
\[ N_\alpha^{(\nu)} = \left[ \langle \tilde{v}_\alpha^{(\nu)} | \left( P^{(\nu)} + D^{(\nu)} C^{(\nu)} \right) | v_\alpha^{(\nu)} \rangle \right]^{-1}. \quad (5.17) \]

Moreover, putting
\[ \left( A^{(\nu)} \right)^{-1} = P^{(\nu)} + D^{(\nu)} C^{(\nu)}, \quad (5.18) \]

we obtain
\[ \left( A^{(\nu)} \right)^{-1} = \sum_{\alpha} |v_\alpha^{(\nu)}\rangle \langle N_\alpha^{(\nu)} \right)^{-1} \langle \tilde{v}_\alpha^{(\nu)}|. \quad (5.19) \]

and its inverse operator in \( P^{(\nu)} \) subspace\(^7\)
\[ A^{(\nu)} = P^{(\nu)} \left( 1 + D^{(\nu)} C^{(\nu)} \right)^{-1} = \sum_{\alpha} |v_\alpha^{(\nu)}\rangle \langle N_\alpha^{(\nu)} \right) \langle \tilde{v}_\alpha^{(\nu)}|. \quad (5.20) \]

\(^7\text{In general, } f(A^{(\nu)}) \neq \sum_{\alpha} |v_\alpha^{(\nu)}\rangle f(N_\alpha^{(\nu)}) \langle \tilde{v}_\alpha^{(\nu)}|. \text{ Therefore, this is not the spectral decomposition of } A^{(\nu)}.\)
Hence, we have

\[ \langle \langle \hat{u}_\alpha^{(\nu)} | A^{(\nu)} | v_\beta^{(\nu)} \rangle \rangle = 2 \delta_{\alpha,\beta} \delta_{\nu,0} = \langle \langle \hat{u}_\alpha^{(\nu)} | A^{(\nu)} \theta_D^{(\nu)} | v_\beta^{(\nu)} \rangle \rangle. \]  

(5.21)

This leads to the intertwining relation of \( A^{(\nu)} \) with the collision operators [24]

\[ \theta_C^{(\nu)} A^{(\nu)} = A^{(\nu)} \theta_D^{(\nu)}. \]  

(5.22)

As mentioned, we have, in general, \( \theta_D^{(\nu)} \neq \theta_C^{(\nu)} \). However, to the lowest order contribution (i.e., to \( \lambda^2 \) order) of \( \theta_D^{(\nu)} \), we obtain the same collision operator as \( \theta_C^{(\nu)} \) in (4.38), i.e.,

\[ \theta_D^{(\nu)} \approx L_0 P^{(\nu)} + \lambda^2 \theta_2^{(\nu)}. \]  

(5.23)

In summary, we have obtained the explicit form of the "complex spectral representation" of \( L_H \) (see (4.6)), and therefore, of the the evolution operator \( U(t) \),

\[ \langle \langle M | U(t) | \rho(0) \rangle \rangle = \sum_\nu \sum_\alpha \langle \langle M | F^{(\nu)}_\alpha \rangle \rangle e^{-i2 \theta_2^{(\nu)} t} \langle \langle \hat{F}^{(\nu)}_\alpha | \rho(0) \rangle \rangle. \]  

(5.24)

This spectral decomposition involves the spectral decomposition of the dissipative collision operators. However, the existence of the collision operator is only a necessary condition to observe irreversibility. To observe dissipation, we have to discuss the class of distribution functions \( \rho \) on which our complex spectral decomposition acts. In the subsequent sections, we shall apply our spectral representation to various situations. In simple cases (finite number of particles and normalizable distributions), we recover the usual results of trajectory dynamics without any dissipation in spite of the fact that we deal with LPS. Still, there are many situations where our new "non-Newtonian" effects can be observed (see Sections 9–12).

6. NONUNITARY TRANSFORMATIONS AND SUBDYNAMICS

Once we have obtained the spectral decomposition (4.6) of \( L_H \), we can construct nonunitary transformation operators which lead to similitude relations between the total Liouvillian \( L_H \) and the collision operators [8,18] (hereafter the index \( B \) stands for \( C \) or \( D \))

\[ \Lambda_B L_H \Lambda_B^{-1} = \Theta_B, \]  

(6.1)

where

\[ \Theta_B \equiv \sum_\nu \theta_B^{(\nu)}. \]  

(6.2)

The nonunitary transformations \( \Lambda \) and their inverses are given by

\[ \Lambda_C = \sum_\nu \sum_\alpha \langle \langle \hat{u}_\alpha^{(\nu)} \rangle \rangle \langle \langle \hat{F}_\alpha^{(\nu)} \rangle \rangle N_\alpha^{(\nu)}/2 = \sum_\nu A^{(\nu)} \hat{\Phi}^D_\nu, \]  

(6.3a)

\[ \Lambda_C^{-1} = \sum_\nu \sum_\alpha \langle \langle \hat{F}_\alpha^{(\nu)} \rangle \rangle \langle \langle \hat{u}_\alpha^{(\nu)} \rangle \rangle N_\alpha^{(\nu)}/2 = \sum_\nu \hat{\Phi}^C_\nu \]  

(6.3b)

and

\[ \Lambda_D = \sum_\nu \sum_\alpha \langle \langle \hat{F}_\alpha^{(\nu)} \rangle \rangle \langle \langle \hat{u}_\alpha^{(\nu)} \rangle \rangle N_\alpha^{(\nu)} /2 = \sum_\nu \hat{\Phi}^D_\nu, \]  

(6.3c)

\[ \Lambda_D^{-1} = \sum_\nu \sum_\alpha \langle \langle \hat{u}_\alpha^{(\nu)} \rangle \rangle \langle \langle \hat{F}_\alpha^{(\nu)} \rangle \rangle N_\alpha^{(\nu)} /2 = \sum_\nu \hat{\Phi}^C_\nu A^{(\nu)} , \]  

(6.3d)

where the operators \( \hat{\Phi}^B_\nu \) are defined by

\[ \hat{\Phi}^C_\nu \equiv P^{(\nu)} + C^{(\nu)}, \quad \hat{\Phi}^D_\nu \equiv P^{(\nu)} + D^{(\nu)}. \]  

(6.4)
Because $L_H$ shares the same eigenvalues with $\theta_{B}(\nu)$, we have the “intertwining relations” [8]

$$L_H \hat{\phi}_\nu^C = \hat{\phi}_\nu^C \theta_{B}(\nu), \quad \hat{\phi}_\nu^D L_H = \theta_{D}(\nu) \hat{\phi}_\nu^D. \quad (6.5)$$

One can easily verify these relations by operating on the eigenstates of the collision operators. We note that the similitude relations (6.1) lead to the intertwining relations (6.5), and vice versa. These relations were already obtained previously [8,18].

As is well known, there exist for integrable systems unitary transformations $U$ which lead to

$$UL_H U^\dagger = L_0. \quad (6.6)$$

We expect that in the situations where dissipative effects are negligible the relations (6.1) would reduce to

$$\Lambda_B L_H \Lambda_B^{-1} = L_0. \quad (6.7)$$

We shall verify this fact later (see (8.15)). However, as the complex spectral representation uses both analytic continuations, (6.7) is not a unitary transformation even for the integrable case. As a result, integrable LPS are diagonalized both through a nonunitary transformation, as well as through a unitary one. We shall come back to this problem in Section 8.

Using $\Lambda$, we may introduce the transformed distribution function $\rho_B$ and the transformed observables $\hat{M}_B$,

$$\langle \rho_B(t) \rangle \equiv \Lambda_B \langle \rho(t) \rangle, \quad \langle \hat{M}_B(t) \rangle \equiv \langle \hat{M}(t) \rangle \Lambda_B^{-1}. \quad (6.8)$$

The new states $\rho_B$ obey (see (6.2))

$$i \frac{\partial}{\partial t} \langle \rho_B(t) \rangle = \Theta_B \langle \rho_B(t) \rangle. \quad (6.9)$$

Since $\theta_{B}(\nu)$ are operators acting on $P^{(\nu)}$ subspace, equation (6.9) actually represents “kinetic equations” for $P^{(\nu)} \langle \rho_B(t) \rangle$ in each correlation subspace,

$$i \frac{\partial}{\partial t} P^{(\nu)} \langle \rho_B(t) \rangle = \theta_{B}(\nu) P^{(\nu)} \langle \rho_B(t) \rangle. \quad (6.10)$$

This represents a set of the kinetic equations of the Fokker-Planck type [19]. Each component $P^{(\nu)} \langle \rho_B(t) \rangle$ evolves independently.

Similarly, the new observables $\hat{M}_B(t)$ obey

$$i \frac{\partial}{\partial t} \langle \hat{M}_B(t) \rangle = \langle \hat{M}_B(t) \rangle \Theta_B, \quad (6.11)$$

which leads again to a set of equations

$$i \frac{\partial}{\partial t} \langle \hat{M}_B(t) \rangle P^{(\nu)} = \langle \hat{M}_B(t) \rangle P^{(\nu)} \theta_{B}(\nu). \quad (6.12)$$

The transformation (6.8) preserves the expectation value of $M$,

$$\langle M \rangle_t = \langle \hat{M}(0) \rangle \rho(t) \rangle = \langle \hat{M}_B(0) \rangle \rho_B(t) \rangle. \quad (6.13)$$

Using the solution of the eigenvalue problem of the collision operator $\theta_{C}(\nu)$, for example, the expectation value is

$$\langle M \rangle_t = \sum_{\nu} \sum_{\omega} \langle \hat{M}_C(0) | u_\omega^{(\nu)} \rangle e^{-i \omega^{(\nu)} t} \langle \hat{u}_\omega^{(\nu)} | \rho_C(0) \rangle. \quad (6.14)$$

---

8In general, the diagonalization of the Liouvillian $L_H$ by unitary transformations leads to a renormalized Liouvillian $L_0'$ (instead of $L_0$) which gives frequency shifts associated with diagonal transitions. However, for the case where there is no bounded motion (i.e., periodic motion), the renormalization effects are negligible as for these interactions they lead to terms of order $\Omega^{-1}$. 

We note that the nonunitary transformations $A$ preserve the reality of the states $\langle q, p | \rho \rangle$ (see [2]). But the transformed states $\langle q, p | \rho_B \rangle$ cannot be considered as probability distribution functions, as $A$ does not preserve positivity. This is a direct consequence of the causal evolution of dynamics combined with the analytic continuations (4.17) and (5.4) (see [2]). However, these states play an important role as they lead to block diagonal equations and permit us to introduce "Lyapounov functions" for dynamical systems (see the next section).

In our earlier work, we have repeatedly introduced the concept of "subdynamics" [24–35]. To see the relation of subdynamics to the complex spectral representation, let us introduce projection operators $\Pi^{(\nu)}$ (see (5.20), (6.3), and (6.4))

$$
\Pi^{(\nu)} = \Lambda_B^{-1} P^{(\nu)} \Lambda_B = \sum_\alpha |F^{(\nu)}_\alpha \rangle \langle F^{(\nu)}_\alpha|.
$$

(6.15)

This leads to the familiar form [24–35]

$$
\Pi^{(\nu)} = \hat{\Phi}_\nu A^{(\nu)} \hat{\Phi}_\nu^D = \left( P^{(\nu)} + C^{(\nu)} \right) A^{(\nu)} \left( P^{(\nu)} + D^{(\nu)} \right).
$$

(6.16)

These operators satisfy the orthogonality and completeness relations,

$$
\Pi^{(\nu)} \Pi^{(\mu)} = \delta_{\nu, \mu}, \quad \sum_\nu \Pi^{(\nu)} = 1,
$$

as well as the commutation relation with $L_H$,

$$
L_H \Pi^{(\nu)} = \Pi^{(\nu)} L_H.
$$

(6.18)

$\Pi^{(\nu)}$ is an extension of $P^{(\nu)}$ to the total Liouvillian $L_H$.

Because these projection operators commute with the Liouvillian, each component $U(t)\Pi^{(\nu)}$ satisfies separate equations of motion,

$$
\langle \hat{M} | U(t) \Pi^{(\nu)} | \rho(0) \rangle = \langle \hat{M} | \hat{\Phi}_\nu e^{-i\theta^{(\nu)}_\nu t} A^{(\nu)} \hat{\Phi}_\nu^D | \rho(0) \rangle = \langle \hat{M} | \hat{\Phi}_\nu A^{(\nu)} e^{-i\theta^{(\nu)}_\nu t} \hat{\Phi}_\nu^D | \rho(0) \rangle.
$$

(6.19)

For this reason, the projection operators $\Pi^{(\nu)}$ are associated with "subdynamics".

As an illustration of subdynamics, let us consider the evolution of a state which is initially in the vacuum of correlations,

$$
| \rho(0) \rangle = P^{(0)} | \rho(0) \rangle.
$$

(6.20)

We now show that the time evolution leads to the correlations which satisfy the volume dependence given in (3.15). From (6.17)–(6.19), we have

$$
| \rho(t) \rangle = \left( P^{(0)} + C^{(0)} \right) e^{-i\theta^{(0)}_1 t} A^{(0)} P^{(0)} | \rho(0) \rangle + \sum_{\nu \neq 0} C^{(\nu)} e^{-i\theta^{(\nu)}_1 t} A^{(\nu)} D^{(\nu)} P^{(0)} | \rho(0) \rangle
$$

(6.21)

$$
= \left( P^{(0)} + \lambda C^{(0)} + \lambda^2 \ldots \right) e^{-i1A^{(0)}_1 t} \left( 1 + \lambda^2 A^{(0)}_2 + \lambda^3 \ldots \right) | \rho(0) \rangle
$$

$$
+ \lambda^2 C^{(2)} e^{-i(L_0 P^{(2)} + \lambda^2 A^{(2)}_2) \nu} D^{(2)} P^{(0)} | \rho(0) \rangle + \lambda^3 \ldots,
$$

where the subscripts $n$ in the operators represent their $\lambda^n$ order contributions, and the superscript $(\nu)$ corresponds to $\nu^{th}$ order correlations. Applying (3.17) and (3.18) to each term in (6.21), one can easily verify that the volume dependence for all correlation components are in agreement with (3.15). The reader can find the detailed estimation of the volume dependence in our earlier articles [19,22]. This shows that the class of singular distribution functions (3.15) is not only form invariant but it acts even as an attractor. In Section 12, we shall see that (3.15) acts as an attractor in the thermodynamic limit even for trajectories.
7. LYAPOUNOV FUNCTIONS—$\mathcal{H}$ THEOREMS

The nonunitary transformations have led to the similitude relation (6.1) between the total Liouvillian $L_H$ and the collision operators. As a consequence, we may introduce transformed states and observables (6.8) whose time evolutions are described only by the $P^{(\nu)}$ components in each correlation subspace. This permits us to introduce “Lyapunov functions” which are the dynamical analogue of Boltzmann's $\mathcal{H}$-function (i.e., “entropy”) for dynamical systems [8,9]. Entropy is the consequence of the complex, irreducible spectral representation of the Liouvillian.

To illustrate this statement, let us consider first the generic reduced single particle momentum distribution function defined by

$$\varphi_1 (p_j, t) = \left< \hat{\varphi}_{p_j} | \rho(t) \right> = \int dp' \delta (p'_j - p_j) \rho_0 (|p', t),$$

(7.1)

with

$$\left< \hat{\varphi}_{p_j} \right> = \int dq \int dp' \delta (p'_j - p_j) \left< q, p' \right> = L^{3N/2} \int dp' \delta (p'_j - p_j) \left< 0, p' \right> |P^{(0)}).$$

(7.2)

where the right-hand side of (7.2) is written in the wave number representation. We have, e.g., (see (3.22))

$$\left< \hat{p}_j \right> = \int dp_j p_j \left< \hat{\varphi}_{p_j} \right>.$$  

(7.3)

We note

$$\left< 0, p' | \hat{\varphi}_{\nu} \right> \left< \hat{\varphi}_{\nu} | \rho \right> = L^{3N/2} \delta (p'_j - p_j) \varphi_1 (p_j).$$

(7.4)

Hence, the Hermitian operator $|\hat{\varphi}_{p_j}\rangle \langle \hat{\varphi}_{p_j}|$ preserves positivity. The reduction does not change the sign of the distribution function.

We now consider the transformed distribution function (see (6.8)), e.g., for $j = 1$,

$$\varphi^B_1 (p_1, t) = \left< \hat{\varphi}_{p_1} | \rho_B(t) \right>.$$ 

(7.5)

Then, a Lyapunov function associated with this distribution function may be defined by

$$\mathcal{H}^B_{\varphi} (t) = \int dp_1 |\varphi^B_1 (p_1, t)|^2,$$

(7.6)

where

$$|\varphi^B_1 (p_1, t)|^2 = \left< \rho(t) | \Lambda^B_1 | \hat{\varphi}_{p_1} \right> \left< \hat{\varphi}_{p_1} | \rho_B(t) \right>.$$ 

(7.7)

We have from (6.10) (e.g., for $B = C$)

$$|\varphi^B_1 (p_1, t)|^2 = \sum_{\alpha, \beta} e^{-i (x^{(0)}_\alpha - x^{(0)}_\beta)} \left< \rho_C(0) | u^{(0)}_\alpha \right> \left< u^{(0)}_\beta | \hat{\varphi}_{p_1} \right> \left< \hat{\varphi}_{p_1} | u^{(0)}_\alpha \right> \left< u^{(0)}_\beta | \rho_C(0) \right>.$$ 

(7.8)

All decay modes are damped for $t > 0$. Moreover, we now show that the damping is monotonous. Taking the time derivative of (7.7), we obtain

$$\frac{\partial}{\partial t} |\varphi^B_1 (p_1, t)|^2 = -\left< \rho_B(t) | \mathcal{K}^{(0)}_B (p_1) | \rho_B(t) \right>,$$

(7.9)

where $\mathcal{K}^{(0)}_B$ is defined by

$$\mathcal{K}^{(0)}_B (p_1) \equiv \left< \hat{\varphi}_{p_1} \right> \left< \hat{\varphi}_{p_1} | i \partial^{(0)}_B \right| \left< \hat{\varphi}_{p_1} \right>.$$ 

(7.10)

The Lyapunov functions are defined for the generic distribution functions. For a trajectory (as an specific distribution function), we have divergence for $|\varphi_1 (p_j)|^2$ because of the square of the delta function of the momentum.

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9 The Lyapunov functions are defined for the generic distribution functions. For a trajectory (as an specific distribution function), we have divergence for $|\varphi_1 (p_j)|^2$ because of the square of the delta function of the momentum.
$\mathcal{K}_B^{(0)}$ is a Hermitian operator. Thus its eigenvalues are real and the left-eigenstates are Hermitian conjugates of the right-eigenstates.\(^{10}\) Let us assume that the spectral decomposition of $\mathcal{K}_B^{(0)}$ is known

$$\mathcal{K}_B^{(0)}(P_1) = \sum_{\beta} \gamma_{\beta}(P_1) \langle w_{\beta}(P_1) \rangle \langle w_{\beta}(P_1) \rangle,$$

(7.11)

where $\gamma_{\beta}$ are real numbers and

$$\langle \langle w_{\beta}(P_1) \rangle w_{\beta}(P_1) \rangle = \delta_{\beta,\beta'},$$

$$\sum_{\beta} \langle w_{\beta}(P_1) \rangle \langle w_{\beta}(P_1) \rangle = \int dp^{N-1} \langle \langle 0, P_1, \{p\}^{N-1} \rangle \rangle \langle \langle 0, P_1, \{p\}^{N-1} \rangle \rangle.$$

(7.12)

As mentioned, the operator $|\varphi_{P_1}\rangle \langle \varphi_{P_1}|$ preserves the positivity. The reduction does not change the sign of the collision operator. Therefore, $\mathcal{K}_B^{(0)}$ is a nonnegative operator, i.e.,

$$\gamma_{\beta}(P_1) \geq 0.$$

(7.13)

Then we have

$$\frac{\partial}{\partial t} |\varphi_{P_1}(P_1, t)\rangle^2 = -\sum_{\beta} \gamma_{\beta}(P_1) \langle \langle w_{\beta}(P_1) \rangle \rho(t) \rangle^2 \leq 0.$$

(7.14)

The evolution of $|\varphi_{P_1}(P_1, t)\rangle^2$ is therefore monotonic. As a consequence, (see (7.6))

$$\frac{d}{dt} \mathcal{H}_\rho(t) \leq 0.$$

(7.15)

Hence, the $\mathcal{H}$ theorem holds. For the nonintegrable case, we have the even stronger condition $\gamma_{\beta} > 0$ for some components. Then, $\mathcal{H}_\rho(t)$ monotonically decreases for $t > 0$, until all decay modes disappear and the system approaches equilibrium. Contrary to Boltzmann's $\mathcal{H}$ theorem, our $\mathcal{H}$ theorem is valid for all $\lambda$ (or concentrations) for which the spectral decomposition of $\mathcal{K}_B^{(0)}$ can be determined.

Instead of the Lyapounov function (7.6), we can introduce the more familiar forms of the $\mathcal{H}$-function, such as

$$\mathcal{H}_\rho(t) = \int dp_1 |\varphi_{P_1}(P_1, t)| \log |\varphi_{P_1}(P_1, t)|.$$

(7.16)

Taking the time derivative, we obtain

$$\frac{d}{dt} \mathcal{H}_\rho(t) = \frac{1}{2} \int dp_1 \frac{1}{|\varphi_{P_1}(P_1, t)|} (\log |\varphi_{P_1}(P_1, t)| + 1) \frac{\partial}{\partial t} |\varphi_{P_1}(P_1, t)|^2 \leq 0.$$

(7.17)

Again we recover the $\mathcal{H}$ theorem. In lowest order of $\lambda$ (or of the concentration), the transformation (7.5) is not necessary (i.e., $\Lambda_B \approx 1$) and Boltzmann's formulation is recovered.

For the more general case of generic reduced distribution functions $f_s$, we have

$$f_s(q_1 \cdots q_s, P_1 \cdots P_s, t) = \langle \langle \hat{f}_1, \cdots, q_s, P_1, \cdots, P_s | \rho(t) \rangle \rangle$$

$$= \frac{N!}{(N-s)!} \int dq' \int dp' \delta(q'_1 - q_1) \cdots \delta(q'_s - q_s) \delta(p'_1 - p_1) \cdots \delta(p'_s - p_s) \rho(q', p', t),$$

(7.18)

with

$$\langle \langle \hat{f}_1, \cdots, q_s, P_1, \cdots, P_s | \rangle \rangle = \frac{1}{L^{3r}} \sum_{k_1} \cdots \sum_{k_s} e^{i(k_1 \cdot q_1 + \cdots + k_r \cdot q_r)}$$

$$\times L^{3N/2} \int dp' \delta(p'_1 - p_1) \cdots \delta(p'_s - p_s) \langle \langle k_1, \cdots, k_r, 0^{N-r}, p' \rangle \rangle.$$

(7.19)

We may now introduce the Lyapounov functions through

$$\mathcal{H}_\rho^f(t) = \int dq_1 \cdots dq_r \int dp_1 \cdots dp_s \left| \langle \langle \hat{f}_1, \cdots, q_r, P_1, \cdots, P_s | \rho(t) \rangle \rangle \right|^2.$$

(7.20)

The extension of the above arguments is straightforward.

\(^{10}\) In the reduced subspace of $P_1$, eigenvalues of $\mathcal{K}_B^{(0)}$ are normalizable. Hence the eigenvalues are real. This is a striking difference from the eigenvalue problem of the Liouvillian $L_B$. 
The Extension of Classical Dynamics

8. LINEAR AND NONLINEAR LIPPIMANN-SCHWINGER EQUATIONS

In the previous sections, we have derived the complex spectral representation of $L_H$ through the solutions of the “nonlinear” eigenvalue problem of the collision operator $\psi^{(v)}$ in (4.24) and (5.8). Also, if we first determine the operators $C^{(v)}$ and $D^{(v)}$, we can construct the global collision operators $\theta_{B}^{(v)}$ which do not explicitly depend on the eigenvalues $Z_{\alpha}^{(v)}$ (see (4.32) and (5.13)).

Then, using the solutions of the “linear” eigenvalue problem for $\theta_{B}^{(v)}$, we can construct the solutions of the eigenvalue problem of $L_H$ through the intertwining relations (6.5) (see [8,18]). In this approach, the nonlinearity of the problem appears in the equations for $C^{(v)}$ and $D^{(v)}$. Indeed, the intertwining relations (6.5) with (4.32) and (5.13) lead to nonlinear equations for $\hat{C}^{(v)}$ and $\hat{D}^{(v)}$, through which we can determine $C^{(v)}$ and $D^{(v)}$ (see [18,27,28]):

$$L_0 \hat{C}^{(v)} - \hat{C}^{(v)} L_0 = -L_V \hat{C}^{(v)} + \hat{C}^{(v)} L_V \hat{C}^{(v)},$$
$$L_0 \hat{D}^{(v)} - \hat{D}^{(v)} L_0 = \hat{D}^{(v)} L_V - \hat{D}^{(v)} L_V \hat{D}^{(v)}.$$

Let us operate $\hat{C}^{(v)}$ and $\hat{D}^{(v)}$ on the eigenstates of the unperturbed Liouvillian $L_0$, $|\Phi^{(v)}_\nu\rangle \equiv \hat{C}^{(v)} |\nu\rangle$, $\langle \Phi^{(v)}_\nu | \equiv \langle \nu | \hat{D}^{(v)}$.

In general, these states are not the eigenstates of $L_H$.

From (8.1), we derive the nonlinear equations

$$|\Phi^{(v)}_\nu\rangle = |\nu\rangle + \lim_{\Omega \to \infty} \sum_{\mu} \frac{-1}{l_{\mu} - l_{\nu} + i\epsilon_{\mu\nu}} P^{(\mu)} Q^{(v)} \lambda L_V |\Phi^{(v)}_\nu\rangle,$$
$$\langle \Phi^{(v)}_\nu | = \langle \nu | + \lim_{\Omega \to \infty} \sum_{\mu} \langle \Phi^{(v)}_\nu | \lambda L_V Q^{(v)} P^{(\mu)} \rangle \frac{1}{l_{\nu} - l_{\mu} + i\epsilon_{\mu\nu}}.$$

We have imposed the boundary conditions

$$|\Phi^{(v)}_\nu\rangle = |\nu\rangle \quad \text{and} \quad \langle \Phi^{(v)}_\nu | = \langle \nu |, \quad (\text{for } \lambda = 0).$$

The analytic continuations of the denominators in (8.3) are given by the $\epsilon$-rule (4.16).

By iterating (8.3), we can construct the explicit form of $C^{(v)}$ and $D^{(v)}$ in powers of $\lambda$. We can then construct $A^{(v)}$ through (5.20), and thus, $\Pi^{(v)}$ as well as $\theta_{B}^{(v)}$ in powers of $\lambda$. We shall call equations (8.3) the “nonlinear Lippmann-Schwinger equations” (NLLS), as we shall show that they are corresponding to a “nonlinear extension” of the classical version of the “Lippmann-Schwinger equations”. The nonlinear terms of NLLS involve the contribution from the diagonal transitions associated with the collision operators (see (4.32) and (5.13))

$$\langle \nu | \lambda L_V |\Phi^{(v)}_\nu\rangle = \langle \nu | \theta_{C}^{(v)} |\nu\rangle - l_{\nu}, \quad \langle \Phi^{(v)}_\nu | \lambda L_V |\nu\rangle = \langle \nu | \theta_{D}^{(v)} |\nu\rangle - l_{\nu}.$$

Let us consider the case when the contribution from the diagonal transitions in the left-hand sides of these expressions are negligible. In the next section, we shall discuss the conditions when this is satisfied. Then, we have

$$\theta_{B}^{(v)} = L_0 P^{(v)}.$$

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$$\langle \nu | \lambda L_V |\Phi^{(v)}_\nu\rangle = \langle \nu | \theta_{C}^{(v)} |\nu\rangle - l_{\nu}, \quad \langle \Phi^{(v)}_\nu | \lambda L_V |\nu\rangle = \langle \nu | \theta_{D}^{(v)} |\nu\rangle - l_{\nu}.$$
where $B$ stands as before for $C$ or $D$. This implies that the eigenstate of $\theta_0^{(\nu)}$ is the unperturbed state $|\nu\rangle$, and the eigenvalues of $L_H$ are $l_\nu$, the same as for $L_0$. Dissipation is negligible, i.e., the evolution is time-symmetric. As the result, we have (again neglecting the diagonal transitions: see (5.17))

$$N_\alpha^{(\nu)} = 1,$$

as well as

$$A^{(\nu)} = P^{(\nu)}.$$

Combining them with (6.5), we have

$$L_H |\Phi^C_\nu\rangle = l_\nu |\Phi^C_\nu\rangle,$$

i.e., for this special case the states $\Phi^C_\nu$ and $\Phi^D_\nu$ are eigenstates of $L_H$ with real eigenvalues $l_\nu$. We shall show later that this situation corresponds to "integrable systems" in the sense of Poincaré.

Then equations (8.3) reduce to the "linear" equations

$$|\Phi^C_\nu\rangle = |\nu\rangle + \sum_{\mu} \frac{-1}{l_\mu - l_\nu + i\epsilon_{\mu\nu}} P^{(\mu)} Q^{(\nu)} \lambda L_V |\Phi^C_\nu\rangle,$$

$$\langle\Phi^D_\nu | L_H = \langle\Phi^D_\nu | l_\nu,$$

where we have abbreviated the notation of the limit $\Omega \to \infty$. These are the "classical" versions of the Lippmann-Schwinger equations. We emphasize that (8.10) as well as (8.9) are valid only for the integrable systems where the diagonal transitions associated with the collision operator are negligible. For this case, we have

$$\langle\Phi^D_\nu | = \delta_{\nu,\mu}, \quad \sum_{\nu} |\Phi^C_\nu\rangle \langle\Phi^D_\nu | = 1,$$

and the spectral decomposition of the evolution operator,

$$e^{-iL_H t} = \sum_{\nu} |\Phi^C_\nu\rangle e^{-i l_\nu t} \langle\Phi^D_\nu |.$$

Moreover, the transformations $\Lambda_B$ reduce to

$$\Lambda_B = \Lambda_I,$$

where

$$\Lambda_I = \sum_{\nu} |\nu\rangle \langle\Phi^D_\nu |, \quad \Lambda_I^{-1} = \sum_{\nu} |\Phi^C_\nu\rangle \langle\nu |,$$

which lead to

$$\Lambda_B L_H \Lambda_B^{-1} = \Lambda_I L_H \Lambda_I^{-1} = L_0.$$

We have put the index $I$ in order to emphasize that $\Lambda_I$ is associated with integrable systems, as (8.15) holds only for this case.

Let us consider the case that interaction among the particles is "transient". For this situation, there exist asymptotic states before and after scattering. This is the situation to which the $S$-matrix theory in quantum mechanics applies. In analogy to the quantum $S$-matrix theory, we can introduce the asymptotic states which are the classical version of the "Möller scattering states" $\Phi^\pm_\nu$ defined as the solution of the equations [38-40]

$$|\Phi^\pm_\nu\rangle = |\nu\rangle + \frac{1}{l_\nu - L_0 \mp i\epsilon} Q^{(\nu)} \lambda L_V |\Phi^\pm_\nu\rangle,$$

$$\langle\Phi^\pm_\nu | = \langle\nu | + \langle\Phi^\pm_\nu | \lambda L_V Q^{(\nu)} \frac{1}{l_\nu - L_0 \mp i\epsilon}.$$
They also satisfy
\[ L_H |\Phi_\nu^\pm\rangle = \lambda_\nu |\Phi_\nu^\pm\rangle, \] (8.17)
as well as (for the integrable systems)
\[ \langle \Phi_\nu^+ | \Phi_\mu^+ \rangle = \delta_{\nu,\mu}, \quad \sum_\nu |\Phi_\nu^+\rangle \langle \Phi_\nu^+| = 1, \] (8.18)
and
\[ e^{-iL_H t} = \sum_\nu |\Phi_\nu^+\rangle e^{-i\lambda_\nu t} \langle \Phi_\nu^+|, \] (8.19)
and similar relations for \( \Phi_\nu^- \). The states \( \Phi_\nu^+ \) correspond to the "retarded" solutions of the scattering, while \( \Phi_\nu^- \) to the "advanced" solutions.

Equation (8.19) is the unitary spectral decomposition of the evolution operator. Moreover, we can introduce the unitary transformations (for repulsive forces)
\[ U_\pm = \sum_\nu |\nu\rangle \langle \Phi_\nu^\pm|, \quad U_\pm^* = \sum_\nu |\Phi_\mu^\pm\rangle \langle \nu|, \] (8.20)
which lead to
\[ U_+ L_H U_+^* = I_0, \] (8.21)
and a similar relation for \( U_- \).

The structure of \( \Lambda_I \) is quite similar to that of \( U_\pm \). However, due to the difference in the analytic continuations between (8.10) and (8.16), these transformations are not the same. For example, the eigenstates corresponding to the vacuum of correlations (i.e., the states with zero eigenvalue \( l_0 = 0 \)) are given for (8.10) by
\[ |\Phi_0^\pm\rangle = |\Phi_0^\pm\rangle, \quad \langle \Phi_0^\pm| = \langle \Phi_0^-|. \] (8.22)
As the complex spectral representation uses both analytic continuations in (8.14), \( \Lambda_I \) is a nonunitary transformation even for the integrable case. Nevertheless, because of the bicompleteness relation in (8.11), the spectral representations (8.12) and (8.19) lead to the same evolution of the distribution function \( \rho(t) \).

It is remarkable that integrable LPS admit both the nonunitary transformation (8.14), as well as to the unitary ones (8.20).\(^{11}\) However, there is a significant difference between the two. To see this, let us evaluate the inner product \( \langle \Phi_{0,0,0}^- | \Phi_{0,0,0}^- \rangle \) for the unitary transformations. Because the inner product is a distribution, we evaluate this with the integration over \( p' \) as (e.g., with the momentum \( p_1 \))
\[ \int dp' p_1 \langle \Phi_{0,0}^- | \Phi_{0,0}^- \rangle = p_1 - \frac{\lambda^2}{\Omega} \sum_{n,j=1}^N \sum_k \int dp' p_1 \cdot d_{jin} \frac{|V_k|^2}{|k \cdot g_{jin} + ic|^2} k \cdot d_{jin} \delta(p' - p) + O(\lambda^3) \]
\[ = p_1 - \frac{\lambda^2}{\Omega} \sum_{n=2}^N \sum_k \frac{|V|^2}{|k \cdot g_{jn} + ic|^2} \cdot d_{kn} \delta(p' - p) + O(\lambda^3) \] (8.23)
To obtain the second equality in (8.23), we have performed an integration by parts over the momenta. The nonvanishing contribution comes only from the terms which are "connected" to the labeled particle 1. All "disconnected" terms vanish by integration by parts over the

\(^{11}\) The nonuniqueness of the spectral decomposition including a nonunitary spectral decomposition has also been observed for the Friedrichs model in quantum mechanics [9].
momentum $p_j$ for $j \neq 1$. As the result, the number of terms of $\lambda^2$ contribution in (8.23) reduces from $N^2$ to $N$. We note that this is a general property associated with reduced quantities (3.20) (see also (4.8)). Whenever we consider the reduced observables, all disconnected terms vanish.

Due to the Poincaré resonances, there appears a singularity $\sim \epsilon^{-1}$ in (8.23). However, for $N$ finite, this singularity is harmless, as we have to take first the limit $\Omega \to \infty$ before taking the limit $\epsilon \to 0^+$. Nevertheless, the unitary transformations cannot be extended to nonintegrable systems in the thermodynamic limit, since $\Omega^{-1}$ is compensated by $N$ in this limit. In contrast, the nonunitary transformation regularizes the Poincaré divergence as

$$
\int dp' \left< \left( \Phi_{0,p'}^D, \Phi_{0,p}^C \right) \right> \sim p_1 + \frac{N}{\Omega^2} \sum_k \left( \frac{1}{(k \cdot v + i c)^2} + \text{c.c.} \right) \sim p_1 + O \left( \frac{N}{\Omega} \right).
$$

(8.24)

Hence, (8.14) has a natural extension for the nonintegrable systems where the time-symmetry is broken.

9. INVARIANTS OF MOTION AND INTEGRABILITY CONDITIONS

Let us discuss the relation between $\Lambda$ and the invariants of motion for integrable systems. We consider the transformations for observables,

$$
\left< \hat{f}_B(t) \right> = (\Lambda \hat{f}_B(\omega)). \ P^{-1}
$$

We note the difference of this quantity from $\left< \hat{f}_B(t) \right>$ introduced in (6.8). The time evolution of $\left< \hat{f}_B(t) \right>$ is generated by the Liouvillian $L_H$, while $\left< \hat{f}_B(t) \right>$ by the collision operator $\Theta_B$.

The important property of $\hat{M}$ is that when $\hat{M}$ is in a single correlation subspace $P^{(\nu)}$, then $\hat{M}$ is in the $\Pi^{(\nu)}$ subspace. For example, let us assume

$$
\left< \hat{f}_D(0) \right> = (\nu^{(\nu)}(\omega)). \ W
$$

Then we have indeed (see (6.3))

$$
\left< \hat{f}_D(t) \right> = (\nu^{(\nu)}(\omega)) e^{-i\theta(t)} \left< \Phi_D^{(\nu)} \right> = (\nu^{(\nu)}(\omega)) e^{-i\theta(t)} \hat{f}_D^{(\nu)}.
$$

(9.4)

Of special interest is the case where $v = 0$, because this leads to “invariants” of motion for integrable systems. To see this, let us consider the transformed “momenta” (see (3.22))

$$
\left< \hat{p}_D(t) \right> = (\Lambda \hat{p}_D(t)). \ P^{-1}
$$

We have

$$
\left< \hat{p}_D(t) | \rho(0) \right> = (\nu^{(\nu)}(\omega)) e^{-i\theta(t)} \hat{p}_D^{(\nu)} | \rho(0) \rangle.
$$

(9.6)

When the diagonal transitions are negligible, i.e., $\theta^{(0)} = 0$, the transformed momenta reduce to the invariants of motion (see (8.14)),

$$
\left< \hat{p}_D(t) | \rho(0) \right> \rightarrow \left< \hat{p}_D | \Lambda | \rho(0) \right> = \int dp' \left< \hat{p}_D | 0, p' \right> \left< \Phi_{0, p'}^D | \rho(0) \right>.
$$

(9.7)
The invariants evaluated on a single trajectory are of special interest. This corresponds to $|\rho(0)\rangle = |q^0, p^0\rangle$,

$$
P_i^D (q^0, p^0) \equiv \langle \langle \hat{p}_i^D | q^0, p^0 \rangle \rangle = L^{3N/2} \int dp' p'_i \langle \langle \hat{p}_i^D | q^0, p^0 \rangle \rangle. \quad (9.8)$$

This defines a set of $3N$ "new" momenta. Therefore, when the conditions (a) diagonal transitions are negligible, and (b) the right-hand side of (9.8) exists, the $P_i^D (q^0, p^0)$ are invariants of motion, and the system is integrable in the sense of Poincaré. We shall call the conditions (a) and (b) the "integrability conditions". We shall discuss later (as well as in the subsequent sections) these conditions in detail for various situations.

In analogy to the quantum $S$-matrix theory, we can write the solution of the Möller state $\Phi_{0,p}$ in (8.22) in terms of the classical version of the $T$-matrix,\(^\text{12}\)

$$
\langle \langle \Phi_{0,p}^D \rangle \rangle = \langle \langle 0, p | T(\pm i\epsilon) \frac{1}{1 + i\epsilon - L_0} \rangle \rangle, \quad (9.9)
$$

where the $T$-matrix is the solution of the integro-differential equation (cf. (5.3)),

$$
T(z) = \lambda L_V + T(z) \frac{1}{z - L_0} \lambda L_V. \quad (9.10)
$$

Then the invariants of motion (9.8) are given by (for integrable systems)

$$
P_i^D (q^0, p^0) = p_i + \lim_{\Omega \to -\infty} \int dp' p'_i \sum_k \langle \langle 0, p' | T(\pm i\epsilon) | k, p \rangle \rangle \frac{1}{1 + i\epsilon - k \cdot q^0} e^{-ik \cdot q^0}. \quad (9.11)
$$

Hence, the existence of the $T$-matrix corresponds to the condition (b) of integrability. As we shall show in the next section, for short-range repulsive interactions and not too large number of particles $N$, this condition is satisfied.\(^\text{13}\) The system is then integrable in the sense of Poincaré. Even when there is no analytic solution described by the Born series in $\lambda$ of the $T$-matrix, there may exist nonanalytic solutions of (9.10), such as they occur for attractive forces in quantum scattering. We hope to present a classical analogue of this situation elsewhere.

The invariants (9.11) are examples of "singular invariants" (as the Fourier components of the invariants are singular at the resonance $k \cdot v = 0$) first introduced by one of the authors [19,41] (see also [42,43]). It is worthwhile to compare our result with the usual canonical transformation theory based on Hamilton-Jacobi's equation for the generating function $F(p', q)$, where $p'$ are the generalized momenta which are also invariants of motion [44]. By the standard perturbation analysis for $F(p', q)$, one can easily show that the generalized momentum $P'_1$ is the same as (9.11) to first order in $\lambda$ (see also (9.14)). Hence, assuming the analyticity of the $T$-matrix at $\lambda = 0$, the invariants (9.11) are the Hamilton-Jacobi invariants of motion.

Let us now discuss in detail the integrability conditions for (9.6). We first consider the case where the number of particles $N$ is finite, and the distribution functions are regular as given by (3.1) with no delta function singularity in their Fourier representation. Expanding (9.6) in powers of $\lambda$, we have

$$
\langle \langle \hat{p}_i^D (t) \rho(0) \rangle \rangle = \lim_{\Omega \to -\infty} \sum_k \int dp \int dp' p_i \langle \langle 0, p | e^{-i \lambda D_0^{(0)} t} (1 + \lambda D_0^{(0)} + \lambda^2 D_2^{(0)}) | k, p' \rangle \rangle \bar{\rho}_k (0) + \lambda^3 \cdots. \quad (9.12)
$$

\(^\text{12}\) For integrable systems, we can remove the restriction expressed by $Q^{(\nu)}$ in (8.10) (see [2]).

\(^\text{13}\) For more than two-body systems, we need a careful discussion of the analyticity of the $T$-matrix, as performed by Padéev for the three-body collision. We shall not discuss this problem here.
Here $\lambda^n \theta_n^{(0)}$ are $\lambda^n D_n^{(0)}$ are the $n^\text{th}$ order approximation of the corresponding operators (see (4.38)). To the second order in $\lambda$, we obtain

$$
(\langle \tilde{p}^D_i (t) | p(0) \rangle) = \lim_{\Omega \to \infty} \frac{1}{\Omega^2} \sum_{n=2}^{N} \sum_{k} \int dp \int dp' p_i \times \langle 0, p' | \left[ 1 + \lambda D_1^{(0)} + \lambda^2 \left( D_2^{(0)} - i\theta_2^{(0)} t \right) + \lambda^3 \cdots \right] | k, p \rangle \rho_k (0).
$$

(9.13)

The contribution from $D_2^{(0)}$ corresponds to off-diagonal transitions, while $\theta_2^{(0)}$ corresponds to diagonal transitions in the space $P^{(0)}$.

As an example, we consider a single trajectory corresponding to (9.8). To first order in $\lambda$, we have (e.g., for $i = 1$)

$$
P_1^D (q^0, p^0, t) = p_1^0 - \lambda \lim_{\Omega \to \infty} \sum_{n=2}^{N} \sum_{k} \int dp \ p_1 \cdot d_j \frac{V_{|k|}}{k \cdot g_{jn} - i\epsilon} e^{-i k \cdot (q^0_j - q_0^0)} \delta (p - p^0)
$$

$$
+ O (\lambda^2)
$$

(9.14)

To obtain the last line in (9.14) we have again retained the "connected" contribution to the labeled particle 1 (see (8.23)).

Similarly, the second order contribution $D_2$ is given by

$$
\bar{P}_1^D (q^0, p^0, t) = -\lambda^2 \lim_{\Omega \to \infty} \sum_{n=2}^{N} \sum_{k} \sum' \int dp \ p_1 \cdot d_1 \frac{V_{|k|}}{k \cdot g_{1n} - i\epsilon} k e^{-i k \cdot (q_1^1 - q_0^0)} + O (\lambda^2),
$$

(9.15)

where the bar denotes the particular term at which we are looking. This term comes from binary correlations. To this order we have also to retain the effect of ternary correlations, which we do not write here. The prime on the summation sign over $k'$ denotes that we exclude $k' = 0$. This restriction is the result of the fact that $D^{(0)}$ is the off-diagonal transition (expressed by $Q^{(0)}$ in (5.5)).

For the diagonal transition we have (see (4.38))

$$
[\bar{P}_1^D (q^0, p^0, t)]_{\lambda^2 \theta_2} = i \lambda^2 t \lim_{\Omega \to \infty} \frac{1}{\Omega^2} \sum_{n=2}^{N} \sum_{k} \int dp \ p_1 \cdot d_1 \frac{|V_{|k|}|^2}{k \cdot g_{1n} - i\epsilon} k e^{-i k \cdot (q_1^1 - q_0^0)} \delta (p - p^0) .
$$

(9.16)

For any finite $N$, the diagonal transition (9.16) is negligible as this term is proportional to $\Omega^{-1}$.

For a short-range Gaussian repulsive interaction, we can explicitly integrate (9.14) over $k$. Let us assume that

$$
V (q) = V_0 e^{-x^2/4a^2} = \frac{1}{\Omega} \sum_{l} B e^{-a^2 x^2} e^{i q l},
$$

(9.17)

where $B \equiv V_0 a^3 / \pi^{3/2}$. To first order of $\lambda$, we have for (9.14),

$$
P_1^D (q, p) = p_1 + \lambda B \sum_{n=2}^{N} \int dk \frac{1}{k \cdot g_{1n} - i\epsilon} k e^{-a^2 k^2} e^{i k \cdot r_n},
$$

(9.18)

where

$$
r_n = q_n - q_1 .
$$

(9.19)
and we have abbreviated the superscript 0 on $q$ and $p$ for the initial condition to simplify the notations. Let us denote the unit vectors of the polar coordinates of $\mathbf{g}_{1n}$ in an arbitrary reference system by $(\hat{v}_n, \hat{\theta}_n, \hat{\phi}_n)$, where $\hat{v}_n$ is the unit vector in the longitudinal direction of $\mathbf{g}_{1n}$, $\hat{\theta}_n$ in the transversal direction of $\mathbf{g}_{1n}$ parallel to the direction of the angle $\theta_n$, and $\hat{\phi}_n$ in the transversal direction of $\mathbf{g}_{1n}$ parallel to the angle $\phi_n$. Let us also introduce the notations

$$r_{n1} = (r_n \cdot \hat{v}_n), \quad r_{n2} = (r_n \cdot \hat{\theta}_n), \quad r_{n3} = (r_n \cdot \hat{\phi}_n),$$

and

$$k_1 = (k \cdot \hat{v}_n), \quad k_2 = (k \cdot \hat{\theta}_n), \quad k_3 = (k \cdot \hat{\phi}_n).$$

We can write (9.18) as

$$p_1^{(0)} = p_1 + \lambda B \sum_{n=2}^{N} \int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 \int_{-\infty}^{+\infty} dk_3 \frac{1}{k_1 v_{1n} - i\epsilon} \times \left( k_1 \dot{v}_n + k_2 \dot{\theta}_n + k_3 \dot{\phi}_n \right) e^{-a^2(k_1^2 + k_2^2 + k_3^2)} e^{i(k_1 r_{n1} + k_2 r_{n2} + k_3 r_{n3})},$$

where $v_{1n} = |\mathbf{g}_{1n}|$. We assume that $v_{1n} \neq 0$. Note that the factor $k_1$ in the numerator of the longitudinal component cancels with $k_1 v_{1n}$ in the denominator. Hence, there is no resonance singularity at $k_1 v_{1n} = 0$ in the longitudinal component. The resonance effect appears only in the transversal components.

We can perform the integration in (9.22), and obtain

$$P_1^D(q, p) = p_1 + \frac{\pi^2 \lambda B}{a^4} \sum_{n=2}^{N} \frac{1}{v_{1n}} e^{-\frac{1}{4a^2}(r_{n2}^2 + r_{n3}^2)} \times \left( \frac{\hat{v}_n e^{-\frac{r_{n1}^2}{4a^2}} - r_{n2} \dot{\theta}_n + r_{n3} \dot{\phi}_n}{\sqrt{\pi}} 2a \left[ 1 + \text{erf}\left( \frac{r_{n1}}{2a} \right) \right] \right),$$

where the error function is defined by

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} dt.$$

We have

$$\text{erf}(-x) = -\text{erf}(x),$$

and

$$\lim_{x \to +\infty} \text{erf}(x) = 1.$$

We note that in spite of the short range interaction, the effect of the interaction in the transversal direction does not disappear for $r_{n1} \to +\infty$. After this limit is taken in (9.23), we have

$$P_1^D(q, p) \to p_1 - \frac{\pi^2 \lambda B}{a^4} \sum_{n=2}^{N} \frac{1}{v_{1n}} e^{-\frac{1}{4a^2}(r_{n2}^2 + r_{n3}^2)} \left( r_{n2} \dot{\theta}_n + r_{n3} \dot{\phi}_n \right).$$

This results from the resonance singularity at $k \cdot \mathbf{g}_{1n}^0 = 0$ in (9.14). The resonance effect leads to the "long range correlations" between the particle 1 and 2 regardless of their distance. Hence, the order of this contribution is $O(\lambda N)$. Similarly, one can show that the order of (9.15) from the binary correlations is $\lambda^2 N$, and from the ternary correlations in $\lambda^3$ the contribution is $O(\lambda^3 N^2)$, and so on (see the discussion below). As a result, if the number of particles $N \to \infty$, then...
(9.14) generally diverges. In order for (9.14) to be an invariant of motion, \( N \) should be finite. Even if \( N \) is finite, but too large, then the series expansion in \( \lambda \) may not converge.

We can easily extend the above estimations for the diagonal transition and the off-diagonal transitions to all order of \( \lambda \). Indeed, by increasing \( \lambda \) in the off-diagonal transition, we multiply by the factor \( \Omega^{-1} \sum_k \) (see (2.24)). This factor does not lead to any extra volume factor in the limit of \( \Omega \rightarrow \infty \) (see (2.16)). A new particle may or may not participate in the interaction. On the other hand, the diagonal transition is a point contribution in the summation over \( k \), so that it leads to a factor \( \Omega^{-1} \) without any summation over the wave vector. Hence, this vanishes in the limit \( \Omega \rightarrow \infty \). As a consequence, all diagonal transitions are negligible for the regular distribution functions for finite \( N \). Therefore, the integrability condition (a) is satisfied.

Moreover, we note that the restriction expressed by \( Q(0) \) in the off-diagonal transition can also be removed for this situation. Indeed, the term corresponding to \( k' = 0 \) in (9.15) is of order \( \epsilon^{-1} \) and can be neglected as we have to take first the limit \( \Omega \rightarrow \infty \) before the limit \( \epsilon \rightarrow 0+ \).

Extension of these estimations to more general observables in equation (9.4) is straightforward. Applying these results to NLLS (8.3), we see that they reduce to the linear Lippmann-Schwinger equation (8.10).

In summary, systems described by regular distribution functions are expected to be integrable. On the contrary, if the distribution functions are singular, or the number of particles approaches infinity, the system is no longer integrable. Then, one can observe the dissipative effects in LPS. In the following sections, we shall discuss these nonintegrable situations which cannot be described by Newtonian trajectory theory.

10. PERSISTENT INTERACTIONS AND SINGULAR DISTRIBUTION FUNCTIONS

In the previous sections, we have constructed the invariants of motion (9.11) for systems with a finite number of particles and described by regular distribution functions. We now show that the new momenta defined in (9.8) are no longer invariants of motion when they are associated with singular distribution functions.

Let us integrate (9.8) over the coordinate \( q \),

\[
I(p, t) = \int dq \mathcal{D}^D_1(q, p, t).
\]

(10.1)

The diagonal transition in (9.16) now gives a finite contribution, while the off-diagonal transitions in (9.14) and (9.15) vanish because of the restriction by \( Q(0) \) in the \( \mathcal{D}^{(0)} \) operator. Therefore we obtain from (9.16) (e.g., \( N = 1 \), and dropping the index of particle 1)

\[
\frac{d}{dt} I(p, t) = \lambda^2 \int dk \int dp' p' |V_k|^2 k \cdot \frac{\partial}{\partial p'} \pi \delta (k \cdot v') k \cdot \frac{\partial}{\partial p'} \delta (p' - p) + O(\lambda^3).
\]

(10.2)

We see that \( I(p, t) \) evolves in time.

One can understand this result as follows. The integration corresponds to the introduction of a nonlocal ensemble which has a delta function singularity in its Fourier representation,

\[
\rho_k(0) = \rho_0^D(p, 0) \delta_\Omega(k) + \rho_k(p, 0).
\]

(10.3)

where we assume that \( \rho_0^D \) and \( \rho_k^D \) do not depend on \( \Omega \) in the limit of large volumes. Because of this singularity, the effects of the diagonal transitions are amplified \( \Omega \) times. As the result, \( I(p, t) \) evolves in time.\(^\dagger\)

\(^\dagger\)For this case, nonnegligible diagonal transitions appear only in the vacuum of correlation. Hence, the analytic continuation for the diagonal operators are also uniquely determined with the complex distribution, as in the case of the thermodynamic limit discussed in (4.38).
However, we note that the normalization of this singular distribution function diverges,
\[
\int dq \int dp \rho(q, p, 0) = \int dp [\Omega \rho_0(p, 0) + \rho_0(p, 0)] \to \infty.
\] (10.4)

Physically, this corresponds to a situation where we continuously send "test" particles towards a single potential. We assume that the interaction between the test particles are negligible as compared with their interaction with the potential. Moreover, we assume the test particles are distributed with a finite concentration in space. Therefore, the interaction between the particles with the potential is "persistent". There are no asymptotic states for this scattering process. This situation goes beyond the usual S-matrix theory.

Corresponding to (10.2), we obtain for the ensemble (10.3),
\[
\frac{d}{dt} \langle \hat{p}^D(t) | \rho(0) \rangle = \lambda^2 \int dk \int dp |V_k|^2 k \cdot \frac{\partial}{\partial p} \pi \delta(k \cdot \mathbf{v}) k \cdot \frac{\partial}{\partial p} \rho_0(p, 0) + O(\lambda^3). \tag{10.5}
\]

Therefore \( \langle \hat{p}^D(t) | \rho(0) \rangle \) evolves in time when associated with the singular distribution function (10.3). In the right-hand side of (10.5), we recognize the Fokker-Planck operator (see (4.36)). Dissipative processes are enhanced by the delta function singularity in (10.3). The system is non-integrable for persistent interaction described by the singular distribution functions.

In the evolution of \( \langle \hat{p}^D(t) | \rho(0) \rangle \), there appear generally higher order contributions in time, as \((-i\partial_a^{(0)} t)^n\) with \(n \geq 2\) (see (6.19)). However, as one can easily see, a repetition of diagonal transitions always leads to an extra volume factor \(\Omega^{-1}\) for the singular case we consider in this section. All higher order contributions \(t^n\) in time with \(n \geq 2\) are negligible in the large volume limit. The evolution of \( \hat{p}^D(t) \) is strictly linear in time. In previous papers, we have investigated in detail this situation and performed numerical simulations [5,6,21]. The agreement is excellent.

Because of the linear time dependence of \( \langle \hat{p}^D(t) | \rho(0) \rangle \) in (10.5), however, the system cannot approach equilibrium in a finite time. This is in contrast to the systems studied in the next section, where we shall investigate the evolution of dynamical systems which are described by singular but \(L_1\) normalizable distributions in the thermodynamic limit such as (3.15).

In the above example, we have shown that the evolution in the \(\Pi^{(0)}\) subspace gives a finite contribution in the limit of large volumes for the singular distribution function. This is generally true for all contributions in the \(\Pi^{(0)}\) subspace, whenever the contributions involve the effect of the interaction \(\lambda \mathbf{v}\). However, there is an exceptional component which leads to a divergence in the \(\Lambda\) transformations. That is the contribution coming from the free motion. For example, the unperturbed component of \( \langle \hat{p}^D(t) | \rho(0) \rangle \) diverges when it is associated with the singular function (10.3), in spite of the fact that its time derivative gives the finite contribution (10.5). The integration of the momentum \(p^0_l\) in (9.14) over space diverges. Physically, this divergence can be easily understood, as we are continuously sending test particles towards the potential. A detector behind the potential registers this incident flow of test particles. Simply by putting the detector in a direction which is not parallel to the flow, one may avoid this diverging contribution.

11. SINGULAR DISTRIBUTION FUNCTIONS AND THE THERMODYNAMIC LIMIT

We now consider the singular distribution functions of class (3.15) corresponding to the thermodynamic limit. As mentioned in Section 3, canonical equilibrium belongs to this class. The main differences from the one considered in the previous section is that the distribution functions, while singular in the Fourier representation, have well-defined \(L_1\) norm. The time evolution of this class of ensembles is the main subject of Nonequilibrium Statistical Mechanics (NESM). Its time dependence has been already investigated in our earlier work [19,22,23]. All results obtained from NESM can be recovered by our complex spectral representation. This includes the derivation of the Fokker-Planck equation, of the Boltzmann equation, and more generally of non-Markovian
master equations, and so on. As this class of ensembles leads to non-Newtonian contributions, we concluded at this time that these contributions result from approximations introduced in the solution of the Liouville equation. We see now that these results are exact consequences of the solution of the eigenvalue problem of the Liouvillian for singular distribution functions outside the Hilbert space.

It has also been shown that this class of distribution functions approaches equilibrium for $t \to \infty$ (see [19]). This is confirmed by our formulation of the $\mathcal{H}$ theorem in Section 7.

Let us now show that this class of distribution functions belongs to the domain of the nonunitary transformation $\Lambda$. To illustrate this, let us evaluate the transformed momentum $\tilde{p}_1(0)$ on the ensemble (3.15). As in (9.14), we have to first order in $\lambda$:

$$\langle \tilde{p}_1^D(0)|\rho(0)\rangle = \int dp\, p_0(p,0) - \frac{\lambda}{\Omega^2} \sum_{n=2}^{N} \sum_{k} \int dp\, p_1\, k \times \frac{V_k}{\partial p_1\, k \cdot g_{kn}} - i\epsilon \rho_{k,-k}(p_1, p_n | p_{n-1}^N, 0) + O(\lambda^2).$$

(11.1)

Note the difference in the volume dependence between (11.1) and (9.14). Now the transformed momentum has a well-defined value of order $c$ in the thermodynamic limit (1.2).

One can easily verify that (11.1) is well defined to an arbitrary order of $\lambda$, as follows: in the second order contribution $\lambda^2$, there are three possible contributions; the first is the diagonal transition coming from the vacuum of correlation $\rho_k(p)$, the second from the binary correlations $\rho_{k',-k'(p_1, p_n)}$, and the third from the ternary correlations $\rho_{k,k',-k-k'(p_1, p_j, p_n)}$. All other terms in the second order terms do not contribute, as they are not "connected" to particle 1 through the interactions (see the discussion in (9.14)). In all the three cases, there appears an extra volume factor $\Omega^{-1}$ through the new interaction (see (2.24)) as compared with the first order contribution in (11.1).

However, for the first case with $\rho_0$, we have an extra factor $\Omega$ as compared to $\rho_{k,-k}$ in (11.1), which compensates the factor $\Omega^{-1}$ coming from the interaction. Hence, the first contribution is also of order $c$. In the second case with $\rho_{k',-k'}$, we have an extra summation over $k'$. This summation, together with the factor $\Omega^{-1}$ from the interaction, leads to the well-defined result in the thermodynamic limit. Hence, the second contribution is also of order $c$. Similarly, one can easily show that any term in $\lambda$ from binary correlations gives the contribution of order $c^2$. In the third case with $\rho_{k,k',-k-k'}$, we obtain a contribution which is of order $^3$. Similarly, one can show that any term in $\lambda$ from ternary correlations gives contribution of order $c^2$, as the summation over the third particle gives a contribution of order $N$ which compensates the factor $\Omega^{-1}$. One can in this way verify that all terms coming from $n^{th}$ order correlations lead to contributions of order $c^{n-1}$. Therefore, assuming convergence of the series\footnote{This may involve resummations.} the transformed momentum $\tilde{p}_1^D(0)$ in (11.1) is well defined to arbitrary order in $\lambda$. Similarly, the transformed observables (9.1) are finite in the thermodynamic limit. Ensembles described by the distribution function in (3.15) are in the domain of the nonunitary transformations $\Lambda$.

In order to compare the behaviour of $\tilde{p}_1^D(t)$ in association with the ensembles (3.15) to the results in the previous section, let us evaluate its time evolution. As mentioned before, $\tilde{p}_1^D(t)$ is in the $\Pi^{(0)}$ subspace. Hence, we can apply the formula (6.19). Then, we obtain

$$\frac{d}{dt}\langle \tilde{p}_1^D(t)|\rho(0)\rangle = \int dp\, p_0(p,t) \frac{\partial}{\partial t} \rho_0(p,t) + O(\lambda^3),$$

(11.2)
equation,
\[
\frac{\partial}{\partial t} \rho_0(p, t) = \lim_{\Omega \to \infty} \frac{\lambda^2}{\Omega^2} \sum_{n=2}^{N} \sum_{k} |V_k|^2 k \cdot d_{1n} \pi \delta(k \cdot g_{1n}) k \cdot d_{1n} \rho_0(p, t) + O(\lambda^3).
\]  
(11.3)

In the thermodynamic limit, the right-hand side of (11.3) gives a finite contribution of order c.

In this equation, we can neglect the contribution of \( \frac{\partial}{\partial p_n} \) in the derivative operator \( d_{1n} \) at the left because of the boundary condition (2.1). This is possible because we understand (11.3) together with the inner product together with the observable \( p_1^2 \) that leads to the integration over the momentum in (11.2).

The result (11.2) is quite similar to (10.5), but there is an interesting difference. The right-hand side of (11.3) depends on time, while it does not in (10.5). In the situation considered here, there appear summations over new particles due to repeated collisions \((-i\theta_B^{(0)} t)^n\). As each summation over particles leads to a factor \( N \), we can no longer neglect higher contribution of \( t^n \) with \( n \geq 2 \) (see the discussion in (10.5)). Because of this nonlinear contribution in time, the system approaches equilibrium in a finite time scale \( t_\infty \sim (\lambda^2 c)^{-1} \).

We shall not try to summarize the results we obtain starting from the singular distribution functions (3.15) and applying our complex spectral decomposition. This would involve a summary of most of Nonequilibrium Statistical Mechanics [19]. We want only to emphasize that here we have a striking example of the emergence of non-Newtonian contributions.

We already mentioned that the ensembles (3.15) are form invariant. Are there other form invariant distributions? This leads us to the basic question: are trajectories conserved in the thermodynamic limit? Can non-Newtonian effects be observed starting from a single trajectory? These are the questions we want to consider now.

12. THE THERMODYNAMIC LIMIT
AND THE COLLAPSE OF THE TRAJECTORIES

We now start with the initial condition (1.4) and consider the limit \( N \to \infty \). In the previous section, we have considered the time evolution in the thermodynamic limit described by the class of singular distribution functions (3.15). A single trajectory does not belong to this class. As we shall show in this section, time dependent perturbation analysis may lead for trajectories to diverging contributions due to the Poincaré resonances. However, there is a generic class of initial conditions for trajectories which are in the domain of \( \Lambda \). For this class, time going on, trajectories are destroyed by the Poincaré resonances and the distribution function approaches the class of (3.15).

Let us consider the time evolution of momentum \( p_1 \) with the initial condition (1.4) corresponding to a trajectory. The evolution operator \( U(t) \) satisfies the integro-differential equation
\[
U(t) = e^{-i\lambda_0 t} - i \int_0^t dt' e^{-i\lambda_0 (t-t')} \lambda L V U(t').
\]  
(12.1)

The iteration of this equation leads to a perturbation expansion of \( U(t) \). Applying the expansion to the momentum in (3.22) for \( j = 1 \), we obtain the first order contribution of \( \lambda \),
\[
\begin{align*}
 p_1(t) & \approx p_1^0 + \lim_{\Omega \to \infty} \lambda \int dp \ p_1 \sum_k (L_V)_{0, \nu, \nu, \nu, \nu} \frac{1}{k \cdot \nu_0 - i\epsilon} (e^{-ik \cdot \nu_0 t} - 1) e^{-ik \cdot q_0} \\
 & - p_1^0 + \lim_{\Omega \to \infty} \frac{\lambda}{\Omega} \sum_{k} \sum_{n=2}^{N} \frac{V_k}{k \cdot g_{1n}^0 - i\epsilon} (e^{-ik \cdot q_{1n}^0 t} - 1) e^{-ik \cdot (q_{1n}^0 - q_0)}.
\end{align*}
\]  
(12.2)

where we have added \(-i\epsilon \) with the positive infinitesimal \( \epsilon \) in the denominator. This addition does not change the value of the right-hand side, since \( k \cdot \nu_0 = 0 \) is not the singular point of the integrand in (12.2).
Let us first consider the case where \( N \) is finite. With nonvanishing initial velocity of the particle, the interaction terminates after a finite time scale. Hence, the interaction among the particles is transient, and the value of \( p_1(t) \) reaches asymptotically a constant. Indeed, for \( t \to +\infty \), the time dependent term in (12.2) vanishes, as the pole at \( k \cdot g_{1n} = +ie \) in this term does not contribute for \( t > 0 \) (see [2]). Then we obtain (for \( t \to +\infty \))

\[
p_1(t) \to p_1^0 + \lambda \sum_{n=2}^{N} \int \frac{dk}{k \cdot g_{1n}^{(0)} - ie} k e^{-ik \cdot (q_1^n - q_2^n)} + O(\lambda^2) = P_1^D(q^0, p^0).
\]

(12.3)

This corresponds to \( P_1^D(q^0, p^0) \) in (9.14). Recall that the contributions to the invariant come only from the space \( \Pi^{(0)} \). In contrast, the time dependent term in (12.2) is the contribution from the creation operator \( \lambda C_{1}^{(2)} \) in the \( \Pi^{(2)} \) subspace associated with the binary correlations \( P^{(2)} \). Hence, the asymptotic contribution comes only from the \( \Pi^{(0)} \) subspace.

As mentioned (see after (9.16)), the resonance singularity at \( k \cdot g_{1n} = 0 \) in the denominator in (12.3) leads to a nonvanishing contribution in the limit of \( |q_1^n - q_2^n| \to \infty \), even for the short-range interaction. Due to the collisions, long-range correlations are built up. As a result, (12.3) may diverge in the limit \( N \to \infty \). Then, trajectories do not belong to the domain of \( D^{(0)} \), and neither to the domain of \( A \). As the thermodynamic limit implies the existence of "intensive variables", this limit does not exist when \( p_1(t) \) diverges for \( N \to \infty \).

However, there are classes of initial conditions that give a finite contribution to \( p_1(t) \) as well as to \( P_1^D(q^0, p^0) \), even in the limit \( N \to \infty \). For example, let us suppose that the initial positions of the particles \( q_0^n \) are chosen randomly. Here, random means that the algorithm to write the sequence \( q_1^n, q_2^n, q_3^n, \ldots \) is "incompressible" [45]. Then, in the thermodynamic limit, the summation over \( n \) and \( k \) in (12.2) gives a contribution of order

\[
\frac{1}{\Omega} \sum_{k} \sum_{n}^{N} f_k e^{-ik \cdot (q_1^n - q_2^n)} \sim \frac{\sqrt{N \lambda^3}}{L^3}.
\]

(12.4)

As a consequence, the right-hand side of (12.2) gives a finite contribution of order \( \sqrt{c} \) in this limit. One can verify this estimate by taking the average of the square of the absolute value of (12.4) over \( q_0^n \) with the assumption of an uniform distribution of \( q_0^n \) in space. In this estimate, we have to take the thermodynamic limit after taking the average. This then shows that the square is of order \( c \) in the thermodynamic limit.

Let us remark that this estimate of the concentration dependence is valid only for the ensemble average over the random distribution of the initial positions. For each given sequence \( q_1^n, q_2^n, q_3^n, \ldots \), the value of the summation (12.4) may change significantly. However, the interest of this estimate is that it guarantees a finite value of (12.4) for almost all choices of the initial condition \( q_1^n, q_2^n, q_3^n, \ldots \) for a single trajectory in the thermodynamic limit, as the average of the square of absolute value is finite. The random numbers are generic points in phase space [45].

Note that if we would first replace the summation over the wave vector by the integral in each individual term in the summation over \( n \) in (12.2) (such as has been done in (12.3)), then take the limit \( N \to \infty \) assuming a random distribution of the particles, we would obtain a diverging contribution of order \( \sqrt{N} \). This shows that we have to perform the summation over \( N \) and over \( k \) simultaneously.

As the result of a random initial condition, the destruction operator in (9.14), as well as in (9.15), gives a finite contribution for the trajectory in the thermodynamic limit. Moreover, the collision operator \( \theta_2 \) (which corresponds to a diagonal transition) in (9.16) also gives a finite

\[\text{\footnotesize \textsuperscript{16}}\text{The above argument holds in any order of } \lambda \text{ whenever the } T\text{-matrix exists, as the long-range correlation is the result of the resonance at } k \cdot \psi^0 = 0 \text{ in the denominator of } (9.11). \text{ In quantum mechanics, there are many examples whose explicit form of the } T\text{-matrix are known, such as the delta-shell potential, separable potential, \ldots.}\]
contribution in the thermodynamic limit, which is of order $c$ regardless of the random or coherent choice of the initial values $q_n^0$, as $\theta$ does not depend on $q_n^0$. One can easily see that for every order in $\lambda$ the destruction operator gives finite contribution. Moreover, one can extend these estimates for the reduced observables (3.20) depending on a finite number of particles. This shows that this class of initial conditions belongs to the domain of the nonunitary transformations.

It is interesting to compare the trajectory in the thermodynamic limit $N \to \infty$ with the one with a random distribution of $q_n^0$ but for a finite number $N$ of particles. If $N$ is large but finite, then (12.4) vanishes as $L^{-3/2}$ in the large volume limit. As a result, the interactions in (12.3) vanish. Hence, the value of $p_1(t)$ approaches to its initial value (for $t \to \infty$)

$$p_1(t) \to p_1^0, \quad \text{(in the average).}$$  \hspace{1cm} (12.5)

This contrasts with the situation in the thermodynamic limit with the random distribution of the scatterers. In this limit, the collision operator is nonnegligible and leads to diffusion processes. The trajectory is not maintained in time. The trajectory “collapses” due to the Poincaré resonances. For example, one can evaluate $\langle p_1(t) \rangle$ as well as $\langle |p_1(t)|^2 \rangle$ for a given initial condition of a single trajectory. We have, of course, $\langle p_1(0) \rangle^2 = \langle |p_1(0)|^2 \rangle$. But, because of the nonnegligible contribution of the collision operator, we have $\langle p_1(t) \rangle^2 \neq \langle |p_1(t)|^2 \rangle$ for $t > 0$. The momentum $p_1(t)$ becomes a stochastic variable and obeys a Langevin type of stochastic equation. The usual sense of the trajectory is thus destroyed. An explicit calculation of this for the “perfect Lorentz gas” can be found in [2].

In [2], we have also shown that all effects of initial correlations in $\Pi^{(\omega)}$ subspace except for $\Pi^{(0)}$ vanish asymptotically. In the $\Pi^{(0)}$ subspace, the correlation is generated from the vacuum of correlation $P^{(0)}$ through the creation operator $C^{(0)}$ (see (4.34)). As illustrated in (3.18), the interaction $\lambda L_V$ (hence, the creation operator) introduces an extra volume factor $\Omega^{-1}$ as compared with the states in the vacuum of correlation. This is a general property of the $\Pi^{(0)}$ subspace, and one can easily verify that the states in the $\Pi^{(0)}$ subspace satisfy the delta function singularity in (3.15). Therefore, the delta function singularity in Fourier space emerges as time goes on, even if we start from a nonsingular distribution function. The class of singular distribution functions (3.15) acts again as an attractor.

In conclusion, the maintenance of the volume dependence of the trajectory (1.4) and the existence of a thermodynamic limit are incompatible. Whenever the thermodynamic limit exists, the trajectory becomes stochastic and approaches the class of singular distribution functions (3.15) in the sense of distribution.

13. HARMONIC LATTICES

Next we consider the other typical systems in classical mechanics, i.e., harmonic and anharmonic lattices. We first summarize briefly the situation for harmonic lattices. For simplicity, we consider one-dimensional lattices. We assume that $N$ atoms with mass $m$ are equally spaced with a distance $a$ in the equilibrium position, and the equilibrium potential energy $U_0$. For the excited lattice, the potential energy $U$ is the quadratic form

$$U - U_0 = \frac{1}{2} \sum_{n,n'} A_{n,n'} u_n u_{n'}, \quad (13.1)$$

where $u_n$ is the displacement of the $n^{th}$ atom from its equilibrium position. We impose cyclic boundary conditions $u_{n+N} = u_n$.

We then introduce normal coordinates $q_k$ (for more details, see [19])

$$u_n = \sum_k q_k e^{ika}, \quad (13.2)$$
where (with integer \( j \))

\[
    k = \frac{2\pi}{Na} j,
\]

(13.3)

and angle \( \alpha_k \) and action variable \( J_k \) related to \( q_k \) through \( (\omega_k = \omega_{-k}) \)

\[
    q_k = \frac{1}{\sqrt{2Nm}} \left\{ \left( \frac{J_k}{\omega_k} \right)^{1/2} e^{i\alpha_k} + \left( \frac{J_{-k}}{\omega_{-k}} \right)^{1/2} e^{-i\alpha_{-k}} \right\},
\]

(13.4)

Neglecting anharmonic terms, we obtain the expected form for the Hamiltonian

\[
    H_0 = \sum_k \omega_k J_k.
\]

(13.5)

The equations of motion are obviously

\[
    \dot{J}_k = 0,
    \dot{\alpha}_k = \omega_k.
\]

(13.6)

We next consider the statistical description in terms of distribution functions \( \rho(J, \alpha, t) \) which satisfy the Liouville equation

\[
    i\frac{\partial \rho}{\partial t} = L_0 \rho, \quad L_0 \equiv -i\omega \frac{\partial}{\partial \alpha}.
\]

(13.7)

The eigenfunctions \( \varphi_{(n)} \) and eigenvalues \( l_{(n)} \) are

\[
    \varphi_{(n)} = N_0 \exp \left[ i \sum_k n_k \alpha_k \right] \quad \text{and} \quad l_{(n)} = \sum_k n_k \omega_k,
\]

(13.8)

where \( N_0 \) is a normalization constant.

Now let us consider more closely the limit \( N \to \infty \). Using (13.2) and (13.4), we obtain terms of the form

\[
    u_n = \sqrt{\frac{2}{Nm}} \sum_k e^{i\kappa_n} \sqrt{\frac{J_k}{\omega_k}} e^{i\alpha_k}.
\]

(13.9)

In the limit \( N \to \infty \),

\[
    \frac{2\pi}{Na} \sum_k \to \int dk.
\]

(13.10)

The condition

\[
    u_n \to \text{finite} \quad \text{for} \ N \to \infty,
\]

(13.11)

imposes that

\[
    \sum_k e^{i\alpha_k} \sim \sqrt{N} \quad \text{for} \ N \to \infty.
\]

(13.12)

The angle variables must therefore behave as "stochastic variables" to which we can apply the law of large numbers. Not all initial conditions are compatible with (13.11). If (13.12) is not satisfied, we have to leave the model of a harmonic solid. Note that this condition means that the sequence \( \alpha_{k_1}, \alpha_{k_2}, \ldots \) with \( k_j = (2\pi j/Na) \) is again "incompressible" [45] and have, therefore, a larger probability to realize the situation (13.12). They correspond to a stochastic sequence among the real number sequences for \( 0 \leq \alpha_{k_j} < 2\pi \). We hope to come back to this problem in a forthcoming publication.
We now turn to the statistical description (13.7). As could be expected, there is here a complete equivalence of this description to the individual descriptions (see [19]). Now let us impose Hilbert space structure for the statistical description. We expand $\rho(J, \alpha)$ in a Fourier series. With obvious notations,
\[
\rho(J, \alpha) = \sum_{\{n\}} \rho_{\{n\}}(J) \exp \left[ i \sum n_k \alpha_k \right].
\]
(13.13)

The Hilbert norm is therefore
\[
\langle \rho | \rho \rangle = \int dJ \sum_{\{n\}} |\rho_{\{n\}}(J)|^2.
\]
(13.14)

This norm is preserved in time. To obtain a finite Hilbert norm for $N \to \infty$, well-defined conditions have to be satisfied. Indeed, the norm (13.14) contains such terms as (with $n_k = \ldots, -1_k, 0, 1_k, 2_k, \ldots$)
\[
|\rho_0|^2 + \sum_k |\rho_{1_k}|^2 + \sum_{kk'} |\rho_{1_k 1_{k'}}|^2 + \sum_{kk'k''} |\rho_{1_k 1_{k'} 1_{k''}}|^2 + \cdots,
\]
(13.15)

which have to converge for $N \to \infty$. This implies
\[
\rho_0 \sim 0(1), \quad \rho_{1_k} \sim \frac{1}{\sqrt{N}}, \quad \rho_{1_k 1_{k'} 1_{k''}} \sim \frac{1}{N}
\]
(13.16)

(the summation $\sum_{kk'k''}$ is over $k + k' + k'' = 0$ or a vector of the reciprocal lattice). To guarantee that (13.14) is finite, we could of course also have, e.g., $\rho_{1_k 1_{k'} 1_{k''}} \sim N^{-3/2}$. But if $\rho_{1_k 1_{k'} 1_{k''}} \sim N^{-1/2}$, the norm diverges and the limit $N \to \infty$ leads outside the Hilbert space. This is the situation we shall meet for anharmonic solids in the next section.

The Hilbert space structure is equivalent to the trajectory description including the randomness condition (13.12). Indeed using (13.9), (13.13), and (13.16), we have
\[
\langle u_n \rangle \sim \frac{1}{\sqrt{N}} \sum_k \int dJ \sqrt{J} \rho_{-1_k} \sim 0(1).
\]
(13.17)

We may calculate in the same way other averages such as $\langle u_n u_{n'} \rangle$ or $\langle u_n u_{n'} u_{n''} \rangle$.

Note that using (13.9) and (13.16)
\[
\langle u_{n_1} u_{n_2} u_{n_3} \rangle \sim \frac{1}{N^{3/2}} \sum_{k_1 k_2 k_3} \int dJ \rho_{1_{k_1} 1_{k_2} 1_{k_3}}
\sim \frac{1}{N^{3/2}} N^2 \frac{1}{N} \sim \frac{1}{\sqrt{N}} \to 0
\]
(13.18)

(again with the condition $k_1 + k_2 + k_3 = 0$). There appear only "even" correlations for the harmonic lattice.

14. ANHARMONIC LATTICES

We come now to anharmonic lattices. The potential energy is now (see (13.1))
\[
U - U_0 = \frac{1}{2} \sum_{nn'} A_{nn'} u_n u_{n'} + \frac{1}{6} \sum_{nn'n''} B_{nn'n''} u_n u_{n'} u_{n''}.
\]
(14.1)

The Hamiltonian $H$ becomes
\[
H = H_0 + \lambda V.
\]
(14.2)
with after a few calculations (see [19])

$$V = \sum_{kk'k''} \left( \frac{J_k J_{k'} J_{k''}}{\omega_k \omega_{k'} \omega_{k''}} \right)^{1/2} \left[ V_{kk'k''} e^{i(\alpha_k + \alpha_{k'} + \alpha_{k''})} + 3V_{k'k''} e^{i(\alpha_k - \alpha_{k'} - \alpha_{k''})} + \text{c.c.} \right], \quad (14.3)$$

where we have introduced the parameter \( \lambda \) for the coupling constant. Note that as can be easily verified (see [19])

$$V_{kk'k''} \sim \frac{1}{\sqrt{N}}. \quad (14.4)$$

Also here the summation over \( k, k', k'' \) is restricted to vectors on the reciprocal lattice.

We shall show that both the trajectory description and the Hilbert space structure are incompatible with the thermodynamic limit \( N \to \infty \). In thermodynamic equilibrium (equipartition theorem),

$$\langle V \rangle \sim N. \quad (14.5)$$

In contrast, using (13.16) corresponding to the Hilbert space structure, we obtain at most

$$\langle V \rangle \sim \sum_{kk'k''} \int dJ V_{kk'k''} \rho_{111} \sim \frac{1}{\sqrt{N}} N^2 \frac{1}{N} \sim \sqrt{N}. \quad (14.6)$$

This shows already that thermodynamic equilibrium (14.5) lies outside the Hilbert space (see also [19, and its Appendix III]). To obtain (14.5), we need stronger "correlations", such as

$$\rho_{1111} \sim \frac{1}{\sqrt{N}}, \quad (14.7)$$

but then the Hilbert space norm diverges.

This is a strong indication that the approach to equilibrium requires one to give up the Hilbert space description as for interacting particles. There is, however, an interesting difference. In the case of interacting particles, the Hilbert space norm vanishes in the limit \( N \to \infty \) (see (3.19), while here it diverges.

Let us now describe the time evolution of anharmonic lattices in the Liouville formulation [19]. For interacting systems, we have

$$L = L_0 + \lambda L_V. \quad (14.8)$$

We use the matrix notation

$$\langle \{n\} | L_V | \{n'\} \rangle = \frac{1}{(2\pi)^N} \int_0^{2\pi} \cdots \int_0^{2\pi} d\alpha_1 \cdots d\alpha_N$$

$$\times \exp \left[ -i \sum_k n_k \alpha_k \right] \exp \left[ i \sum_k n'_k \alpha_k \right]. \quad (14.9)$$

We obtain directly for the only nonvanishing matrix elements [19]

$$\langle n_k n_{k'} n_{k''} | L_V | n_k \pm 1, n_{k'} \pm 1, n_{k''} \pm 1 \rangle$$

$$= V_{\mp, \mp, \mp} \left[ \frac{n_k}{2J_k} + \frac{n_{k'}}{2J_{k'}} + \frac{n_{k''}}{2J_{k''}} \pm \frac{\partial}{\partial J_k} \pm \frac{\partial}{\partial J_{k'}} \pm \frac{\partial}{\partial J_{k''}} \right] (J_k J_{k'} J_{k''})^{1/2}. \quad (14.10)$$

Note that this is still an operator acting on the actions \( J_k \).

Starting from (14.8), we can now introduce the dynamics of correlations similarly to the interacting particles. The contribution \( \rho_0 \) is called the "vacuum of correlations" and plays an
especially important role. As the result of (14.7), we may have “destruction (of correlation) processes” such as represented graphically in Figure 1.

Now using (14.4) and (14.10), we see immediately that Figure 2 leads precisely to (14.7). Correlations are amplified by anharmonic effects and bring us outside the Hilbert space.

The trajectory description is destroyed as well. Indeed because of Poincaré resonances, we now also have “diffusive processes” such as represented in Figure 3. Each vertex contains de-
rivative operators $\frac{\partial}{\partial J}$; Figure 3 leads, therefore, to diffusive processes containing second order operators $\frac{\partial^2}{\partial J^2}$ characteristic of diffusive processes.

Let us mention that these diffusive processes to order $\lambda^2$ represent Fokker-Planck type of contributions which break time symmetry [19]. The operator appearing in Figure 3 can be easily obtained explicitly (see [19, (2.8.6)]). It is

$$\lim_{N \to \infty} \sum_{k,k',k''} \pi \delta (\omega_k + \omega_{k'} - \omega_{k''}) \left| \frac{V_{kk'} - V_{k''}}{\omega_k \omega_{k'} \omega_{k''}} \right|^2$$

$$\times \left( \frac{\partial}{\partial I_k} + \frac{\partial}{\partial I_{k'}} - \frac{\partial}{\partial I_{k''}} \right) J_k J_{k'} J_{k''} \left( \frac{\partial}{\partial I_k} + \frac{\partial}{\partial I_{k'}} - \frac{\partial}{\partial I_{k''}} \right).$$

(14.11)

The action variable now becomes a stochastic variable. As a result, even if we would start with well-defined action variables $\prod (J_k - J^2_k)$ trajectories are destroyed by diffusion. Equation (14.11) leads for times of the order of the relaxation time ($\sim \lambda^{-2}$ for weak interactions) to

$$\langle J_k^2 \rangle \sim \langle J_k \rangle^2 \sim t.$$  

(14.12)

There are "non-Newtonian contributions". In this sense, the trajectory again collapses.

There are, of course, many comments which could be made, but this would bring us outside the range of this article. Let us only emphasize the role of the $\delta$ function for the frequency in (14.11) which comes from Poincaré resonances. For Poincaré integrable systems, there would be no "collapse" of the trajectory and the Hilbert space structure would be preserved as then we could introduce cyclic action-angle variables. The problem would then be similar to that of harmonic oscillators.

The main difference of anharmonic lattices from the problem of interacting particles is that even if we start with a Hilbert space structure (that means with $\rho$ corresponding to a finite Hilbert norm), anharmonic forces lead, time going on, outside the Hilbert space.

15. CONCLUDING REMARKS

As is well known since the fundamental work by von Neumann, quantum mechanics has been associated with the Hilbert space [46]. Koopman applied the Hilbert space structure to statistical mechanics [47]. To include the observed irreversibility, however, we have to go beyond the Hilbert space as the evolution in classical or quantum mechanics is ruled by the Hermitian Liouville operator.

The main result of this paper is the extension of the Liouville operator $L_H$ for LPS to the class of functions which are singular in their Fourier expansions for the space variables (interacting particles) or for angle variables (anharmonic lattices): Sections 4, 5 and 14, 15. These functions play an essential role in statistical mechanics: Section 3. The spectral decomposition of $L_H$ in this function space has quite unique features. The eigenvalues are complex and are given by the spectral decomposition of the collision operator $\Theta$. Non-Newtonian contributions appear in this representation. They will be "hidden" in the spectral representation in the Hilbert space, if this representation could be obtained (even its existence is in doubt).

There is of course much overlapping with our early work [19–23, 27–29]. The main difference is that at this time we assumed that we had to limit ourselves to the Hilbert space. To obtain a semigroup representation (including complex eigenvalues), we had to introduce a nonunitary transformation from the distribution function $\rho$ to a new distribution function $\tilde{\rho} = \Lambda \rho$ (the so-called "physical" representation). Now irreversibility appears already in $\tilde{\rho}$. The nonunitary transformation theory appears naturally as the result of the intertwining relation between $L_H$ and $\Theta$ (see Section 6).

This nonunitary transformation is necessary to formulate $\mathcal{H}$-quantities which decrease with time until equilibrium is reached. The existence of $\mathcal{H}$-functions has nothing to do with extra-dynamical
assumptions such as coarse graining but is a consequence of the time symmetry breaking due to Poincaré resonances.

The value of the $H$-function depends on the deviation from equilibrium. It is natural to assume the existence of an entropy behavior. Only states which lead to finite values of $H$ are found in nature (or can be prepared). In more anthropomorphic terms that means that only systems involving a "finite information" exist in nature. From the mathematical point of view, this means only distribution functions which are in the domain of the nonunitary transformation $\Lambda$. Of special interest to us is the so-called thermodynamical limit. The existence of this limit requires special conditions as the result of the long-range correlations due to Poincaré resonances. As shown in Section 12, this leads to the conclusion that the thermodynamic limit is always associated with a singular distribution function lying outside the Hilbert space. If we would start with a trajectory, it would "collapse". The concept of a trajectory is no more the basic, primitive concept as assumed in classical dynamics as in general for LPS we need a statistical description. But this is not due to our "ignorance" but to the effect of the non-Newtonian terms due to resonances.

The extension to "non-Hilbert" spaces is an element which is common with the spectral theory associated with deterministic chaos [18]. But the nature of the function space is quite different. Here the extension is introduced to avoid the difficulties associated with "sensitivity to initial conditions". Here the main new element is the role of resonances associated with persistent interactions. This latter condition means that we have to consider the system as a whole. If we would extract any $N$ particles and treat them in isolation, all dissipative effects would vanish and we would come back to the traditional trajectory description.

We are well aware that there are many interesting mathematical and physical questions which need further elaboration. We limited ourselves to repulsive forces for the interacting particles. It would be interesting to consider also the effect of attractive forces. Also we have used formal expressions in the coupling constant $\lambda$ without studying their radius of convergence. In concrete situations we may need partial resummations.

We have shown that irreversibility can be included in the classical dynamic description. This unification of dynamics and thermodynamics requires a statistical formulation of the laws of dynamics and gives to them a new meaning in agreement with the evolutionary patterns of nature.

The situation studied here is closely related to quantum mechanics (interacting particles and nonlinear quantum field). There also we expect that we have in general to go outside the Hilbert space. The parallel results in quantum mechanics mean also giving up the wave function description and the Hilbert space. It becomes, therefore, interesting to reconsider some of the basic problems of modern physics from this point of view.

REFERENCES