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Poincaré Resonances and the Extension of Classical Dynamics

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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 non-integrable Poincaré systems (LPS) the two descriptions are not equivalent. Practically all dynamical systems studied in statistical mechanics belong to the class of LPS. The basic step is the extension of the Liouville operator L_H outside the Hilbert space to functions singular in their Fourier transforms. This generalized 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 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 part refers to the various irreversible processes such as relaxation times, diffusion etc. Irreducible means that these representations cannot be implemented by trajectory theory. As a result, the dynamical group of evolution splits into two semi-groups. 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'.

The reason for the new features is the appearance of new, non-Newtonian effects due to Poincaré resonances. The resonances couple dynamical events and lead to 'collision operators' (such as the Fokker–Planck operator) well-known from various phenomenological approaches to non-equilibrium physics. These 'collision operators' represent diffusive processes and mark the breakdown of the deterministic description which was always associated with classical mechanics. 'Subdynamics' as discussed in previous publications, is derived from the spectral representation.

The eigenfunctions of the Liouville operator have remarkable properties as they lead to long-range correlations due to resonances even if the interactions as included in the Hamiltonian are short-range (only equilibrium correlations remain short-range). This is in agreement with the results of non-equilibrium thermodynamics as the appearance of dissipative structures is connected to long-range correlations.

In agreement with previous results, it is shown that there exists an intertwining relation between L_H and the collision operator Θ as defined in the text. Both have the same eigenvalues and are connected by a non-unitary similitude $\Lambda L_H \Lambda^{-1} = \Theta$. The various forms of Λ and their symmetry properties are discussed. A consequence of the intertwining relation are 'non-linear Lippmann–Schwinger' equations which reduce to the classical linear Lippmann–Schwinger equations when the dissipative effects due to the Poincaré resonances can be neglected.

Using the transformation operator Λ, we can define new distribution functions and new observables whose evolution equations take a specially simple form (they are 'bloc diagonalized'). Dynamics is transformed in an infinite set of kinetic equations. Starting with these equations, we can derive $\mathcal{H}$-functions which present a monotonous time behavior and reach their minimum at equilibrium. This requires no extra-dynamical assumptions (such as coarse graining, environment effects ...). Moreover, our formulation is valid for strong coupling (beyond the so-called Van Hove's $\lambda^2 t$ limit).

We then study the conditions under which our new non-Newtonian effects are observable. For a finite number N of particles and transient interactions (such as realized in the usual scattering experiments) we recover traditional trajectory theory. To observe our new effects we need persistent interactions associated to singular distribution functions. We have studied in detail two examples, both analytically and by computer simulations. These examples are persistent scattering in which test particles are continuously interacting with a scattering center, and the Lorentz model in which a 'light' particle is scattered by a large number of 'heavy' particles. The agreement between our theoretical predictions and the numerical simulations is excellent. The new results are also essential in the thermodynamic limit as introduced in statistical mechanics. We recover also, the results of non-equilibrium statistical mechanics obtained by various phenomenological approximations.

Of special interest is the domain of validity of the trajectory description as a trajectory is traditionally considered as a primitive, irreducible concept. In the Liouville description the natural variables are wave vectors $\mathbf{k}$ which are constants in free motion and modified by interactions and resonances. A trajectory can be considered as a coherent superposition of plane waves corresponding to wave vectors $\mathbf{k}$. Resonances correspond to non-local processes in space-time. They threaten therefore the persistence of trajectories. In fact, we show that whenever the thermodynamic limit exists, trajectories are destroyed and transformed into singular distribution functions. We have a 'collapse' of trajectories, to borrow the terminology from quantum mechanics. The trajectory becomes a stochastic object as in Brownian motion theory.

In conclusion, we obtain a unified formulation of dynamics and of thermodynamics. This involves the introduction of LPS which leads to dissipation together with the consideration of delocalized situations. From this point of view, there is a strong analogy with phase transitions which are also defined in the thermodynamic limit. Irreversibility is, in this sense, an 'emergent' property which could not be included in classical dynamics as long as its study was limited to local, transient situations.

1. INTRODUCTION

In the past it has been repeatedly asked if quantum mechanics is 'complete'. The reason to ask this question is the difficulty to incorporate measurement and more generally dissipative processes in the frame of the conventional formulation of quantum theory. Similar questions can also be asked in the frame of classical mechanics. In previous papers [1–14] we have already indicated that these questions can be answered by formulating classical or quantum mechanics on the statistical level for classes of unstable dynamical systems (deterministic chaos, large Poincaré systems (LPS) which are non-integrable and for which the frequencies are continuous functions of wave length). Here we shall present an overview of our extension of classical mechanics for LPS.

In classical mechanics trajectories occupy a privileged position (somewhat as pure states in quantum theory) as equations of motion correspond to point transformations. In addition, there exists the ensemble description introduced by Gibbs and Einstein. The statistical description has been considered to be only a question of practical convenience or approximation. It was always admitted that the 'individual' description in terms of trajectories and the statistical description in terms of ensembles were equivalent. It is this equivalence which is destroyed for the classes of unstable systems we consider. There appear new solutions on the statistical level which cannot be implemented by trajectory dynamics. As a result the laws of dynamics take a new form for LPS. They now express 'possibilities' and not 'certitudes'. Moreover, they incorporate time-symmetry breaking as they lead to a semi-group description. We can in this way construct $\mathcal{H}$-functions on a purely dynamical basis and unify dynamics and thermodynamics.

We consider Hamiltonians which are of the form

$$H(q, p) = H_0(p) + \lambda V(q) = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} + \lambda \sum_{j>i}^{N} V(|\mathbf{q}_i - \mathbf{q}_j|), \tag{1}$$

where λ is the coupling constant, and q and p are N-component vectors, i.e., $q \equiv (\mathbf{q}_1, \ldots, \mathbf{q}_N)$ with three-dimensional vectors $\mathbf{q}_j$, and so on. The system is put into a large box with volume L^3. These are the systems studied in equilibrium and non-equilibrium statistical mechanics. It is well known that these systems are in general non-integrable in the sense of Poincaré. In the large limit $L^3 \to \infty$ we obtain LPS. The number of particles N may be finite or infinite. We shall be especially interested in the 'thermodynamic limit',

$$N \to \infty, \quad \text{and} \quad L^3 \to \infty \quad \text{with} \quad c = N/L^3 = \text{finite}. \tag{2}$$

The statistical description in classical dynamics is expressed by the Liouville equation for the distribution function [17–19],

$$i\frac{\partial}{\partial t}\rho(t) = L_H\rho(t). \tag{3}$$

Here $L_H\rho \equiv i\{H, \rho\}$ is the Poisson bracket of ρ 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 non-local ensembles. A special case of localized ensembles are single trajectories,*

$$\rho(q, p, 0) = \frac{1}{L^{3N}}\prod_{j=1}^{N}\sum_{\mathbf{k}_j} e^{i\mathbf{k}_j(\mathbf{q}_j - \mathbf{q}_j^0)}\delta(\mathbf{p}_j - \mathbf{p}_j^0) \to \prod_{j=1}^{N}\delta(\mathbf{q}_j - \mathbf{q}_j^0)\delta(\mathbf{p}_j - \mathbf{p}_j^0) \quad \text{for} \quad L \to \infty. \tag{4}$$

Associated to a finite number of particles, localized distributions ρ describe transient interactions (free in and out states) as studied in quantum S-matrix theory. In contrast non-local ensembles describe persistent interactions as studied in statistical mechanics. They are, as just mentioned, characterized by singularities in their Fourier transforms (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 to collision operators 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 non-unitary transformation operators Λ 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 [14, 20–31]. In the previous work subdynamics has been constructed by using an ansatz for the analytic continuation (the so-called $i\epsilon$ rule) (see for example [31]). We now may derive subdynamics from the complex spectral representation. Using our non-unitary transformation theory we can transform the Liouville equation for ρ into an infinite set of 'kinetic equations' (see Section 6). We also obtain a new formulation of the Heisenberg type of equation for the evolution of observables which makes explicit

*In the box normalization formalism which we shall consider in this paper, the delta function in space is replaced by a periodic delta function with 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 a single point of phase space.

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 '$\mathcal{H}$-functions' derived usually through phenomenological assumptions (Sections 7 and 8). Our non-unitary transformation theory allows us 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 the collision operator Θ lead to a non-linear extension of the Lippmann–Schwinger type equations, well known from quantum scattering theory (see Section 9). When dissipative effects can be neglected, the non-linear terms vanish and we come back to the classical version of the Lippmann–Schwinger equation.

However, our equations differ from the Lippmann–Schwinger equation by our analytic continuation. There appears a degeneracy for LPS. The existence of Poincaré resonances[†] even in the non-dissipative 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 10–13 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 to 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 to distribution functions which are singular in their Fourier transforms (Sections 11 and 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 non-equilibrium statistical mechanics [17] (such as Fokker–Planck equations, Boltzmann equations, generalized master equations etc.). 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.

It is very interesting that the functional form of these distribution functions (see (45)) is invariant in respect to time. This form even acts as an attractor (see (143)). 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. Trajectories have always 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 $\mathbf{k}$.

Now in the statistical description the natural variables are precisely the wave vectors (see Section 2). The trajectory becomes a construct. Resonances correspond to non-local 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 then have a 'collapse' of trajectories to borrow the terminology from quantum mechanics (see Section 13).

[†]Here, 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 appear already for repulsive interactions. These resonances are not related to 'resonance poles' associated to the so-called resonance scattering.

We first ask: under which conditions does (4) in the limits $L \to \infty$ and $N \to \infty$ 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 Sections 8, 13, and Appendix J).

The results described here can easily be extended to quantum theory. There is 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 [32]).

Our predictions have been verified analytically and by computer simulations in simple situations such as the Lorentz model (see Appendices F, G and Refs [1, 2, 16]).

2. THE LIOUVILLIAN FORMALISM

The evolution of the system is governed by the Liouville equation (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,

$$\lim_{|p|\to\infty} \rho(q, p) \to 0. \tag{5}$$

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 non-local ensembles in phase space as considered in typical situations in statistical mechanics.

The formal solution of the Liouville equation is

$$\rho(t) = \mathcal{U}(t)\rho(0), \tag{6}$$

with

$$\mathcal{U}(t) = \mathrm{e}^{-iL_H t}. \tag{7}$$

$\mathcal{U}(t)$ 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 are defined by (with $\int \mathrm{d}q \equiv \int \mathrm{d}\mathbf{q}_1 \ldots \int \mathrm{d}\mathbf{q}_N$ and so on)

$$\langle\langle f|g\rangle\rangle \equiv \int \mathrm{d}q \int \mathrm{d}p \langle\langle f|q, p\rangle\rangle\langle\langle q, p|g\rangle\rangle = \int \mathrm{d}q \int \mathrm{d}p f^*(q, p)g(q, p), \tag{8}$$

and their Hilbert norms by

$$\|f\| \equiv \sqrt{\langle\langle f|f\rangle\rangle}. \tag{9}$$

We have introduced Dirac's 'bra' and 'ket' notations, i.e. $\langle\langle f|$ and $|g\rangle\rangle$, analogous to quantum mechanics. This permits us to use various representations. The Liouvillian L_H is a hermitian operator and $\mathcal{U}(t)$ unitary. That means as long as we remain in Hilbert space the eigenvalues l of L_H are real, and the eigenvalues $\exp(-ilt)$ of $\mathcal{U}(t)$ 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 to 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 $|\rho(0)\rangle\rangle = |q^0, p^0\rangle\rangle$ is represented by Dirac's delta function,

$$\rho(q, p, 0) = \langle\langle q, p|\rho(0)\rangle\rangle = \delta(q - q^0)\delta(p - p^0), \tag{10}$$

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

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

$$\langle\langle \hat{M}| = \int dq \int dp M(q, p)\langle\langle q, p|. \tag{11}$$

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

$$M(q, p) = \langle\langle \hat{M}|q, p\rangle\rangle. \tag{12}$$

The evolution of the observables is given by

$$\langle\langle \hat{M}(t)| = \langle\langle \hat{M}|^0 U(t). \tag{13}$$

They satisfy the classical 'Heisenberg equations' of motion,

$$i\frac{\partial}{\partial t}|\hat{M}(t)\rangle\rangle = -L_H|\hat{M}(t)\rangle\rangle. \tag{14}$$

The Hamiltonian equations of motion correspond to a special case of the Heisenberg equations for the set of observables $(\hat{\mathbf{q}}_j, \hat{\mathbf{p}}_j)$ associated to trajectories. Similarly, the Liouville equation (3) corresponds to the classical 'Schrödinger' picture of the equation of motion.

The expectation value of M is given by

$$\langle M\rangle_t = \langle\langle \hat{M}(0)|\rho(t)\rangle\rangle = \langle\langle \hat{M}(t)|\rho(0)\rangle\rangle. \tag{15}$$

Let us consider a system described by the Hamiltonian (1). For simplicity, we assume short-range repulsive interactions. Corresponding to the decomposition of the Hamiltonian (1), we have also (with $L_0 \equiv L_{H_0}$)

$$L_H = L_0 + \lambda L_V. \tag{16}$$

The unperturbed Liouvillian is the derivative operator $L_0 = -iv \cdot \partial/\partial q$, where $\mathbf{v}_j \equiv \mathbf{p}_j/m_j$ is the velocity of the particle j. Then the eigenstate of L_0 is given by

$$L_0|k, p\rangle\rangle = (k \cdot v)|k, p\rangle\rangle. \tag{17}$$

Here, $k \cdot v \equiv \mathbf{k}_1 \cdot \mathbf{v}_1 + \ldots + \mathbf{k}_N \cdot \mathbf{v}_N$, and

$$\langle\langle q, p'|k, p\rangle\rangle = L^{-3N/2} e^{ik \cdot q}\delta(p' - p), \tag{18}$$

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

$$\mathbf{k}_j = \mathbf{n}_j \Delta k. \tag{19}$$

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

$$\Omega^{-1}\sum_k \to \int d\mathbf{k}, \qquad \delta_\Omega(\mathbf{k}) \equiv \Omega\delta^{kr}(\mathbf{k}) \to \delta(\mathbf{k}). \tag{20}$$

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

[‡]Following the tradition for non-equilibrium statistical mechanics [19], we use the convention that the distribution functions are associated to ket-states, while the observables are associated to bra-states. See also the comment below [50].

Note that the eigenfunctions (18) 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,

$$\langle\langle k, p|k', p'\rangle\rangle = \delta^{kr}(k - k')\delta(p - p'), \qquad \sum_k \int dp|k, p\rangle\rangle\langle\langle k, p| = 1. \tag{21}$$

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

$$\rho(q, p, t) = \frac{1}{L^{3N/2}} \sum_k e^{ik\cdot(q-vt)} \langle\langle k, p|\rho(0)\rangle\rangle. \tag{22}$$

For a trajectory we have (see (4))

$$\langle\langle k, p|\rho(0)\rangle\rangle = \frac{1}{L^{3N/2}} e^{-ik\cdot q^0} \delta(p - p^0). \tag{23}$$

This leads with (22) to

$$\rho(q, p, t) = \delta(q - q^0 - vt)\delta(p - p^0). \tag{24}$$

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 λL_V is *off-diagonal* and leads to transitions from one set of wave vectors to another. Let us consider the matrix elements $(L_V)_{k',p';k,p}$ defined as

$$(L_V)_{k',p';k,p} \equiv \langle\langle k', p'|L_V|k, p\rangle\rangle = \frac{1}{L^{3N}} \int dq \int dq' \, e^{-ik'\cdot q} \langle\langle q, p'|L_V|q', p\rangle\rangle e^{ik\cdot q'}. \tag{25}$$

In this example, the only non-vanishing matrix elements are [17]

$$\begin{aligned}\langle\langle \mathbf{k}_j', \mathbf{k}_n', \{k\}^{N-2}, p'|L_V|\mathbf{k}_j, \mathbf{k}_n, \{k\}^{N-2}, p\rangle\rangle \\ = -\frac{1}{\Omega}\sum_{\mathbf{l}} \delta^{kr}(\mathbf{k}_j - \mathbf{k}_j' + \mathbf{l})\delta^{kr}(\mathbf{k}_n - \mathbf{k}_n' - \mathbf{l}) V_l[\mathbf{l}\cdot\mathbf{d}_{jn}\delta(p - p')], \\ = \frac{1}{\Omega}\sum_{\mathbf{l}} \delta^{kr}(\mathbf{k}_j - \mathbf{k}_j' + \mathbf{l})\delta^{kr}(\mathbf{k}_n - \mathbf{k}_n' - \mathbf{l}) V_l[\mathbf{l}\cdot\mathbf{d}_{jn}'\delta(p' - p)],\end{aligned} \tag{26}$$

where

$$\mathbf{d}_{jn} \equiv \partial/\partial\mathbf{p}_j - \partial/\partial\mathbf{p}_n, \tag{27}$$

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

$$V(|\mathbf{q}|) = \frac{1}{\Omega}\sum_l V_l e^{i\mathbf{l}\cdot\mathbf{q}}. \tag{28}$$

We assume $V_0 = 0$, i.e.,[§]

$$\int \mathrm{d}\mathbf{q} V(|\mathbf{q}|) = 0. \tag{29}$$

All indices k in (26) keep their values, except the two indices $\mathbf{k}_j$, $\mathbf{k}_n$; moreover, we have the conservation law of wave vectors,

$$\mathbf{k}'_n + \mathbf{k}'_j = \mathbf{k}_n + \mathbf{k}_j. \tag{30}$$

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 non-local ensembles. Let us first consider local ensembles. We consider the Fourier expansion of the distribution function

$$\rho(q, p, t) = \frac{1}{L^{3N}} \sum_k \mathrm{e}^{ik \cdot q} \bar{\rho}_k(p, t), \tag{31}$$

where (see the volume factor in (18))

$$\bar{\rho}_k(p, t) \equiv L^{3N/2} \langle\langle k, p | \rho(t) \rangle\rangle. \tag{32}$$

For local ensembles, the coefficients $\bar{\rho}_k(p)$ do not depend of the volume in the limit $\Omega \to \infty$. As we shall see later, this is not the case for non-local ensembles where $\rho(q, p) \neq 0$ in the limit $|\mathbf{q}_j| \to \infty$. In order to emphasize this fact and to distinguish (31) from the Fourier coefficients $\rho_k(p)$ for non-local ensembles, we put the bar on the coefficients $\bar{\rho}_k$. The distribution function (31) is normalizable as

$$\int \mathrm{d}q \int \mathrm{d}p \rho(q, p) = \int \mathrm{d}p \bar{\rho}_0(p) = 1. \tag{33}$$

A single trajectory belongs to this class (see (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 non-vanishing elements $\mathbf{k}_j$ in the wave vector $k = (\mathbf{k}_1, \ldots, \mathbf{k}_N)$.

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

$$\langle\langle \rho | \rho \rangle\rangle = \frac{1}{L^{3N}} \sum_k \int \mathrm{d}p |\bar{\rho}_k(p)|^2 \to \frac{1}{(2\pi)^{3N}} \int \mathrm{d}k \int \mathrm{d}p |\bar{\rho}_k(p)|^2. \tag{34}$$

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

On the other hand, statistical mechanics (equilibrium and non-equilibrium) deals mainly with non-local distributions, such as canonical distribution function. As in equilibrium problems it is useful to introduce reduced distribution functions f_s referring to s paticles. From the normalized distribution function ρ we may deduce the probability $\rho_s(\mathbf{q}_1 \cdots \mathbf{q}_s, \mathbf{p}_1 \cdots \mathbf{p}_s)$ of finding, at a given time t, a set of s specific particles 1, 2, ..., s with

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

*Trajectories are a special case of this class of distributions. They satisfy (33) but have no Hilbert space norm.

momenta $\mathbf{p}_1, \ldots, \mathbf{p}_s$ and coordinates $\mathbf{q}_1, \ldots, \mathbf{q}_s$

$$\rho_s(\mathbf{q}_1 \cdots \mathbf{q}_s, \mathbf{p}_1 \cdots \mathbf{p}_s) = \int \mathrm{d}q^{N-s}\, \mathrm{d}p^{N-s} \rho(q, p, t). \tag{35}$$

Distribution functions that refer to specified particles are called *specific* distribution functions [17]. We shall in general be more interested in the probability of finding s arbitrary particles at positions $\mathbf{q}_1, \ldots, \mathbf{q}_s, \mathbf{p}_1, \ldots, \mathbf{p}_s$. This probability, which we shall call f_s is found by multiplying ρ_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

$$\begin{aligned} f_s(\mathbf{q}_1 \cdots \mathbf{q}_s, \mathbf{p}_1 \cdots \mathbf{p}_s) &= \frac{N!}{(N-s)!} \rho_s(\mathbf{q}_1 \cdots \mathbf{q}_s, \mathbf{p}_1 \cdots \mathbf{p}_s) \\ &= \frac{N!}{(N-s)!} \int \mathrm{d}q^{N-s}\, \mathrm{d}p^{N-s} \rho(q, p). \end{aligned} \tag{36}$$

We shall also use distribution function φ_s in momentum space and n_s in coordinate space defined by

$$\begin{aligned} \varphi_s(\mathbf{p}_1 \cdots \mathbf{p}_s) &= \frac{(N-s)!}{N!} \int \mathrm{d}p^s f_s, \\ n_s(\mathbf{q}_1 \cdots \mathbf{q}_s) &= \int \mathrm{d}p^s f_s. \end{aligned} \tag{37}$$

The reduced distribution functions f_s, φ_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 non-local distributions. For this case distribution functions have 'delta function singularities' in their Fourier representation [17]. For example, let us consider the reduced number density in space given by $n_1(\mathbf{q}) = c + h(\mathbf{q})$, where c is a constant and h is an absolutely integrable function. In the Fourier representation we have (see (20))

$$n_1(\mathbf{q}) = \frac{1}{\Omega} \sum_{\mathbf{k}} (c\delta_\Omega(\mathbf{k}) + h_k) \mathrm{e}^{i\mathbf{k}\cdot\mathbf{q}}. \tag{38}$$

In the limit of large volume, the uniform part has a delta function singularity at $\mathbf{k} = 0$.

We note that the Hamiltonian (1) is also a non-local phase function, which has again a delta function singularity in its Fourier representation,

$$H(q, p) = \frac{1}{\Omega} \sum_{\mathbf{k}} \sum_{i}^{N} \left[\frac{\mathbf{p}_i^2}{2m_i} \delta_\Omega(\mathbf{k}) + \lambda \sum_{j(>i)}^{N} V_k \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{q}_j} \right] \mathrm{e}^{i\mathbf{k}\cdot\mathbf{q}_i}. \tag{39}$$

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

$$\rho^{eq}(q, p) = \frac{f(H_0 + \lambda V)}{\int \mathrm{d}q\, \mathrm{d}p f(H_0 + \lambda V)}. \tag{40}$$

We assume the normalization

$$\int \mathrm{d}p f(H_0) = 1. \tag{41}$$

Then, using (29) we have the power series expansion in the coupling constant λ for the Hamiltonian (1),

$$\rho^{eq} = \frac{1}{L^{3N}}\Bigg[1 + \frac{1}{2!}\lambda\sum_{i,j}^{N} V_{ij}\frac{\partial}{\partial H_0} + \frac{\lambda^2}{2}\Bigg(\frac{1}{2!}\sum_{i,j}^{N} V_{ij}V_{ij} + \frac{1}{3!}\sum_{i,j,m}^{N} V_{ij}V_{jm} + \frac{1}{4!}\sum_{i,j,m,n}^{N} V_{ij}V_{mn}\Bigg)\frac{\partial^2}{\partial H_0^2}$$
$$- \frac{\lambda^2}{2L^{3N}}\int \mathrm{d}qV^2\int \mathrm{d}p\left(\frac{\partial^2 f(H_0)}{\partial H_0^2}\right) + \lambda^3\cdots\Bigg]f(H_0), \tag{42}$$

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)

$$f(H) = \left(\frac{\beta}{2\pi m}\right)^{3N/2} \mathrm{e}^{-\beta(H_0+\lambda V)}. \tag{43}$$

We then obtain (with (39))

$$\rho^{eq}(q, p) = \frac{1}{L^{3N}}\left(\frac{\beta}{2\pi m}\right)^{3N/2} \mathrm{e}^{-\beta H_0}\Bigg[(1 + \lambda^2 \ldots)$$
$$+ \frac{1}{2!\Omega}\sum_{i,j}\sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{q}_i-\mathbf{q}_j)}\left(-\lambda\beta V_{|k|} + \lambda^2\beta^2\frac{1}{\Omega}\sum_{k'} V_{|\mathbf{k}'|}V_{|\mathbf{k}'-\mathbf{k}|} + \lambda^3 \ldots\right) \tag{44}$$
$$+ \frac{1}{3!\Omega^2}\sum_{i,j,n}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} \mathrm{e}^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{q}_i-\mathbf{k}\cdot\mathbf{q}_j-\mathbf{k}'\cdot\mathbf{q}_n}(\lambda^2\beta^2 V_{|\mathbf{k}|}V_{|\mathbf{k}'|} + \lambda^3 \ldots) + \ldots\Bigg].$$

Here, the first term in the bracket does not depend on the coordinates, so that this term is associated to a Fourier coefficient which has only vanishing wave vectors. The second term corresponds to contributions which have non-vanishing wave vectors $\mathbf{k}_i = \mathbf{k}$ and $\mathbf{k}_j = -\mathbf{k}$ 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 $\mathbf{q}_j \Rightarrow \mathbf{q}_j + \mathbf{a}$ for all j, then the total wave vector vanishes $\mathbf{k}_i + \mathbf{k}_j + \ldots = 0$).

The remarkable feature of the equilibrium distribution is that ρ^{eq} can be decomposed into the 'vacuum of correlations' (i.e. the first term in the bracket of (44)), binary correlations (the second term), ternary correlations (the third term) etc. Moreover, we see the appearence of delta function singularities as in (38). 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 ρ in terms of correlation functions which have a finite range of correlations in the thermodynamics limit [17, 18].

In our previous work in non-equilibrium statistical mechanics we used the class of ensembles which corespond to the natural generalization of the canonical distribution: [17, 18]

$$\rho(q, p) = \frac{1}{L^{3N}}\sum_{k} \mathrm{e}^{ik\cdot q}\Bigg[\rho_0(|p)\delta^{kr}(k) + \frac{1}{\Omega}\sum_{j>i}^{N}\rho_{\mathbf{k}_i,-\mathbf{k}_i}(\mathbf{p}_i, \mathbf{p}_j|p^{N-2})\delta_{\mathbf{k}_i+\mathbf{k}_j,0}\delta_{ij}^{kr}(k)$$
$$+ \frac{1}{\Omega^2}\sum_{n>j>i}^{N}\rho_{\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_n}(\mathbf{p}_i, \mathbf{p}_j, \mathbf{p}_n|p^{N-3})\delta_{\mathbf{k}_i+\mathbf{k}_j+\mathbf{k}_n,0}\delta_{ijn}^{kr}(k) + \ldots \tag{45}$$
$$+ \frac{1}{\Omega}\sum_{j}^{N}\rho'_{\mathbf{k}_j}(\mathbf{p}_j|p^{N-1})\delta_j^{kr}(k) + \frac{1}{\Omega^2}\sum_{j>i}^{N}\rho'_{\mathbf{k}_i,\mathbf{k}_j}(\mathbf{p}_i, \mathbf{p}_j|p^{N-2})\delta_{ij}^{kr}(k) + \ldots\Bigg].$$

Here, $\delta^{kr}(k)$ is a product of N Kronecker's delta, $\delta_j^{kr}(k)$ a product of $N-1$ Kronecker's delta which excludes the particle j, and $\delta_{ij}^{kr}(k)$ 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 non-vanishing elements $\mathbf{k}_j$ in the wave vector k. In the expression $\rho_{\mathbf{k}_i,\mathbf{k}_j,\ldots}(\mathbf{p}_i, \mathbf{p}_j, \ldots | p^{N-r})$, the momentum arguments on the left side of bar denote the particle i with a non-vanishing wave vector $\mathbf{k}_i$, the particle j with $\mathbf{k}_j$, ... 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 $\rho_{\mathbf{k}_i,\mathbf{k}_j,\ldots}$ and $\rho'_{\mathbf{k}_i,\mathbf{k}_j,\ldots}$ does not depend on the volume Ω, 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 (31), we have introduced the new notations $\rho_{\mathbf{k}_i,\mathbf{k}_j,\ldots}$ and $\rho'_{\mathbf{k}_i,\mathbf{k}_j,\ldots}$ instead of $\bar{\rho}_{\mathbf{k}_i,\mathbf{k}_j,\ldots}$ for the Fourier coefficients in (45). Here, the coefficients $\rho_{\mathbf{k}_i,\mathbf{k}_j,\ldots}$ are associated to the homogenous components of the distribution function in space (i.e., the component with the total wave vector vanishes $\mathbf{k}_i + \mathbf{k}_j + \ldots = 0$), while the coefficients $\rho'_{\mathbf{k}_i,\mathbf{k}_j,\ldots}$ are associated to the 'inhomogeneous' components (with $\mathbf{k}_i + \mathbf{k}_j + \ldots \neq 0$). This form of expansion leads to an extension of the cluster expansion in terms of the correlation functions in non-equilibrium statistical mechanics: i.e., the coefficients $\rho_0(p)$, $\rho_{\mathbf{k}_i,\mathbf{k}_j}(p)$, $\rho_{\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_n}(p)$, $\cdots$ are just the Fourier components of the momentum distribution functions (which correspond to the 'vacuum of correlation'), of the binary correlations, of the ternary correlations, and so on [17, 18]. As we have seen, interactions leads to transitions from one set of wave vectors to another. This corresponds to a 'dynamics of correlations' [17].

A characteristic feature of the distributions (45) is that all reduced quantities are well defined. For example, the expectation value of $\mathbf{q}_1 - \mathbf{q}_2$ is given by (in the thermodynamic limit)

$$\int dq \int dp(\mathbf{q}_1 - \mathbf{q}_2)\rho(q, p) = -i\left[\frac{\partial}{\partial \mathbf{k}} \int dp \rho_{\mathbf{k},-\mathbf{k}}(\mathbf{p}_1, \mathbf{p}_2 | p^{N-2})\right]_{\mathbf{k}=0} \tag{46}$$

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 (45) invariant. For example, let us assume that the system is initially in the vacuum of correlation. Because of the volume dependence in (18), we first note the relation between the Fourier coefficients $\rho_k(p)$ and the (k, p)-components $\langle\langle k, p|\rho\rangle\rangle$ of the distribution function,

$$\begin{aligned} \langle\langle 0, p|\rho\rangle\rangle &= \frac{1}{L^{3N/2}}\rho_0(|p), \\ \langle\langle \mathbf{k}_i, -\mathbf{k}_i, \{0\}^{N-2}, p|\rho\rangle\rangle \delta_{ij}^{kr}(k) &= \frac{1}{L^{3N/2}} \frac{1}{\Omega}\rho_{\mathbf{k}_i,-\mathbf{k}_i}(\mathbf{p}_i, \mathbf{p}_j | p^{N-2}), \\ &\vdots \end{aligned} \tag{47}$$

Also

$$\begin{aligned} \langle\langle \mathbf{k}_j, \mathbf{k}_n, \{0\}^{N-2}, p|\lambda L_V|\rho\rangle\rangle &= \int dp' \langle\langle \mathbf{k}_j, \mathbf{k}_n, \{0\}^{N-2}, p|\lambda L_V|0, p'\rangle\rangle \langle\langle 0, p'|\rho\rangle\rangle \\ &= -\frac{1}{L^{3N/2}} \frac{1}{\Omega} \lambda V_{|k_j|} \mathbf{k}_j \cdot \mathbf{d}_{jn} \rho_0(|p) \delta_{\mathbf{k}_j+\mathbf{k}_n,0}. \end{aligned} \tag{48}$$

This gives the same volume dependence as in the second expression in (47). One can extend this result to all orders of λ and to all Fourier components (see [17, 18] 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, as well as Appendix F).

We note the distribution function ρ (45) satisfies (33). In contrast, the Hilbert space norm of (45) vanishes as in the thermodynamic limit

$$\langle\langle \rho|\rho\rangle\rangle = \frac{1}{L^{3N}}\left(\int \mathrm{d}p|\rho_0(|p)|^2 + \frac{1}{\Omega^2}\sum_j^N\sum_{\mathbf{k}}\int \mathrm{d}p|\rho'_{\mathbf{k}}(\mathbf{p}_j|p^{N-1})|^2 + \ldots\right) \to 0. \tag{49}$$

Hence, distribution functions 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 $s \leqslant N$)

$$M(\mathbf{q}_1, \ldots, \mathbf{q}_r, \mathbf{p}_1, \ldots, \mathbf{p}_s) = \frac{1}{\Omega^N}\sum_k \mathrm{e}^{ik\cdot q} M_k(\mathbf{p}_1, \ldots, \mathbf{p}_s)\delta_\Omega(\mathbf{k}_{r+1}) \cdots \delta_\Omega(\mathbf{k}_N). \tag{50}$$

Hence, these observables also do not belong to the Hilbert space.

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

$$\begin{aligned} P^{(0)} &= \int \mathrm{d}p|k,\ p\rangle\rangle\langle\langle k,\ p|\delta^{kr}(k), \quad P_{ij}^{(k_i,-k_i)} = \int \mathrm{d}p|k,\ p\rangle\rangle\langle\langle k,\ p|\delta_{\mathbf{k}_i+\mathbf{k}_j,0}\delta_{ij}^{kr}(k), \ldots \\ P_j^{(k_j)} &= \int \mathrm{d}p|k,\ p\rangle\rangle\langle\langle k,\ p|\delta_j^{kr}(k), \quad P_{ij}^{(k_i,k_j)} = \int \mathrm{d}p|k,\ p\rangle\rangle\langle\langle k,\ p|\delta_{ij}^{kr}(k), \ldots \end{aligned} \tag{51}$$

The index a in $P_a^{(\nu)}$ denotes the particles associated to non-vanishing wave vectors, while the index ν denotes the value of their wave vectors. The projection operators in the first line in (51) extract the homogenous components in the Fourier expansion of the phase functions, while the projection operators in the second line in (51) extract the inhomogeneous components of the phase functions.

Note that the momentum $\hat{\mathbf{p}}_j$ as defined in (11) lies in the vacuum of correlation subspace $P^{(0)}$,

$$\langle\langle \hat{\mathbf{p}}_j| = \int \mathrm{d}q\int \mathrm{d}p\int \mathrm{d}p'\sum_k \mathbf{p}_j\langle\langle q,\ p|k,\ p'\rangle\rangle\langle\langle k,\ p'| = L^{3N/2}\int \mathrm{d}p\mathbf{p}_j\langle\langle 0,\ p|P^{(0)}. \tag{52}$$

The projection operators $P_a^{(\nu)}$ commute with the unperturbed Liouvillian,

$$L_0 P_a^{(\nu)} = (k\cdot v)P_a^{(\nu)} = P_a^{(\nu)}L_0. \tag{53}$$

Moreover

$$P_a^{(\nu)}P_b^{(\mu)} = P_a^{(\nu)}\delta_{\nu,\mu}\delta_{a,b}, \qquad \sum_\nu\sum_a P_a^{(\nu)} = 1. \tag{54}$$

To shorten the notation we have not written the delta functions for the momenta (c.f. (21)). We also introduce the projection operators $Q_a^{(\nu)}$,

$$Q_a^{(\nu)} = 1 - P_a^{(\nu)}, \tag{55}$$

which are orthogonal to $P_a^{(\nu)}$, i.e.

$$P_a^{(\nu)}Q_a^{(\nu)} = Q_a^{(\nu)}P_a^{(\nu)} = 0. \tag{56}$$

We note that

$$P_a^{(\nu)} L_V P_a^{(\nu)} = 0. \tag{57}$$

In the following discussion we shall often use the notation,

$$P^{(\nu)} = |\nu\rangle\rangle\langle\langle\nu|, \tag{58}$$

as well as l_ν for the eigenvalue of L_0. Then, the spectral decomposition of the L_0 is

$$L_0 = \sum_\nu |\nu\rangle\rangle l_\nu \langle\langle\nu|. \tag{59}$$

We now come 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 non-integrable systems, the spectral decomposition of the Liouvillian corresponding to Hamiltonian (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 (49), we have to extend the eigenvalue problem outside the Hilbert space. This has already been done in the case of deterministic chaos [9–14]. Our extension introduced here is quite natural, as the class of functions we consider includes the equilibrium distribution. 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 [1]

$$L_H |F_\alpha^{(\nu)}(\lambda)\rangle\rangle = Z_\alpha^{(\nu)} |F_\alpha^{(\nu)}(\lambda)\rangle\rangle, \tag{60}$$

with the boundary condition

$$|F_\alpha^{(\nu)}(\lambda)\rangle\rangle \to P^{(\nu)} |F_\alpha^{(\nu)}(0)\rangle\rangle \qquad \text{for} \qquad \lambda \to 0. \tag{61}$$

The indices α (together with ν) are the parameters characterizing the eigenfunctions.

As we shall show, the eivenvalues $Z_\alpha^{(\nu)}$ are generally complex numbers. The time evolution of LPS splits into two semi-groups. For the semi-group corresponding to $t > 0$, the eigenstates are associated to the eigenvalues with $\operatorname{Im} Z_\alpha^{(\nu)} \leq 0$ (including the case $\operatorname{Im} Z_\alpha^{(\nu)} < 0$) and equilibrium is reached in our future for $t \to +\infty$ (see Appendix A), while for the other 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 semi-group 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 $\langle\langle \tilde{F}_\alpha^{(\nu)}|$, i.e.

$$\langle\langle \tilde{F}_\alpha^{(\nu)}| L_H = \langle\langle \tilde{F}_\alpha^{(\nu)}| Z_\alpha^{(\nu)}, \tag{62}$$

again with the boundary condition

$$\langle\langle \tilde{F}_\alpha^{(\nu)}(\lambda)| \to \langle\langle \tilde{F}_\alpha^{(\nu)}(0)|P^{(\nu)} \qquad \text{for} \qquad \lambda \to 0. \tag{63}$$

We assume the bi-orthogonality and bi-completeness relations

$$\langle\langle \tilde{F}_\alpha^{(\nu)}|F_\beta^{(\mu)}\rangle\rangle = \delta_{\nu,\mu}\delta_{\alpha,\beta}, \qquad \sum_\nu \sum_\alpha |F_\alpha^{(\nu)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(\nu)}| = 1. \tag{64}$$

We assume also that the eigenstates of the Liouvillian are not degenerate for the different indices of ν and α. The bi-orthogonality relation is the direct consequence of the assumption of the non-degeneracy. This assumption, as well as bi-completeness of the eigenstates, should be verified for each specific Hamiltonian.*

Moreover we assume that the Liouvillian is diagonalizable

$$L_H = \sum_\nu \sum_\alpha |F_\alpha^{(\nu)}\rangle\rangle Z_\alpha^{(\nu)} \langle\langle \tilde{F}_\alpha^{(\nu)}|. \tag{65}$$

In this paper we shall not consider more general situations which would lead to Jordan blocks (see [14, 28]).

Let us first consider the eigenvalue problem (60) for the right eigenstates. As mentioned, we consider eigenfunctions which have the structure (45). 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:

$$\begin{aligned}\langle\langle q, p|F_\alpha^{(\nu)}\rangle\rangle = \frac{1}{L^{3N/2}} \sum_k e^{ik\cdot q} \Bigg[& F_0^{(\nu)}(p, \alpha)\delta^{kr}(k) + \frac{1}{\Omega} \sum_{j>i}^{N} F_{\mathbf{k}_i,\mathbf{k}_j}^{(\nu)}(p, \alpha)\delta_{\mathbf{k}_i+\mathbf{k}_j,0}\delta_{ij}^{kr}(k) \\ & + \frac{1}{\Omega^2} \sum_{n>j>i}^{N} F_{\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_n}^{(\nu)}(p, \alpha)\delta_{\mathbf{k}_i+\mathbf{k}_j+\mathbf{k}_n,0}\delta_{ijn}^{kr}(k) + \ldots \Bigg].\end{aligned} \tag{66}$$

We assume that the Fourier coefficients $F_{\mathbf{k}_i,\mathbf{k}_j,\ldots}^{(\nu)}$ do not depend on the volume in the limit of the large volumes $\Omega \to \infty$. $F_0^{(\nu)}$ correspond to the vacuum of correlation, $F_{\mathbf{k}_i,-\mathbf{k}_i}^{(\nu)}$ to binary correlations, ... as ρ in (45).

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

We formulate the eigenvalue problem for an arbitrary number N of particles, including $N \to \infty$. For this case, special care is necessary, as the perturbed Liouvillian L_V in (26) contains N^2 terms involving all pairs of particles j and n. We therefore take the inner product of the eigenvalue equation (60) with observables (50) which depend on an arbitrary but finite number of particles:

$$\langle\langle \hat{M}|L_H|F_\alpha^{(\nu)}\rangle\rangle = Z_\alpha^{(\nu)} \langle\langle \hat{M}|F_\alpha^{(\nu)}\rangle\rangle. \tag{67}$$

This operation reduces the number of pairs and leads to a finite contribution in the thermodynamic limit (2). In our discussion of the eigenvalue problem, we shall always understand our formulae as in (67). We shall come back this problem later in Sections 8 and 10 (see also [17]).

Applying the projection operators $P^{(\nu)}$ and $Q^{(\nu)}$ in (55) to (60), we derive the set of equations:

$$P^{(\nu)}L_H(P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle + Q^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle) = Z_\alpha^{(\nu)} P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle, \tag{68a}$$

$$Q^{(\nu)}L_H(P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle + Q^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle) = Z_\alpha^{(\nu)} Q^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle. \tag{68b}$$

*The proof of the bi-orthogonality and bi-completeness for the complex spectral representation for the quantum Friedrichs model as well as potential scattering can be found in [1, 5, 7].

Equation (68b) leads to

$$(Z_\alpha^{(\nu)} - Q^{(\nu)} L_H Q^{(\nu)}) Q^{(\nu)} | F_\alpha^{(\nu)} \rangle\rangle = Q^{(\nu)} \lambda L_V P^{(\nu)} | F_\alpha^{(\nu)} \rangle\rangle. \tag{69}$$

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

$$Q^{(\nu)} | F_\alpha^{(\nu)}(z) \rangle\rangle = \mathscr{C}^{(\nu)}(z) P^{(\nu)} | F_\alpha^{(\nu)}(z) \rangle\rangle, \tag{70}$$

where

$$\mathscr{C}^{(\nu)}(z) = \frac{-1}{Q^{(\nu)} L_H Q^{(\nu)} - z} Q^{(\nu)} \lambda L_V P^{(\nu)}. \tag{71}$$

If this geometrical series converges, we have

$$\mathscr{C}^{(\nu)}(z) = \sum_{n=0}^{\infty} \left(\frac{-1}{L_0 - z} Q^{(\nu)} \lambda L_V Q^{(\nu)} \right)^n \frac{-1}{L_0 - z} Q^{(\nu)} \lambda L_V P^{(\nu)}. \tag{72}$$

This expansion for $\mathscr{C}^{(\nu)}$ corresponds to a sequence of 'irreducible transitions', as the intermediate states are orthogonal to the initial state in the space $P^{(\nu)}$ [17]. The operator $\mathscr{C}^{(\nu)}$ is called the 'creation-of-correlation' operator, or 'creation operator' in short. The creation operator describes off-diagonal transitions from $P^{(\nu)}$ to orthogonal states in $Q^{(\nu)}$ subspace:

$$\mathscr{C}^{(\nu)}(z) = Q^{(\nu)} \mathscr{C}^{(\nu)}(z) P^{(\nu)}. \tag{73}$$

The substitution of z by $Z_\alpha^{(\nu)}$ leads to a solution of (69). However, we have to be careful with the analytic continuation of $(z - L_0)^{-1}$ in (72) to avoid divergences associated to the Poincaré resonances [8]. This is achieved using the so-called '$i\epsilon$-rule' for the analytic continuation [14, 26, 31]. For two-body scattering (or potential scattering) considered in our previous article [1] we have proved that the $i\epsilon$-rule follows the bi-orthogonality condition of the eigenstates of the Liouvillian. Let us recall the $i\epsilon$-rule for the two-body scattering [1] (see also [31]). In order to specify the analytic continuation in accordance with the $i\epsilon$-rule, we define the index d_ν of the 'degree of correlation' of the unperturbed state $|\nu\rangle\rangle$ as the integer which is the minimum number of interactions λL_V required to raise the state $|\nu\rangle\rangle$ from the state $|0, p\rangle\rangle$, the 'vacuum of correlation'. The degree of the correlation for $|0, p\rangle\rangle$ is $d_0 = 0$. The second term of the Fourier component in (66) 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 determine the analytic continuation of the propagators for $t > 0$ as [1]

$$\lim_{\Omega \to \infty} \frac{\langle\langle \mu | \lambda L_V | \nu \rangle\rangle}{l_\mu - l_\nu + i\epsilon_{\mu\nu}}. \tag{74}$$

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

$$i\epsilon_{\mu\nu} = \begin{cases} -i\epsilon, & \text{for } d_\mu \geqslant d_\nu, \\ +i\epsilon, & \text{for } d_\mu < d_\nu, \end{cases} \tag{75}$$

and ϵ is a positive infinitesimal $\epsilon \to 0+$. This limit should be taken after the limit to the continuous spectrum $\Omega \to \infty$ (see Appendix B). 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 (74) we introduce the notation,

$$P^{(\mu)}\frac{-1}{(l_\mu - Z_\alpha^{(\nu)})_{C_{\mu\nu}}} \equiv P^{(\mu)}\frac{-1}{[l_\mu - z]^+_{Z_\alpha^{(\nu)}}}, \qquad \text{for } d_\mu \geqslant d_\nu, \tag{76a}$$

$$P^{(\mu)}\frac{-1}{(l_\mu - Z_\alpha^{(\nu)})_{C_{\mu\nu}}} \equiv P^{(\mu)}\frac{-1}{l_\mu - Z_\alpha^{(\nu)}}, \qquad \text{for } d_\mu < d_\nu. \tag{76b}$$

Here,

$$\int_{\mathbf{R}} dw \frac{f(w)}{[w - z]^+_{Z_\alpha^{(\nu)}}} = \lim_{\epsilon \to 0+} \sum_{n=0}^{\infty} \int_{\mathbf{R}} dw \frac{(-i\gamma)^n}{(w - w' - i\epsilon)^{n+1}} f(w), \tag{77}$$

and

$$\int_{\mathbf{R}} dw \frac{f(w)}{w - Z_\alpha^{(\nu)}} = \lim_{\epsilon \to 0+} \sum_{n=0}^{\infty} \int_{\mathbf{R}} dw \frac{(-i\gamma)^n}{(w - w' + i\epsilon)^{n+1}} f(w), \tag{78}$$

where $Z_\alpha^{(\nu)} = w' - i\gamma$ with w' and $\gamma \geqslant 0$ real, and the integrations are performed with a suitable test functions $f(w)$ on the real axis $\mathbf{R}$. We can perform the summation of the geometrical series (77) by introducing the 'complex distribution' defined by [4]

$$\int_{\mathbf{R}} dw \frac{f(w)}{[w - z]^+_{Z_\alpha^{(\nu)}}} \equiv \lim_{z \downarrow Z_\alpha^{(\nu)}} \int_{\mathbf{R}} dw \frac{f(w)}{w - z} = \int_{\Gamma} dw \frac{f(w)}{w - z}. \tag{79}$$

Here, $z \downarrow Z_\alpha^{(\nu)}$ means that we first evaluate the integration in the upper-half plane of z (i.e. $\operatorname{Im} z > 0$), then take the limit $z \to Z_\alpha^{(\nu)}$ in the lower-half plane. We can perform the integration by changing the contour as shown in Fig. 1.

The relation of (79) to the complex 'δ-function' is presented in Appendix C. Moreover, in Appendix D we present the proof that the analytic continuations (76) (and (102) for the left eigenstates in the next section) lead indeed to a bi-orthonormal set of the eigenstates of L_H for N-body systems. We shall present the proof of the uniqueness of the analytic continuation elsewhere.

There is another branch of the analytic continuation in (72), which corresponds to the complex conjugate of (76). But we shall not consider this branch, as this leads to the eigenstates belonging to other semi-groups oriented towards our past.

Then, with (76) we have the solution of (69)

$$Q^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle = \mathcal{C}^{(\nu)}(Z_\alpha^{(\nu)})P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle, \tag{80}$$

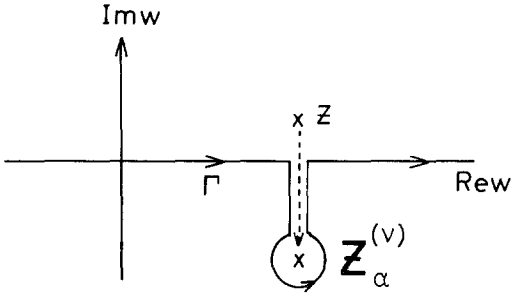

Fig. 1. Contour Γ for the complex distribution in (79).

where

$$P^{(\mu)}\mathscr{C}^{(\nu)}(Z_\alpha^{(\nu)})P^{(\nu)} = P^{(\mu)}\frac{-1}{(l_\mu - Z_\alpha^{(\nu)})_{C_{\mu\nu}}}\mathscr{T}_C^{(\nu)}(Z_\alpha^{(\nu)})P^{(\nu)} \tag{81}$$

Here we have introduced the '$\mathscr{T}$-matrix' which is defined as the solution of the equation

$$\mathscr{T}_C^{(\nu)}(z) = \lambda Q^{(\nu)}L_V + \sum_\mu \lambda Q^{(\nu)}L_V P^{(\mu)}\frac{-1}{(l_\mu - z)_{C_{\mu\nu}}}\mathscr{T}_C^{(\nu)}(z). \tag{82}$$

Substituting (80) into (68), we obtain the non-linear equation [28]

$$\psi^{(\nu)}(Z_\alpha^{(\nu)})|u_\alpha^{(\nu)}\rangle\rangle = Z_\alpha^{(\nu)}|u_\alpha^{(\nu)}\rangle\rangle, \tag{83}$$

where

$$|u_\alpha^{(\nu)}\rangle\rangle \equiv P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle. \tag{84}$$

Equation (84) implies

$$L_0|u_\alpha^{(\nu)}\rangle\rangle = l_\nu|u_\alpha^{(\nu)}\rangle\rangle. \tag{85}$$

Here, $\psi^{(\nu)}$ is the generalization of the 'collision operator' familiar from non-equilibrium statistical mechanics [17]. This operator is associated to diagonal transitions between two states corresponding to the same projection operator $P^{(\nu)}$. The collision operator is defined through

$$\psi^{(\nu)}(Z_\alpha^{(\nu)}) = L_0P^{(\nu)} + \lambda P^{(\nu)}L_V\mathscr{C}^{(\nu)}(Z_\alpha^{(\nu)})P^{(\nu)}. \tag{86}$$

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

$$\langle\langle\tilde{u}_\alpha^{(\nu)}|u_\beta^{(\mu)}\rangle\rangle = \delta_{\nu,\mu}\delta_{\alpha,\beta}, \qquad \sum_\alpha |u_\alpha^{(\nu)}\rangle\rangle\langle\langle\tilde{u}_\alpha^{(\nu)}| = P^{(\nu)}. \tag{87}$$

We have

$$\langle\langle\tilde{u}_\alpha^{(\nu)}|L_0 = \langle\langle\tilde{u}_\alpha^{(\nu)}|l_\nu. \tag{88}$$

We note that the states $\langle\langle\tilde{u}_\alpha^{(\nu)}|$ are generally not the left eigenstates of $\psi^{(\nu)}(Z_\alpha^{(\nu)})$ [27].

Let us then introduce the 'global' collision operator by

$$\theta_C^{(\nu)} \equiv \sum_\alpha \psi^{(\nu)}(Z_\alpha^{(\nu)})|u_\alpha^{(\nu)}\rangle\rangle\langle\langle\tilde{u}_\alpha^{(\nu)}| = \sum_\alpha |u_\alpha^{(\nu)}\rangle\rangle Z_\alpha^{(\nu)}\langle\langle\tilde{u}_\alpha^{(\nu)}|, \tag{89}$$

as well as the 'global' creation operator,

$$\mathbf{C}^{(\nu)} \equiv \sum_\alpha \mathscr{C}^{(\nu)}(Z_\alpha^{(\nu)})|u_\alpha^{(\nu)}\rangle\rangle\langle\langle\tilde{u}_\alpha^{(\nu)}|. \tag{90}$$

We shall call also $\theta_C^{(\nu)}$ the collision operator and $\mathbf{C}^{(\nu)}$ the creation operator for simplicity, as far as no confusion is possible. Then we have [21]

$$\theta_C^{(\nu)} = L_0P^{(\nu)} + \lambda P^{(\nu)}L_V\mathbf{C}^{(\nu)}P^{(\nu)}, \tag{91}$$

and

$$\theta_C^{(\nu)}|u_\alpha^{(\nu)}\rangle\rangle = Z_\alpha^{(\nu)}|u_\alpha^{(\nu)}\rangle\rangle, \qquad \langle\langle\tilde{u}_\alpha^{(\nu)}|\theta_C^{(\nu)} = \langle\langle\tilde{u}_\alpha^{(\nu)}|Z_\alpha^{(\nu)}. \tag{92}$$

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

With the creation operator we have also

$$Q^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle = Q^{(\nu)}\mathbf{C}^{(\nu)}P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle. \tag{93}$$

Formula (84) shows that the privileged components $P^{(\nu)}|F_\alpha^{(\nu)}\rangle\rangle$ are eigenstates of the collision operator, which has the same eigenvalues $Z_\alpha^{(\nu)}$ as the Liouvillian. The solution of the eigenvalue problem of the Liouvillian for our class of singular functions (66) has unique features. The privileged components satisfy closed equations and the $Q^{(\nu)}$ components are 'driven' by the privileged components (see (93)). In the previous work on subdynamic theory (for non-equilibrium statistical mechanics as well as for deterministic chaos) this property has been presented as an 'ansatz' [14, 31]. Here we derive this property through the complex spectrual representation of L_H for the singular class of eigenstates (66).

The collision operators are dissipative operators, and they are the central objects of non-equilibrium statistical mechanics [17, 18]. 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,

$$\theta_C^{(0)} \approx \lambda^2\theta_2^{(0)} = \lambda^2 P^{(0)}L_V Q^{(0)}\frac{1}{i\epsilon - L_0}Q^{(0)}L_V P^{(0)}, \tag{94}$$

which gives

$$\lambda^2\langle\langle 0, p|\theta_2^{(0)}|0, p'\rangle\rangle = \lim_{\Omega\to\infty}\frac{\lambda^2}{\Omega^2}\sum_{j>n}^{N}\sum_{\mathbf{k}}|V_k|^2\mathbf{k}\cdot\mathbf{d}_{jn}\pi\delta(\mathbf{k}\cdot\mathbf{g}_{jn})\mathbf{k}\cdot\mathbf{d}_{jn}\delta(p - p'), \tag{95}$$

where

$$\mathbf{g}_{jn} \equiv \mathbf{v}_j - \mathbf{v}_n. \tag{96}$$

Also in the low concentration limit, $\theta_C^{(0)}$ reduces to the Boltzmann collision operator [17].

The Fokker–Planck operator (94) is an anti-hermitian operator and has non-vanishing negative imaginary eigenvalues (i.e. $\operatorname{Im} Z_\alpha^{(0)} < 0$) associated to diffusive processes in momentum space (see the example given in the Appendix F; see also [17, 18]). This illustrates the consistency of our construction of the eigenstates of the Liouvillian with $\operatorname{Im} Z_\alpha^{(\nu)} \leqslant 0$. Moreover, the contribution of the Fokker–Planck operator comes from the integration over wave vectors satisfying Poincaré's resonances condition $\mathbf{k}\cdot\mathbf{g}_{jn} = 0$. This means that the dissipation has a dynamical origin associated with 'non-integrability' of LPS due to Poincaré's resonances. The Fokker–Planck operator leads to 'Brownian motion'. Instead of separate dynamical events described by each interactions λL_V, we have events 'coupled' by the resonance condition $\delta(\mathbf{k}\cdot\mathbf{g}_{jn})$. 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 kinetic theory. In general the denominators in the operators involves both directions of the analytic continuation (76). Nevertheless, the analytic continuations of the diagonal operators, such as $\theta_C^{(\nu)}$, are uniquely determined in the thermodynamic limit by the complex distributions (76a). This is the result of the so-called Henin's theorem [22]; i.e. for the diagonal transition between the states in $P^{(\nu)}$, the intermediates states should correspond to a higher degree of correlation than $P^{(\nu)}$. Indeed, the diagonal transition restricts the wave vector transfer and leads to extra volume factors Ω^{-1} through the interaction (see (26)). The diagonal transitions give non-vanishing 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 Ω^{-1}. We then obtain for example to the lowest order contribution of $\theta_C^{(\nu)}$ (i.e. to λ^2 order).

$$\theta_C^{(\nu)} \approx L_0 P^{(\nu)} + \lambda^2 \theta_2^{(\nu)} = L_0 P^{(\nu)} + \lambda^2 P^{(\nu)} L_V Q^{(\nu)} \frac{1}{l_\nu + i\epsilon - L_0} Q^{(\nu)} L_V P^{(\nu)}. \tag{97}$$

Combining (93) with (84), we obtain the right eigenstates (60) of the Liouvillian,

$$|F_\alpha^{(\nu)}\rangle\rangle = N_\alpha^{(\nu)1/2}(P^{(\nu)} + \mathscr{C}^{(\nu)}(Z_\alpha^{(\nu)}))|u_\alpha^{(\nu)}\rangle\rangle = N_\alpha^{(\nu)1/2}(P^{(\nu)} + \mathbf{C}^{(\nu)})|u_\alpha^{(\nu)}\rangle\rangle, \tag{98}$$

where $N_\alpha^{(\nu)}$ is a normalization constant which we shall specify later (see (115)).

Let us note that (83) is a 'non-linear eigenvalue problem', as the collision operator $\psi^{(\nu)}$ itself depends on $Z_\alpha^{(\nu)}$. Unknown eigenvalues $Z_\alpha^{(\nu)}$ appear in the propagator inside the collision operator. This corresponds to the Brillouin–Wigner formulation of the eigenvalue problem of the Hamiltonian H for integrable systems when the eigenvalues are real. We can extend this formulation to the eigenvalue problem of L_H for non-integrable classical systems [4]. The Brillouin–Wigner theory gives a systematic approximation scheme for the solution of the eigenvalue problem. We present this method in Appendix E. In Section 9, we shall also construct a non-linear equation [14] for $\mathbf{C}^{(\nu)}$, through which we can determine the explicit form of the creation operator by a perturbation series in powers of λ (see (171)).

Replacing $P^{(\nu)}$ by the projection operators corresponding to the inhomogeneous components, the construction of eigenstates associated to 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 (62) for the left eigenstates. As for the right eigenstates, we obtain

$$\langle\langle \tilde{F}_\alpha^{(\nu)}| = \langle\langle \tilde{v}_\alpha^{(\nu)}|(P^{(\nu)} + \mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)}))N_\alpha^{(\nu)1/2} = \langle\langle \tilde{v}_\alpha^{(\nu)}|(P^{(\nu)} + \mathbf{D}^{(\nu)})N_\alpha^{(\nu)1/2}. \tag{99}$$

The operator $\mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)})$ is called the 'destruction-of-correlation' operator, or 'destruction operator' in short. This operator is defined by

$$P^{(\nu)}\mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)})P^{(\mu)} = P^{(\nu)}\mathscr{T}_D^{(\nu)}(Z_\alpha^{(\nu)}) \frac{1}{(Z_\alpha^{(\nu)} - l_\mu)_{D_{\mu\nu}}} P^{(\mu)}, \tag{100}$$

where we have introduced the '$\mathscr{T}$-matrix' similar to (82),

$$\mathscr{T}_D^{(\nu)}(z) = \lambda L_V Q^{(\nu)} + \sum_\mu \mathscr{T}_D^{(\nu)}(z) \frac{1}{(z - l_\mu)_{D_{\mu\nu}}} P^{(\mu)} \lambda L_V Q^{(\nu)}, \tag{101}$$

using the analytic continuation given by (c.f. (76))

$$\frac{1}{(Z_\alpha^{(\nu)} - l_\mu)_{D_{\nu\mu}}} P^{(\mu)} \equiv \frac{1}{[z - l_\mu]^+_{Z_\alpha^{(\nu)}}} P^{(\mu)}, \quad \text{for } d_\nu < d_\mu, \tag{102a}$$

$$\frac{1}{(Z_\alpha^{(\nu)} - l_\mu)_{D_{\nu\mu}}} P^{(\mu)} \equiv \frac{1}{Z_\alpha^{(\nu)} - l_\mu} P^{(\mu)}, \quad \text{for } d_\nu \geqslant d_\mu. \tag{102b}$$

Again $\mathscr{D}^{(\nu)}(z)$ corresponds to the off-diagonal transitions (see (73))

$$\mathscr{D}^{(\nu)}(z) = P^{(\nu)}\mathscr{D}^{(\nu)}(z)Q^{(\nu)}. \tag{103}$$

$\mathbf{D}^{(\nu)}$ is the global destruction operator defined below (see (110)). We have

$$\langle\langle \tilde{v}_\alpha^{(\nu)}| \equiv \langle\langle \tilde{F}_\alpha^{(\nu)}|P^{(\nu)}, \tag{104}$$

and

$$\langle\langle \tilde{F}_\alpha^{(\nu)}|Q^{(\nu)} = \langle\langle \tilde{F}_\alpha^{(\nu)}|P^{(\nu)}\mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)}) = \langle\langle \tilde{F}_\alpha^{(\nu)}|P^{(\nu)}\mathbf{D}^{(\nu)}. \tag{105}$$

$\langle\langle \tilde{v}_\alpha^{(\nu)}|$ are the left eigenstates of the collision operator $\psi^{(\nu)}$,

$$\langle\langle \tilde{v}_\alpha^{(\nu)}|\psi^{(\nu)}(Z_\alpha^{(\nu)}) = \langle\langle \tilde{v}_\alpha^{(\nu)}|Z_\alpha^{(\nu)}, \tag{106}$$

where

$$\psi^{(\nu)}(Z_\alpha^{(\nu)}) = P^{(\nu)}L_0 + \lambda P^{(\nu)}\mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)})L_V P^{(\nu)}. \tag{107}$$

We note that the analytic continuations in (102) leads to the same collision operator as (86).

We denote $|v_\alpha^{(\nu)}\rangle\rangle$ the functions which are bi-orthogonal to $\langle\langle \tilde{v}_\alpha^{(\nu)}|$. Again we assume

$$\langle\langle \tilde{v}_\alpha^{(\nu)}|v_\beta^{(\mu)}\rangle\rangle = \delta_{\nu,\mu}\delta_{\alpha,\beta}, \qquad \sum_\alpha |v_\alpha^{(\nu)}\rangle\rangle\langle\langle \tilde{v}_\alpha^{(\nu)}| = P^{(\nu)}. \tag{108}$$

We have

$$L_0|v_\alpha^{(\nu)}\rangle\rangle = l_\nu|v_\alpha^{(\nu)}\rangle\rangle, \qquad \langle\langle \tilde{v}_\alpha^{(\nu)}|L_0 = \langle\langle \tilde{v}_\alpha^{(\nu)}|l_\nu. \tag{109}$$

Then the 'global' destruction operator is defined by

$$\mathbf{D}^{(\nu)} \equiv \sum_\alpha |v_\alpha^{(\nu)}\rangle\rangle\langle\langle \tilde{v}_\alpha^{(\nu)}|\mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)}). \tag{110}$$

Similarly to $\mathbf{C}^{(\nu)}$, the operator $\mathbf{D}^{(\nu)}$ satisfies a non-linear equation given later (see (171)). We can also introduce the 'global' collision operator (see (89))

$$\theta_D^{(\nu)} \equiv \sum_\alpha |v_\alpha^{(\nu)}\rangle\rangle Z_\alpha^{(\nu)}\langle\langle \tilde{v}_\alpha^{(\nu)}| = L_0P^{(\nu)} + \lambda P^{(\nu)}\mathbf{D}^{(\nu)}L_V P^{(\nu)}. \tag{111}$$

We have

$$\theta_D^{(\nu)}|v_\alpha^{(\nu)}\rangle\rangle = Z_\alpha^{(\nu)}|v_\alpha^{(\nu)}\rangle\rangle, \qquad \langle\langle \tilde{v}_\alpha^{(\nu)}|\theta_D^{(\nu)} = \langle\langle \tilde{v}_\alpha^{(\nu)}|Z_\alpha^{(\nu)}. \tag{112}$$

We note that

$$\theta_D^{(\nu)} \neq \theta_C^{(\nu)}. \tag{113}$$

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

One can now determine the normalization constant as follows: as the result of the bi-orthogonal relation (64), we have

$$\delta_{\alpha,\beta} = \langle\langle \tilde{F}_\alpha^{(\nu)}|F_\beta^{(\nu)}\rangle\rangle = (N_\alpha^{(\nu)}N_\beta^{(\nu)})^{1/2}\langle\langle \tilde{v}_\alpha^{(\nu)}|(P^{(\nu)} + \mathbf{D}^{(\nu)}\mathbf{C}^{(\nu)})|u_\beta^{(\nu)}\rangle\rangle. \tag{114}$$

This gives us the normalization constant in (98) and (99) as

$$N_\alpha^{(\nu)} = [\langle\langle \tilde{v}_\alpha^{(\nu)}|(P^{(\nu)} + \mathbf{D}^{(\nu)}\mathbf{C}^{(\nu)})|u_\alpha^{(\nu)}\rangle\rangle]^{-1}. \tag{115}$$

Moreover, putting

$$(A^{(\nu)})^{-1} \equiv P^{(\nu)} + \mathbf{D}^{(\nu)}\mathbf{C}^{(\nu)}, \tag{116}$$

we obtain

$$(A^{(\nu)})^{-1} = \sum_\alpha |v_\alpha^{(\nu)}\rangle\rangle(N_\alpha^{(\nu)})^{-1}\langle\langle \tilde{u}_\alpha^{(\nu)}|, \tag{117}$$

and its inverse operator in $P^{(v)}$ subspace[†]

$$A^{(v)} = P^{(v)}(1 + \mathbf{D}^{(v)}\mathbf{C}^{(v)})^{-1} = \sum_{\alpha} |u_\alpha^{(v)}\rangle\rangle N_\alpha^{(v)} \langle\langle \tilde{v}_\alpha^{(v)}|. \tag{118}$$

Hence, we have

$$\langle\langle \tilde{u}_\alpha^{(v)}|\theta_C^{(v)} A^{(v)}|v_\beta^{(v)}\rangle\rangle = Z_\alpha^{(v)} N_\alpha^{(v)} \delta_{\alpha,\beta} = \langle\langle \tilde{u}_\alpha^{(v)}|A^{(v)}\theta_D^{(v)}|v_\beta^{(v)}\rangle\rangle. \tag{119}$$

This leads to the intertwining relation of $A^{(v)}$ with the collision operators [20]

$$\theta_C^{(v)} A^{(v)} = A^{(v)} \theta_D^{(v)}. \tag{120}$$

As mentioned, we have in general $\theta_D^{(v)} \neq \theta_C^{(v)}$. However, to the lowest order contribution (i.e. to λ^2 order) of $\theta_D^{(v)}$ we obtain the same collision operator as $\theta_C^{(v)}$ in (97), i.e.

$$\theta_D^{(v)} \approx L_0 P^{(v)} + \lambda^2 \theta_2^{(v)}. \tag{121}$$

In summary we have obtained the explicit form of the 'complex spectral representation' of L_H (see (65)) and therefore of the evolution operator ${}^{\mathcal{Q}}\mathcal{U}(t)$,

$$\langle\langle M|{}^{\mathcal{Q}}\mathcal{U}(t)|\rho(0)\rangle\rangle = \sum_{v}\sum_{\alpha} \langle\langle M|F_\alpha^{(v)}\rangle\rangle \, \mathrm{e}^{-iZ_\alpha^{(v)}t} \langle\langle \tilde{F}_\alpha^{(v)}|\rho(0)\rangle\rangle. \tag{122}$$

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 ρ 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 inspite of the fact that we deal with LPS. Still there are many situations where our new 'non-Newtonian' effects can be observed (see Sections 9–11, and Appendices F and G).

6. NON-UNITARY TRANSFORMATIONS AND SUBDYNAMICS

Once we have obtained the spectral decomposition (65) of L_H, we can construct non-unitary transformation operators which lead to similitude relations between the total Liouvillian L_H and the collision operators [4, 14] (hereafter the index B stands for C or D)

$$\Lambda_B L_H \Lambda_B^{-1} = \Theta_B, \tag{123}$$

where

$$\Theta_B \equiv \sum_{v} \theta_B^{(v)}. \tag{124}$$

The non-unitary transformations Λ and their inverses are given by

$$\Lambda_C = \sum_{v}\sum_{\alpha} |u_\alpha^{(v)}\rangle\rangle \langle\langle \tilde{F}_\alpha^{(v)}|N_\alpha^{(v)1/2} = \sum_{v} A^{(v)} \hat{\Phi}_v^D, \tag{125a}$$

$$\Lambda_C^{-1} = \sum_{v}\sum_{\alpha} |F_\alpha^{(v)}\rangle\rangle \langle\langle \tilde{u}_\alpha^{(v)}|N_\alpha^{(v)-1/2} = \sum_{v} \hat{\Phi}_v^C, \tag{125b}$$

[†]In general $f(A^{(v)}) \neq \sum_\alpha |u_\alpha^{(v)}\rangle\rangle f(N_\alpha^{(v)}) \langle\langle \tilde{v}_\alpha^{(v)}|$. Therefore, this is not the spectral decomposition of $A^{(v)}$.

and

$$\Lambda_D = \sum_\nu \sum_\alpha |v_\alpha^{(\nu)}\rangle\rangle \langle\langle \tilde{F}_\alpha^{(\nu)}| N_\alpha^{(\nu)-1/2} = \sum_\nu \hat{\Phi}_\nu^D, \tag{125c}$$

$$\Lambda_D^{-1} = \sum_\nu \sum_\alpha |F_\alpha^{(\nu)}\rangle\rangle \langle\langle \tilde{v}_\alpha^{(\nu)}| N_\alpha^{(\nu)1/2} = \sum_\nu \hat{\Phi}_\nu^C A^{(\nu)}, \tag{125d}$$

where the operators $\hat{\Phi}_\nu^B$ are defined by

$$\hat{\Phi}_\nu^C \equiv P^{(\nu)} + \mathbf{C}^{(\nu)}, \qquad \hat{\Phi}_\nu^D \equiv P^{(\nu)} + \mathbf{D}^{(\nu)}. \tag{126}$$

Because L_H shares the same eigenvalues with $\theta_B^{(\nu)}$ we have the 'intertwining relations' [4]

$$L_H \hat{\Phi}_\nu^C = \hat{\Phi}_\nu^C \theta_C^{(\nu)}, \qquad \hat{\Phi}_\nu^D L_H = \theta_D^{(\nu)} \hat{\Phi}_\nu^D. \tag{127}$$

One can easily verify these relations by operating on the eigenstates of the collision operators. We note that the similitude relations (123) lead to the intertwining relations (127), and vice versa. These relations were already obtained previously [4, 14]. The existence of the two different transformations Λ_C and Λ_D suggests the possibility of another transformation operator Λ associated to a more symmetrical form of the collision operator. This will be shown in Appendix H.

As well known there exist for integrable systems unitary transformations U which lead to[‡]

$$UL_H U^\dagger = L_0. \tag{128}$$

We expect that in the situation where dissipative effects are neglegible the relations (123) would reduce to

$$\Lambda_B L_H \Lambda_B^{-1} = L_0. \tag{129}$$

We shall verify this fact later (see (183)). However, as the complex spectral representation uses both analytic continuation, (129) is not a non-unitary transformation even for the integrable case. As the result, integrable LPS are diagonalized both through a non-unitary transformation, as well as through a unitary one. We shall come back to this problem in Section 9.

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

$$|\rho_B(t)\rangle\rangle \equiv \Lambda_B |\rho(t)\rangle\rangle, \qquad \langle\langle \hat{M}_B(t)| \equiv \langle\langle \hat{M}(t)|\Lambda_B^{-1}. \tag{130}$$

The new states ρ_B obey (see (124))

$$i\frac{\partial}{\partial t}|\rho_B(t)\rangle\rangle = \Theta_B |\rho_B(t)\rangle\rangle. \tag{131}$$

Since $\theta_B^{(\nu)}$ are operators acting on $P^{(\nu)}$ subspace, equation (131) actually represents 'kinetic equations' for $P^{(n)}|\rho_B(t)\rangle\rangle$ in each correlation subspace,

$$i\frac{\partial}{\partial t} P^{(\nu)}|\rho_B(t)\rangle\rangle = \theta_B^{(\nu)} P^{(\nu)}|\rho_B(t)\rangle\rangle. \tag{132}$$

[‡]In general the diagonalization of the Liouvillian L_H by unitary transformation leads to a renormalized Liouvillian L_0' (instead of L_0) which gives frequency shifts associated to 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 Ω^{-1}.

This represents a set of the kinetic equations of the Fokker–Planck type [17]. Each component $P^{(\nu)}|\rho_B(t)\rangle\rangle$ evolves independently.

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

$$i\frac{\partial}{\partial t}\langle\langle \hat{M}_B(t)| = \langle\langle \hat{M}_B(t)|\Theta_B, \tag{133}$$

which leads again to a set of equations

$$i\frac{\partial}{\partial t}\langle\langle \hat{M}_B(t)|P^{(\nu)} = \langle\langle \hat{M}_B(t)|P^{(\nu)}\theta_B^{(\nu)}. \tag{134}$$

We shall illustrate in Appendix G these equations in a simple example.

The transformation (130) preserves the expectation value of M,

$$\langle M\rangle_t = \langle\langle \hat{M}(0)|\rho(t)\rangle\rangle = \langle\langle \hat{M}_B(0)|\rho_B(t)\rangle\rangle. \tag{135}$$

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

$$\langle M\rangle_t = \sum_\nu\sum_\alpha \langle\langle \hat{M}_C(0)|u_\alpha^{(\nu)}\rangle\rangle\, \mathrm{e}^{-iZ_\alpha^{(\nu)}t}\langle\langle \tilde{u}_\alpha^{(\nu)}|\rho_C(0)\rangle\rangle. \tag{136}$$

We note that the non-unitary transformations Λ preserve the reality of the states $\langle\langle q, p|\rho\rangle\rangle$ (see Appendix I for the proof). But the transformed states $\langle\langle q, p|\rho_B\rangle\rangle$ cannot be considered as probability distribution functions, as Λ does not preserve positivity. This is a direct consequence of the causal evolution of dynamics combined with the analytic continuations (76) and (102) (see Appendix C). However, these states play an important role as they lead to bloc 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' [20–31]. To see the relation of subdynamics to the complex spectral representation, let us introduce projection operators $\Pi^{(\nu)}$ (see (118), (125) and (126))

$$\Pi^{(\nu)} = \Lambda_B^{-1}P^{(\nu)}\Lambda_B = \sum_\alpha |F_\alpha^{(\nu)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(\nu)}|. \tag{137}$$

This leads to the familiar form [20–31]

$$\Pi^{(\nu)} = \hat{\Phi}_\nu^C A^{(\nu)}\hat{\Phi}_\nu^D = (P^{(\nu)} + \mathbf{C}^{(\nu)})A^{(\nu)}(P^{(\nu)} + \mathbf{D}^{(\nu)}). \tag{138}$$

These operators satisfy the orthogonality and completeness relations,

$$\Pi^{(\nu)}\Pi^{(\mu)} = \Pi^{(\nu)}\delta_{\nu,\mu}, \qquad \sum_\nu \Pi^{(\nu)} = 1, \tag{139}$$

as well as the commutation relation with L_H,

$$L_H\Pi^{(\nu)} = \Pi^{(\nu)}L_H. \tag{140}$$

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

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

$$\langle\langle \hat{M}|{}^{\mathcal{Q}}\mathcal{U}(t)\Pi^{(\nu)}|\rho(0)\rangle\rangle = \langle\langle \hat{M}|\hat{\Phi}_\nu^C\,\mathrm{e}^{-i\theta_C^{(\nu)}t}A^{(\nu)}\hat{\Phi}_\nu^D|\rho(0)\rangle\rangle = \langle\langle \hat{M}|\hat{\Phi}_\nu^C A^{(\nu)}\,\mathrm{e}^{-i\theta_D^{(\nu)}t}\hat{\Phi}_\nu^D|\rho(0)\rangle\rangle. \tag{141}$$

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,

$$|\rho(0)\rangle\rangle = P^{(0)}|\rho(0)\rangle\rangle. \tag{142}$$

We now show that the time evolution leads to the correlations which satisfy the volume dependence given in (45). From (139)–(141), we have

$$\begin{aligned}|\rho(t)\rangle\rangle &= (P^{(0)} + \mathbf{C}^{(0)})\,\mathrm{e}^{-i\theta_C^{(0)}t}A^{(0)}P^{(0)}|\rho(0)\rangle\rangle + \sum_{\nu(\neq 0)}\mathbf{C}^{(\nu)}\,\mathrm{e}^{-i\theta_C^{(\nu)}t}A^{(\nu)}\mathbf{D}^{(\nu)}P^{(0)}|\rho(0)\rangle\rangle \\ &= (P^{(0)} + \lambda\mathbf{C}_1^{(0)} + \lambda^2\cdots)\,\mathrm{e}^{-i\lambda^2\theta_2^{(0)}t}(1 + \lambda^2 A_2^{(0)} + \lambda^3\cdots)|\rho(0)\rangle\rangle \\ &\quad + \lambda^2\mathbf{C}_1^{(2)}\,\mathrm{e}^{-i(L_0P^{(2)}+\lambda^2\theta_2^{(2)})t}\mathbf{D}_1^{(2)}P^{(0)}|\rho(0)\rangle\rangle + \lambda^3\cdots.\end{aligned} \tag{143}$$

where the subscripts n in the operators represent their λ^n order contributions, and the superscript (ν) corresponds to νth order correlations. Applying (47) and (48) to each term in (143) one can easily verify that the volume dependence for all correlation components are in agreement with (45). The reader can find the detailed estimation of the volume dependence in our earlier articles [17, 18]. This shows that the class of singular distribution functions (45) is not only form invariant but it acts even as an attractor. In Section 13, as well as in Appendix F, we shall see that (45) acts as an attractor in the thermodynamic limit even for trajectories.

7. LYAPUNOV FUNCTIONS—$\mathcal{H}$ THEOREMS

The non-unitrary transformations have led to the similitude relation (123) between the total Liouvillian L_H and the collision operators. As the consequence, we may introduce transformed states and observables (130) whose time evolutions are described only by the $P^{(\nu)}$ components in each correlation subspace. This permits us to introduce 'Lyapunov functions' which are dynamical analogue of Boltzmann's $\mathcal{H}$-function (i.e. 'entropy') for dynamcial systems [4, 5]. 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[§]

$$\varphi_1(\mathbf{p}_j, t) = \langle\langle\hat{\varphi}_{\mathbf{p}_j}|\rho(t)\rangle\rangle = \int \mathrm{d}p'\,\delta(\mathbf{p}_j' - \mathbf{p}_j)\rho_0(|p', t), \tag{144}$$

with

$$\langle\langle\hat{\varphi}_{\mathbf{p}_j}| \equiv \int \mathrm{d}q \int \mathrm{d}p'\,\delta(\mathbf{p}_j' - \mathbf{p}_j)\langle\langle q, p'| = L^{3N/2}\int \mathrm{d}p'\,\delta(\mathbf{p}_j' - \mathbf{p}_j)\langle\langle 0, p'|P^{(0)}, \tag{145}$$

where the right-hand side of (145) is written in the wave number representation. We have, for example; (see (52))

$$\langle\langle\hat{\mathbf{p}}_j| = \int \mathrm{d}\mathbf{p}_j\mathbf{p}_j\langle\langle\hat{\varphi}_{\mathbf{p}_j}|. \tag{146}$$

We note

$$\langle\langle 0, p'|\hat{\varphi}_{\mathbf{p}_j}\rangle\rangle\langle\langle\hat{\varphi}_{\mathbf{p}_j}|\rho\rangle\rangle = L^{3N/2}\delta(\mathbf{p}_j' - \mathbf{p}_j)\varphi_1(\mathbf{p}_j). \tag{147}$$

[§]The Lyapunov functions are defined for the generic distribution functions. For a trajectory (as a specific distribution function), we have divergence for $|\varphi_1(\mathbf{p}_j)|^2$ because of the square of the delta function of the momentum.

Hence the hermitian operator $|\hat{\varphi}_{\mathbf{p}_j}\rangle\rangle\langle\langle\hat{\varphi}_{\mathbf{p}_j}|$ preserves positivity. The reduction does not change the sign of the distribution function.

We now consider the transformed distribution function (see (130)), e.g. for $j = 1$,

$$\varphi_1^B(\mathbf{p}_1, t) = \langle\langle\hat{\varphi}_{\mathbf{p}_1}|\rho_B(t)\rangle\rangle. \tag{148}$$

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

$$\mathcal{H}_\varphi^B(t) = \int \mathrm{d}\mathbf{p}_1 |\varphi_1^B(\mathbf{p}_1, t)|^2, \tag{149}$$

where

$$|\varphi_1^B(\mathbf{p}_1, t)|^2 = \langle\langle\rho(t)|\Lambda_B^\dagger|\hat{\varphi}_{\mathbf{p}_1}\rangle\rangle\langle\langle\hat{\varphi}_{\mathbf{p}_1}|\Lambda_B|\rho(t)\rangle\rangle. \tag{150}$$

We have from (132) (e.g. for $B = C$)

$$|\varphi_1^B(\mathbf{p}_1, t)|^2 = \sum_{\alpha,\beta} \mathrm{e}^{-i(Z_\alpha^{(0)} - Z_\beta^{(0)c\,c})t}\langle\langle\rho_C(0)|\tilde{u}_\beta^{(0)}\rangle\rangle\langle\langle u_\beta^{(0)}|\hat{\varphi}_{\mathbf{p}_1}\rangle\rangle\langle\langle\hat{\varphi}_{\mathbf{p}_1}|u_\alpha^{(0)}\rangle\rangle\langle\langle\tilde{u}_\alpha^{(0)}|\rho_C(0)\rangle\rangle. \tag{151}$$

All decay modes are damped for $t > 0$. Moreover, we now show that the damping is monotonous. Taking the time derivative of (150), we obtain

$$\frac{\partial}{\partial t}|\varphi_1^B(\mathbf{p}_1, t)|^2 = -\langle\langle\rho_B(t)|\mathcal{K}_B^{(0)}(\mathbf{p}_1)|\rho_B(t)\rangle\rangle, \tag{152}$$

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

$$\mathcal{K}_B^{(0)}(\mathbf{p}_1) \equiv |\hat{\varphi}_{\mathbf{p}_1}\rangle\rangle\langle\langle\hat{\varphi}_{\mathbf{p}_1}|i\theta_B^{(0)} + (i\theta_B^{(0)})^\dagger|\hat{\varphi}_{\mathbf{p}_1}\rangle\rangle\langle\langle\hat{\varphi}_{\mathbf{p}_1}|. \tag{153}$$

$\mathcal{K}_B^{(0)}$ is a hermitian operator. Thus these eigenvalues are real and the left-eigenstates are a hermitian conjugate of the right-eigenstates¶. Let us assume that the spectral decomposition of $\mathcal{K}_B^{(0)}$ is known

$$\mathcal{K}_B^{(0)}(\mathbf{p}_1) = \sum_\beta \gamma_\beta(\mathbf{p}_1)|w_\beta(\mathbf{p}_1)\rangle\rangle\langle\langle w_\beta(\mathbf{p}_1)|, \tag{154}$$

where γ_β are real numbers and

$$\begin{aligned} &\langle\langle w_\beta(\mathbf{p}_1)|w_{\beta'}(\mathbf{p}_1)\rangle\rangle = \delta_{\beta,\beta'}, \\ &\sum_\beta |w_\beta(\mathbf{p}_1)\rangle\rangle\langle\langle w_\beta(\mathbf{p}_1)| = \int \mathrm{d}p^{N-1}|0, \mathbf{p}_1, \{p\}^{N-1}\rangle\rangle\langle\langle 0, \mathbf{p}_1, \{p\}^{N-1}|. \end{aligned} \tag{155}$$

As mentioned, the operator $|\hat{\varphi}_{\mathbf{p}_1}\rangle\rangle\langle\langle\hat{\varphi}_{\mathbf{p}_1}|$ preserves the positivity. The reduction does not change the sign of the collision operator. Therefore, $\mathcal{K}_B^{(0)}$ is a non-negative operator, i.e.

$$\gamma_\beta(\mathbf{p}_1) \geqslant 0. \tag{156}$$

Then we have

$$\frac{\partial}{\partial t}|\varphi_1^B(\mathbf{p}_1, t)|^2 = -\sum_\beta \gamma_\beta(\mathbf{p}_1)|\langle\langle w_\beta(\mathbf{p}_1)|\rho_B(t)\rangle\rangle|^2 \leqslant 0. \tag{157}$$

The evolution of $|\varphi_1^B(\mathbf{p}_1, t)|^2$ is therefore monotonic. As the consequence, (see (149))

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}_\varphi^B(t) \leqslant 0. \tag{158}$$

¶In the reduced subspace of $\mathbf{1P}_1$, eigenstate of $\mathcal{K}_B^{(0)}$ are normalizable. This is in contrast to the eigenstates of the Liouvillian.

Hence, the $\mathcal{H}$ theorem holds. Then, $\mathcal{H}_\varphi^B(t)$ 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 λ (or concentrations) for which the spectral decomposition of $\mathcal{K}_B^{(0)}$ can be determined.

Instead of the Lyapunov function (149), we can introduce the more familiar form of the $\mathcal{H}$-function, such as

$$\mathcal{H}_\varphi^{B\prime}(t) = \int \mathrm{d}\mathbf{p}_1 |\varphi_1^B(\mathbf{p}_1, t)| \log |\varphi_1^B(\mathbf{p}_1, t)|. \tag{159}$$

Taking the time derivative, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}_\varphi^{B\prime}(t) = \frac{1}{2}\int \mathrm{d}\mathbf{p}_1 \frac{1}{|\varphi_1^B(\mathbf{p}_1, t)|}(\log|\varphi_1^B(\mathbf{p}_1, t)| + 1)\frac{\partial}{\partial t}|\varphi_1^B(\mathbf{p}_1, t)|^2 \leqslant 0. \tag{160}$$

Again we recover the $\mathcal{H}$ theorem. In the lowest order of λ (or of the concentration) the transformation (148) 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

$$\begin{aligned} f_s(\mathbf{q}_1 \cdots \mathbf{q}_s, \mathbf{p}_1 \cdots \mathbf{p}_s, t) &= \langle\langle \hat{f}_{\mathbf{q}_1,\ldots,\mathbf{q}_s,\mathbf{p}_1,\ldots,\mathbf{p}_s} | \rho(t) \rangle\rangle \\ &= \frac{N!}{(N-s)!}\int \mathrm{d}q' \int \mathrm{d}p' \delta(\mathbf{q}_1' - \mathbf{q}_1)\cdots\delta(\mathbf{q}_r' - \mathbf{q}_r)\delta(\mathbf{p}_1' - \mathbf{p}_1)\cdots \\ &\quad \times \delta(\mathbf{p}_s' - \mathbf{p}_s)\rho(q', p', t), \end{aligned} \tag{161}$$

with

$$\begin{aligned} \langle\langle \hat{f}_{\mathbf{q}_1,\ldots,\mathbf{q}_s,\mathbf{p}_1,\ldots,\mathbf{p}_s} | &= \frac{1}{L^{3r}}\sum_{\mathbf{k}_1}\cdots\sum_{\mathbf{k}_r} \mathrm{e}^{i(\mathbf{k}_1\cdot\mathbf{q}_1 + \cdots + \mathbf{k}_r\cdot\mathbf{q}_r)} \\ &\quad \times L^{3N/2}\int \mathrm{d}p' \delta(\mathbf{p}_1' - \mathbf{p}_1)\cdots\delta(\mathbf{p}_s' - \mathbf{p}_s)\langle\langle \mathbf{k}_1, \ldots, \mathbf{k}_r, \{0\}^{N-r}, p' |. \end{aligned} \tag{162}$$

We may now introduce the Lyapunov functions through

$$\mathcal{H}_f^B(t) = \int \mathrm{d}\mathbf{q}_1 \ldots \mathrm{d}\mathbf{q}_r \int \mathrm{d}\mathbf{p}_1 \ldots \mathrm{d}\mathbf{p}_s |\langle\langle \hat{f}_{\mathbf{q}_1,\ldots,\mathbf{q}_r,\mathbf{p}_1,\ldots,\mathbf{p}_s} | \rho_B(t)\rangle\rangle|^2. \tag{163}$$

The extension of the above arguments is straightforward.

8. POINCARÉ RESONANCES, FLOW OF CORRELATIONS AND ENTROPY BARRIER

The complex spectral representation obtained in Sections 4 and 5 as well as the $\mathcal{H}$ theorem in the previous section permit us to understand in an intuitive way the mechanism of irreversibility, which is associated to the 'flow of correlations' [6, 17].

Let us consider the evolution of binary correlations g_2.

$$\begin{aligned} g_2(\mathbf{q}_1, \mathbf{q}_2, \mathbf{p}_1, \mathbf{p}_2, t) &= \int \mathrm{d}q^{N-2}\int \mathrm{d}p^{N-2}\frac{1}{\Omega}\sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{q}_1-\mathbf{q}_2)}\rho_{\mathbf{k},-\mathbf{k}}(\mathbf{p}_1, \mathbf{p}_2 | p^{N-2}, t) \\ &= L^{3N/2}\int \mathrm{d}q^{N-2}\int \mathrm{d}p^{N-2}\sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{q}_1-\mathbf{q}_2)}\langle\langle \mathbf{k}, -\mathbf{k}, \{0\}^{N-2}, p | \rho(t)\rangle\rangle, \end{aligned} \tag{164}$$

where

$$|\rho(t)\rangle\rangle = \sum_{\nu}\sum_{\alpha} e^{-iZ_{\alpha}^{(\nu)}t}|F_{\alpha}^{(\nu)}\rangle\rangle\langle\langle \tilde{F}_{\alpha}^{(\nu)}|\rho(0)\rangle\rangle$$
$$= \sum_{\nu}(P^{(\nu)} + \mathbf{C}^{(\nu)})e^{-i\theta_C^{(\nu)}t}A^{(\nu)}(P^{(\nu)} + \mathbf{D}^{(\nu)})|\rho(0)\rangle\rangle. \tag{165}$$

Let us then consider for example an initial condition with no correlations, i.e. the system is initially in the vacuum of correlation,

$$|\rho(0)\rangle\rangle = P^{(0)}\rho(0)\rangle\rangle. \tag{166}$$

We assume that the coupling is small, i.e. $\lambda \ll 1$. The traditional approximation for a weakly coupled system in kinetic theory is the $\lambda^2 t$-approximation [17]. Then one only retains contribution of the order $(\lambda^2 t)^n$ with $n \geq 0$. For the evolution of correlations, however, this leads to the trivial result that all correlations vanish in the weakly coupled limit $\lambda \to 0$. Hence, we have to go beyond this approximation. We shall keep terms to order $\lambda(\lambda^2 t)^n$ in (165). We call this the '$\lambda(\lambda^2 t)^n$-approximation'. It should be emphasized that the $\lambda^2 t$-approximation describes only the asymptotic evolution in time. As the result, one cannot discuss causality in this approximation. In contrast, our approximation is applicable for all time scales. It is easy to extend this procedure to higher order approximations.

Then we have the contribution from $\Pi^{(0)}$ associated to the vacuum of correlation, and from $\Pi^{(k,-k)}$ associated to binary correlations (all other contributions are neglegible in this approximation):

$$\langle\langle \mathbf{k}, -\mathbf{k}, \{0\}^{N-2}, p|\rho(t)\rangle\rangle$$
$$= \lambda\langle\langle \mathbf{k}, -\mathbf{k}, \{0\}^{N-2}, p|(\mathbf{C}_1^{(0)}e^{-i\lambda^2\theta_2^{(0)}t} + e^{-i(\mathbf{k}\cdot\mathbf{g}_{12}+\lambda^2\theta_2^{(k,-k)})t}\mathbf{D}_1^{(k,-k)})P^{(0)}|\rho(0)\rangle\rangle, \tag{167}$$

where

$$\int dp'\langle\langle \mathbf{k}, -\mathbf{k}, \{0\}^{N-2}, p|\lambda\mathbf{C}_1^{(0)}|0, p'\rangle\rangle\rho_0(p')$$
$$= -\int dp'\langle\langle \mathbf{k}, -\mathbf{k}, \{0\}^{N-2}, p|\lambda\mathbf{D}_1^{(k,-k)}|0, p'\rangle\rangle\rho_0(p')$$
$$= -\lambda\frac{V_k}{\mathbf{k}\cdot\mathbf{g}_{12} - i\epsilon}\mathbf{k}\cdot\mathbf{d}_{12}\rho_0(p). \tag{168}$$

To evaluate (164) explicitly, we have to specify the interaction, and to solve the eigenvalue problem for the collision operators $\lambda^2\theta_2^{(0)}$ and $\mathbf{k}\cdot\mathbf{g}_{12} + \lambda^2\theta_2^{(k,-k)}$. For a simple system, such as the 'perfect Lorentz gas' (see Appendix F), we can solve the eigenvalue problem explicitly. We shall present detailed calculations for the causal evolution of the correlations in separate papers [41, 42] (see Appendix C for a remark on the causality). Here, we shall present a sketch of the results.

We first note that the effects of the two subspaces $\Pi^{(0)}$ and $\Pi^{(k,-k)}$ cancel at $t = 0$. For a short time scale, effects of dissipation coming from the collision operators are negligible. The integration over $\mathbf{k}$ in (164) is quite similar to the calculation of the momentum transfer (218) discussed in Section 11. In Appendix J we present the result of the integration of (218), using a short-range Gaussian repulsive interaction (see (J8) and (J12)). As far as the coordinate dependence is concerned, (164) are essentially the same as (218). Hence, we shall refer here to the results for (218). The results show that the binary correlation in $\Pi^{(0)}$ remains finite for $|\mathbf{q}_1 - \mathbf{q}_2| \to \infty$ (see (J15)). This results from the resonance singularity at

$\mathbf{k} \cdot \mathbf{g}_{12} = 0$ in (168). The resonance effect leads in the $\Pi^{(0)}$ subspace to 'long-range correlations' between the particles 1 and 2 whatever their distance. On the other hand, the effect in the subspace $\Pi^{(k,-k)}$ is simply a shift with an opposite sign of the contribution in $\Pi^{(0)}$ for short time scale, as $\mathbf{q}_1 - \mathbf{q}_2$ is replaced by $\mathbf{q}_1 - \mathbf{q}_2 - \mathbf{g}_{12}t$ (see also (J12)). Hence the total contribution of the binary correlation develops in space, following a causal evolution (see Fig. 2). Due to the Poincaré resonances, the long-range correlations are built up, as time goes on. However, it should be noted that the long-range correlations are associated only to non-equilibrium modes, as for equilibrium mode we have $\rho_0(p) = f(H_0)$ in (168) and it leads to $\mathbf{k} \cdot \mathbf{d}_{12}\rho_0(p) = \mathbf{k} \cdot \mathbf{g}_{12}f'(H_0)$, where the prime denotes the derivative. The factor $\mathbf{g}_{12}$ compensates the denominator in (168) and there is no resonance singularity at $\mathbf{k} \cdot \mathbf{g}_{12} = 0$ for the equilibrium mode.

For large time scales, the effects of the dissipation coming from the collision operators are no longer negligible. Effects from non-equilibrium modes both in $\Pi^{(0)}$ and in $\Pi^{(k,-k)}$ subspaces vanish for large time scales due to the repeated collisions with particles in the medium. In (164) only equilibrium short-range binary correlations remain finite around each particle. However during this process, ternary non-equilibrium correlations are built up, and then also decay to equilibrium correlations, then fourth order correlations etc. As time goes on, the non-equilibrium correlations are propagating over larger distance*, and transfer the correlations among more and more particles. We then have the directed 'flow of correlations'. This flow finally disappears in the 'sea' of highly multiple, incoherent correlations [17]. While the very meaning of irreversibility is difficult to express in terms of the usual dynamics of particles, it acquires a direct intuitive sense in terms of the 'dynamics of correlation' based on the complex spectral representation.

The $\mathcal{H}$-property, as well as flow of correlations, are direct consequences of the existence of the complex spectral representation of the Liouvillian. As mentioned before, the dynamical group splits then into two semi-groups. We have to retain the semi-group for which the system approaches equilibrium in our future. This corresponds to the 'second law of thermodynamics'. This law plays a basic role as it leads to a 'selection principle' for the states which can be observed in nature.

In the previous paper [5] we have already shown for a simple non-integrable quantum system (i.e. the Friedrichs model) that the 'entropy barrier' defined as the difference

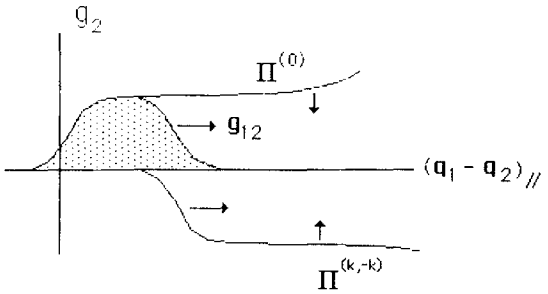

Fig. 2. Causal propagation of binary correlations g_2 in the parallel direction $(\mathbf{q}_1 - \mathbf{q}_2)_{//}$ to the relative velocity $\mathbf{g}_{12}$. The contribution from the $\Pi^{(0)}$ diverges exponentially as a function of $(\mathbf{q}_1 - \mathbf{q}_2)_{//}$ (see the discussion in Appendix C). The contribution in the space $\Pi^{(0)}$ damps in time, while the contribution in the space $\Pi^{(k,-k)}$ shifts with the relative velocity $\mathbf{g}_{12}$ and damps. Outside the non-causal region $(\mathbf{q}_1 - \mathbf{q}_2)_{//} > |\mathbf{g}_{12}|t$ the contribution in the space $\Pi^{(0)}$ is canceled by the contribution in $\Pi^{(k,-k)}$. As time goes on, a long-range correlation is built up by the resonance.

*Due to the existence of diffusion modes in space associated to small wave vectors $\mathbf{k}$, the non-equilibrium correlations can propagate over a larger distance (see Appendices F and K).

between the value of the $\mathcal{H}$-function after and before a 'velocity inversion' increases exponentially as a function of time t_0 at which the velocities are inverted. For this case the 'long-range correlations' between the unstable particles and the emitted photons are built up again due to resonances. The longer the time t_0, the more difficult it becomes to prepare the 'velocity inverted' states. Asymptotically, the entropy barrier diverges. One can no longer prepare the 'inverted' states. As mentioned, the resonances also build up long-range correlations among the particles for the N-body system. We can then extend this argument for the system in the thermodynamic limit. We present this extension in Appendix K. There we shall show that long-range correlations lead again to an 'entropy barrier'. To be consistent with our experience, it is natural to exclude the set of initial conditions which would lead to an infinite value of the $\mathcal{H}$-functions or of the 'entropy'. Therefore, the second law of thermodynamics may be formulated as follows.

Only states which lead to finite values of $\mathcal{H}$ functions are found in nature.

In other words, only states in the domain of Λ are found (or can be prepared) in nature. This seems to us a very natural conclusion.

9. LINEAR AND NON-LINEAR LIPPMANN–SCHWINGER EQUATIONS

In the previous sections we have derived the complex spectral representation of L_H through the solutions of the 'non-linear' eigenvalue problem of the collision operator $\psi^{(\nu)}$ in (83) and (106). Also, if we first determine the operators $\mathbf{C}^{(\nu)}$ and $\mathbf{D}^{(\nu)}$, we can construct the global collision operators $\theta_B^{(\nu)}$ which do not explicitly depend on the eigenvalues $Z_\alpha^{(\nu)}$ (see (91) and (111)). Then, using the solutions of the 'linear' eigenvalue problem for $\theta_B^{(\nu)}$, we can construct the solutions of the eigenvalue problem of L_H through the intertwining relations (127) [4, 14]. In this approach the nonlinearlity of the problem appears in the equations for $\mathbf{C}^{(\nu)}$ and $\mathbf{D}^{(\nu)}$. Indeed, the intertwining relations (127) with (91) and (111) lead to non-linear equations for $\hat{\Phi}_\nu^C$ and $\hat{\Phi}_\nu^C$, through which we can determine $\mathbf{C}^{(\nu)}$ and $\mathbf{D}^{(\nu)}$ [14, 23, 24]:

$$L_0\hat{\Phi}_\nu^C - \hat{\Phi}_\nu^C L_0 = -L_V\hat{\Phi}_\nu^C + \hat{\Phi}_\nu^C L_V\hat{\Phi}_\nu^C, \tag{169a}$$

$$L_0\hat{\Phi}_\nu^D - \hat{\Phi}_\nu^D L_0 = \hat{\Phi}_\nu^D L_V - \hat{\Phi}_\nu^D L_V\hat{\Phi}_\nu^D. \tag{169b}$$

Let us operate $\hat{\Phi}_\nu^C$ and $\hat{\Phi}_\nu^D$ on the eigenstates of the unperturbed Liouvillian L_0,

$$|\Phi_\nu^C\rangle\rangle \equiv \hat{\Phi}_\nu^C|\nu\rangle\rangle, \qquad \langle\langle\Phi_\nu^D| \equiv \langle\langle\nu|\hat{\Phi}_\nu^D. \tag{170}$$

In general these states are not eigenstates of L_H.

From (169) we derive the non-linear equations,

$$|\Phi_\nu^C\rangle\rangle = |\nu\rangle\rangle + \lim_{\Omega\to\infty}\sum_\mu \frac{-1}{l_\mu - l_\nu + i\epsilon_{\mu\nu}} P^{(\mu)}Q^{(\nu)}\lambda L_V|\Phi_\nu^C\rangle\rangle$$

$$+ \lim_{\Omega\to\infty}\sum_\mu \frac{1}{l_\mu - l_\nu + i\epsilon_{\mu\nu}} P^{(\mu)}Q^{(\nu)}|\Phi_\nu^C\rangle\rangle\langle\langle\nu|\lambda L_V|\Phi_\nu^C\rangle\rangle, \tag{171a}$$

$$\langle\langle\Phi_\nu^D| = \langle\langle\nu| + \lim_{\Omega\to\infty}\sum_\mu \langle\langle\Phi_\nu^D|\lambda L_V Q^{(\nu)}P^{(\mu)}\frac{1}{l_\nu - l_\mu + i\epsilon_{\nu\mu}}$$

$$+ \lim_{\Omega\to\infty}\sum_\mu \langle\langle\Phi_\nu^D|\lambda L_V|\nu\rangle\rangle\langle\langle\Phi_\nu^D|Q^{(\nu)}P^{(\mu)}\frac{-1}{l_\nu - l_\mu + i\epsilon_{\nu\mu}}. \tag{171b}$$

We have imposed the boundary conditions

$$|\Phi_\nu^C\rangle\rangle = |\nu\rangle\rangle, \qquad \text{and} \qquad \langle\langle\Phi_\nu^D| = \langle\langle\nu|, \qquad (\text{for } \lambda = 0). \tag{172}$$

The analytic continuations of the denominators in (171) are given by the $i\epsilon$-rule (75).

By iterating (171) we can construct the explicit form of $\mathbf{C}^{(\nu)}$ and $\mathbf{D}^{(\nu)}$ in powers of λ. We can then construct $A^{(\nu)}$ through (118), and thus $\Pi^{(\nu)}$ as well as $\theta_B^{(\nu)}$ in powers of λ. We shall call equations (171) the 'non-linear Lippmann–Schwinger equations' (NLLS), as we shall show that they are corresponding to a 'non-linear extension' of the classical version of the 'Lippmann–Schwinger equations'. The non-linear terms of NLLS involve the contribution from the diagonal transitions associated to the collision operators (see (91) and (111))

$$\langle\langle\nu|\lambda L_V|\Phi_\nu^C\rangle\rangle = \langle\langle\nu|\theta_C^{(\nu)}|\nu\rangle\rangle - l_\nu, \qquad \langle\langle\Phi_\nu^D|\lambda L_V|\nu\rangle\rangle = \langle\langle\nu|\theta_D^{(\nu)}|\nu\rangle\rangle - l_\nu. \tag{173}$$

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

$$\theta_B^{(\nu)} = L_0 P^{(\nu)}, \tag{174}$$

where B stands as before for C or D. This implies that the eigenstate of $\theta_B^{(\nu)}$ is the unperturbed state $|\nu\rangle\rangle$, and the eigenvalues of L_H are l_ν 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 (115))

$$N_\alpha^{(\nu)} = 1, \tag{175}$$

as well as

$$A^{(\nu)} = P^{(\nu)}. \tag{176}$$

Combining them with (127), we have

$$L_H|\Phi_\nu^C\rangle\rangle = l_\nu|\Phi_\nu^C\rangle\rangle, \qquad \langle\langle\Phi_\nu^D|L_H = \langle\langle\Phi_\nu^D|l_\nu, \tag{177}$$

i.e. for this special case the states Φ_ν^C and Φ_ν^D are eigenstates of L_H with real eigenvalues l_ν. We shall show later that this situation corresponds to 'integrable systems' in the sense of Poincaré.

Then equations (171) reduce to the 'linear' equations,

$$\begin{aligned} |\Phi_\nu^C\rangle\rangle &= |\nu\rangle\rangle + \sum_\mu \frac{-1}{l_\mu - l_\nu + i\epsilon_{\mu\nu}} P^{(\mu)} Q^{(\nu)} \lambda L_V |\Phi_\nu^C\rangle\rangle, \\ \langle\langle\Phi_\nu^D| &= \langle\langle\nu| + \sum_\mu \langle\langle\Phi_\nu^D|\lambda L_V Q^{(\nu)} P^{(\mu)} \frac{1}{l_\nu - l_\mu + i\epsilon_{\nu\mu}}, \end{aligned} \tag{178}$$

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 (178) as well as (177) is valid only for the integrable systems where the diagonal transitions associated to the collision operator are negligible. For this case we have

$$\langle\langle\Phi_\nu^D|\Phi_\mu^C\rangle\rangle = \delta_{\nu,\mu} \qquad \sum_\nu |\Phi_\nu^C\rangle\rangle\langle\langle\Phi_\nu^D| = 1, \tag{179}$$

and the spectral decomposition of the evolution operator,

$$\mathrm{e}^{-iL_H t} = \sum_\nu |\Phi_\nu^C\rangle\rangle\, \mathrm{e}^{-il_\nu t} \langle\langle\Phi_\nu^D|. \tag{180}$$

Moreover the transformations Λ_B reduce to

$$\Lambda_B = \Lambda_I, \tag{181}$$

where

$$\Lambda_I = \sum_\nu |\nu\rangle\rangle\langle\langle \Phi_\nu^D|, \qquad \Lambda_I^{-1} = \sum_\nu |\Phi_\nu^C\rangle\rangle\langle\langle \nu|, \tag{182}$$

which lead to

$$\Lambda_B L_H \Lambda_B^{-1} = \Lambda_I L_H \Lambda_I^{-1} = L_0. \tag{183}$$

We have put in the index I in order to emphasize that Λ_I is associated to integrable systems, as (183) holds only for this case. In Appendix L we present the explicit form of the solutions of (178) for Φ_ν^C and Φ_ν^D for two-particle systems (or potential scattering).

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 versions of the 'Möller scattering states' $\Phi_\nu^\pm$ defined as the solution of the equations (33–35)

$$\begin{aligned} |\Phi_\nu^\pm\rangle\rangle &= |\nu\rangle\rangle + \frac{1}{l_\nu - L_0 \pm i\epsilon} Q^{(\nu)} \lambda L_V |\Phi_\nu^\pm\rangle\rangle, \\ \langle\langle \Phi_\nu^\pm| &= \langle\langle \nu| + \langle\langle \Phi_\nu^\pm| \lambda L_V Q^{(\nu)} \frac{1}{l_\nu - L_0 \mp i\epsilon}. \end{aligned} \tag{184}$$

They also satisfy

$$L_H |\Phi_\nu^\pm\rangle\rangle = l_\nu |\Phi_\nu^\pm\rangle\rangle, \tag{185}$$

as well as (for the integrable systems)

$$\langle\langle \Phi_\nu^+ | \Phi_\mu^+\rangle\rangle = \delta_{\nu,\mu} \qquad \sum_\nu |\Phi_\nu^+\rangle\rangle\langle\langle \Phi_\nu^+| = 1, \tag{186}$$

and

$$e^{-iL_H t} = \sum_\nu |\Phi_\nu^+\rangle\rangle\, e^{-il_\nu t} \langle\langle \Phi_\nu^+|, \tag{187}$$

and similar relations for Φ_ν^-. The states Φ_ν^+ correspond to the 'retarded' solutions of the scattering, while Φ_ν^- to the 'advanced' solutions.

Equation (187) is the unitary spectral decomposition of the evolution operator. Moreover we can introduce the unitary transformations (for repulsive forces)

$$U_\pm = \sum_\nu |\nu\rangle\rangle\langle\langle \Phi_\nu^\pm|, \qquad U_\pm^\dagger = \sum_\nu |\Phi_\nu^\pm\rangle\rangle\langle\langle \nu|, \tag{188}$$

which lead to

$$U_+ L_H U_+^\dagger = L_0. \tag{189}$$

and a similar relation for U_-.

The structure of Λ_I is quite similar to that of $U_\pm$. However, due to the difference in the analytic continuations between (178) and (184) 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 (178) by

$$|\Phi_0^C\rangle\rangle = |\Phi_0^+\rangle\rangle, \qquad \langle\langle\Phi_0^D| = \langle\langle\Phi_0^-|. \tag{190}$$

As the complex spectral representation uses both analytic continuation in (182), Λ_I is a non-unitary transformation even for the integrable case. Nevertheless, because of the bi-completeness relation in (179), the spectral representation (180) and (187) lead to the same evolution of the distribution function $|\rho(t)\rangle\rangle$.

It is remarkable that integrable LPS admits both the non-unitary transformation (182), as well as the unitary ones (188).[§] However, there is a significant difference between the two. To see this, let us evaluate the inner product $\langle\langle\Phi_{0,p'}^-|\Phi_{0,p}^-\rangle\rangle$ for the unitary transformations. Because the inner product is a distribution, we evaluate this with an integration over p' as (e.g. with the momentum $\mathbf{p}_1$)

$$\begin{aligned}\int dp'\mathbf{p}_1'\langle\langle\Phi_{0,p'}^-|\Phi_{0,p}^-\rangle\rangle &= \mathbf{p}_1 - \frac{\lambda^2}{\Omega^2}\sum_{n>j}^{N}\sum_{\mathbf{k}}\int dp'\mathbf{p}_1'\mathbf{k}\cdot\mathbf{d}_{jn}'\frac{|V_k|^2}{|\mathbf{k}\cdot\mathbf{g}_{jn}' + i\epsilon|^2}\mathbf{k}\cdot\mathbf{d}_{jn}'\delta(p' - p) + O(\lambda^3)\\ &= \mathbf{p}_1 - \frac{\lambda^2}{\Omega^2}\sum_{n=2}^{N}\sum_{\mathbf{k}}\mathbf{k}\cdot\mathbf{d}_{1n}\frac{|V_k|^2}{|\mathbf{k}\cdot\mathbf{g}_{1n} + i\epsilon|^2}\mathbf{k} + O(\lambda^3) \qquad (191)\\ &= \mathbf{p}_1 + O(N/\epsilon\Omega).\end{aligned}$$

To obtain the second equality in (191) we have performed an integration by parts over the momenta. The non-vanishing contribution comes only from the terms which are 'connected' to the labeled particle 1. All 'disconnected' terms vanish by integration by parts over the momentum $\mathbf{p}_j$ for $j \neq 1$. As the result, the number of terms of the λ^2 contribution in (191) reduce from N^2 to N. We note that this is a general property associated to reduced quantities (50) (see also (67)). Whenever we consider the reduced observables, all disconnected terms vanish.

Due to the Poincaré resonances, there appears a singularity $\sim\epsilon^{-1}$ in (191). However, for N finite this singularity is harmless, as we have to take first the limit $\Omega \to 0+$ before taking the limit $\epsilon \to 0+$ (see (B2)). Nevertheless, the unitary transformations cannot be extended to non-integrable systems in the thermodynamic limit, since Ω^{-1} is compensated by N in this limit. In contrast, the non-unitary transformation regularizes the Poincaré divergence as

$$\int dp'\mathbf{p}_1'\langle\langle\Phi_{0,p'}^D|\Phi_{0,p}^C\rangle\rangle \sim \mathbf{p}_1 + \frac{N}{\Omega^2}\sum_{\mathbf{k}}\left(\frac{1}{(\mathbf{k}\cdot\mathbf{v} + i\epsilon)^2} + c.c\right) \sim \mathbf{p}_1 + O(N/\Omega). \tag{192}$$

Hence, (182) has a natural extension for the non-integrable systems where the time-symmetry is broken (see also the Appendix D).

10. INVARIANTS OF MOTION AND INTEGRABILITY CONDITIONS

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

$$\langle\langle\tilde{M}^B(t)| \equiv \langle\langle\hat{M}(0)|\Lambda_B{}^{\mathcal{U}}(t). \tag{193}$$

[§]The non-uniqueness of the spectral decomposition including a non-unitary spectral decomposition has also been observed for the Friedrichs model in quantum mechanics [5].

We note the difference of this quantity from $\langle\langle \hat{M}_B(t)|$ introduced in (130). The time evolution of $\langle\langle \widetilde{M}^B(t)|$ is generated by the Liouvilian L_H, while $\langle\langle \hat{M}_B(t)|$ is generated by the collision operator Θ_B.

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

$$\langle\langle \hat{M}(0)| = \langle\langle \hat{M}(0)|P^{(\nu)}. \tag{194}$$

Then we have indeed (see (125))

$$\langle\langle \widetilde{M}^D(0)|\Pi^{(\nu)} = \sum_\alpha \langle\langle \hat{M}(0)|v_\alpha^{(\nu)}\rangle\rangle \langle\langle \tilde{F}_\alpha^{(\nu)}|N_\alpha^{(\nu)-1/2}\Pi^{(\nu)} = \sum_\alpha \langle\langle \hat{M}(0)|v_\alpha^{(\nu)}\rangle\rangle \langle\langle \tilde{F}_\alpha^{(\nu)}| \, N_\alpha^{(\nu)-1/2} = \langle\langle \widetilde{M}^D(0)|. \tag{195}$$

For this case we have (see (141))

$$\langle\langle \widetilde{M}^D(t)| = \sum_\alpha \langle\langle \hat{M}(0)|v_\alpha^{(\nu)}\rangle\rangle \, \mathrm{e}^{-iZ_\alpha^{(\nu)}t} \langle\langle \tilde{v}_\alpha^{(\nu)}|\Phi_D^{(\nu)} = \langle\langle \hat{M}(0)| \, \mathrm{e}^{-i\theta_D^{(\nu)}t}\hat{\Phi}_\nu^D. \tag{196}$$

Of special interest is the case where $\nu = 0$, because this leads to 'invariants' of motion for integrable systems. To see this, let us consider the transformed 'momenta' (see (52))

$$\langle\langle \tilde{\mathbf{p}}_i^D(t)| \equiv \langle\langle \hat{\mathbf{p}}_i|\Lambda_D \mathcal{U}(t). \tag{197}$$

We have

$$\langle\langle \tilde{\mathbf{p}}_i^D(t)|\rho(0)\rangle\rangle = \langle\langle \hat{\mathbf{p}}_i| \, \mathrm{e}^{-i\theta_D^{(0)}t}\hat{\Phi}_0^D|\rho(0)\rangle\rangle. \tag{198}$$

When the diagonal transitions are negligible, i.e. $\theta_D^{(0)} = 0$, the transformed momenta reduce to the invariants of motion (see (182))

$$\langle\langle \tilde{\mathbf{p}}_i^D(t)|\rho(0)\rangle\rangle \to \langle\langle \hat{\mathbf{p}}_i|\Lambda_I|\rho(0)\rangle\rangle = \int \mathrm{d}p' \langle\langle \hat{\mathbf{p}}_i|0, \, p'\rangle\rangle \langle\langle \Phi_{0,p'}^D|\rho(0)\rangle\rangle. \tag{199}$$

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

$$\mathbf{P}_i^D(q^0, \, p^0) \equiv \langle\langle \tilde{\mathbf{p}}_i^D|q^0, \, p^0\rangle\rangle = L^{3N/2}\int \mathrm{d}p' \mathbf{p}_i' \langle\langle \Phi_{0,p'}^D|q^0, \, p^0\rangle\rangle. \tag{200}$$

This defines a set of $3N$ 'new' momenta. Therefore, when the conditions (a) diagonal transitions are negligible, and (b) the right-hand side of (200) exists, the $\mathbf{P}_i^D(q^0, p^0)$ are invariants of motion, and the system is integrable in the sense of Poincaré. We shall call the condistions (a) and (b) the 'integrability conditions'. We shall discuss later these conditions in detail for various situations.

In analogy to the quantum S-matrix theory, we can write the solution of the Möller state $\Phi_{0,p}^D$ in (190) in terms of the classical version of the $\mathcal{T}$-matrix,[§]

$$\langle\langle \Phi_{0,p}^D| = \langle\langle 0, \, p| + \langle\langle 0, \, p|\mathcal{T}(+i\epsilon)\frac{1}{+i\epsilon - L_0}, \tag{201}$$

where the $\mathcal{T}$-matrix is the solution of the integro-differential equation (c.f. (101)),

$$\mathcal{T}(z) = \lambda L_V + \mathcal{T}(z)\frac{1}{z - L_0}\lambda L_V. \tag{202}$$

[§]For integrable systems we can remove the restriction expressed by $Q^{(\nu)}$ in (178). See the discussion of the last part in the next section.

Then the invariants of motion (200) are given by (for integrable systems)

$$\mathbf{P}_i^D(q^0, p^0) = \mathbf{p}_i + \lim_{\Omega\to\infty} \int dp' \mathbf{p}_i' \sum_k \langle\langle 0, p' | \mathcal{T}(+i\epsilon) | k, p \rangle\rangle \frac{1}{+i\epsilon - k\cdot v^0} e^{-ik\cdot q^0}. \quad (203)$$

Hence, the existence of the $\mathcal{T}$-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.* The system is then integrable in the sense of Poincaré. Even when there is no analytic solution described by the Born series in λ of the $\mathcal{T}$-matrix, there may exist non-analytic solutions of (202), such as they occur for attractive forces in quantum scattering. We hope to present a classical analogue of this situation elsewhere.

The invariants (203) 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 [17, 36] (see also [37, 38]). It is worthwhile comparing 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 [39]. By the standard perturbation analysis for $F(P', q)$, one can easily show that the generalized momentum $\mathbf{P}_1'$ is the same as (203) to first order in λ (see also (206)). Hence, assuming the analyticity of the $\mathcal{T}$-matrix at $\lambda = 0$, the invariants (203) are the Hamilton–Jacobi invariants of motion.

Let us now discuss in detail the integrability conditions for (198). We first consider the case where the number of particles N is finite, and the distribution functions are regular as given by (31) with no delta function singularity in their Fourier representation. Expanding (198) in powers of λ, we have

$$\langle\langle \tilde{\mathbf{p}}_i^D(t) | \rho(0) \rangle\rangle = \lim_{\Omega\to\infty} \sum_k \int dp \int dp' \mathbf{p}_i \langle\langle 0, p | e^{-i\lambda^2\theta_2^{(0)}t}(1 + \lambda\mathbf{D}_1^{(0)} + \lambda^2\mathbf{D}_2^{(0)}) | k, p' \rangle\rangle \bar{\rho}_k(0) + \lambda^3 \cdots \quad (204)$$

Here $\lambda^n\theta_n^{(0)}$ and $\lambda^n\mathbf{D}_n^{(0)}$ are the nth order approximation of the corresponding operators (see (97)). To the second order in λ, we obtain

$$\langle\langle \tilde{\mathbf{p}}_i^D(t) | \rho(0) \rangle\rangle = \lim_{\Omega\to\infty} \sum_k \int dp \int dp' \mathbf{p}_i \times \langle\langle 0, p | [1 + \lambda\mathbf{D}_1^{(0)} + \lambda^2(\mathbf{D}_2^{(0)} - i\theta_2^{(0)}t) + \lambda^3 \cdots] | k, p' \rangle\rangle \bar{\rho}_k(0). \quad (205)$$

The contribution from $\mathbf{D}_n^{(0)}$ 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 (200). To first order in λ, we have (e.g. for $i = 1$)

$$\begin{aligned} \mathbf{P}_1^D(q^0, p^0, t) &= \mathbf{p}_1^0 - \lambda \lim_{\Omega\to\infty} \frac{1}{\Omega} \sum_{n>j}^N \sum_k \int dp \mathbf{p}_1 \mathbf{k}\cdot\mathbf{d}_{jn} \frac{V_{|\mathbf{k}|}}{\mathbf{k}\cdot\mathbf{g}_{jn} - i\epsilon} e^{-i\mathbf{k}(\mathbf{q}_j^0 - \mathbf{q}_n^0)} \delta(p - p^0) + O(\lambda^2) \\ &= \mathbf{p}_1^0 + \lambda \lim_{\Omega\to\infty} \frac{1}{\Omega} \sum_{n=2}^N \sum_{\mathbf{k}} \frac{V_k}{\mathbf{k}\cdot\mathbf{g}_{1n}^0 - i\epsilon} \mathbf{k}\, e^{-i\mathbf{k}\cdot(\mathbf{q}_1^0 - \mathbf{g}_n^0)} + O(\lambda^2) \end{aligned} \quad (206)$$

*For more than two-body systems, we need a careful discussion of the analyticity of the $\mathcal{T}$-matrix, as performed by Faddeev for the three-body collision. We shall not discuss this problem here.

To obtain the last line in (206) we have again retained the 'connected' contribution to the labeled particle 1 (see (191)).

Similarly, the second order contribution $\mathbf{D}_2$ is given by

$$\overline{[\mathbf{P}_1^D(q^0, p^0, t)]}_{\lambda^2\mathbf{D}_2} = -\lambda^2 \lim_{\Omega\to\infty} \frac{1}{\Omega^2} \sum_{n=2}^{N} \sum_{\mathbf{k}} \sum_{\mathbf{k}'}{}' \int \mathrm{d}p\mathbf{p}_1\mathbf{k}\cdot\mathbf{d}_{1n} \frac{V_{|\mathbf{k}|}}{\mathbf{k}\cdot\mathbf{g}_{1n} - i\epsilon} \times (\mathbf{k}-\mathbf{k}')\cdot\mathbf{d}_{1n} \frac{V_{|\mathbf{k}-\mathbf{k}'|}}{\mathbf{k}'\cdot\mathbf{g}_{1n} - i\epsilon} \mathrm{e}^{-i\mathbf{k}'\cdot(\mathbf{q}_1^0-\mathbf{q}_n^0)} \delta(p-p^0), \quad (207)$$

where the bar denotes the particular term we are looking at. 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 $\mathbf{k}'$ denotes that we exclude $\mathbf{k}' = 0$. This restriction is the result of the fact that $\mathbf{D}^{(0)}$ is the off-diagonal transition (expressed by $Q^{(0)}$ in (103)).

For the diagonal transition we have (see (97))

$$[\mathbf{P}_1^D(q^0, p^0, t)]_{\lambda^2\theta_2} = i\lambda^2 t \lim_{\Omega\to\infty} \frac{1}{\Omega^2} \sum_{n=2}^{N} \sum_{\mathbf{k}} \int \mathrm{d}p\mathbf{p}_1\mathbf{k}\cdot\mathbf{d}_{1n} \frac{|V_k|^2}{\mathbf{k}\cdot\mathbf{g}_{1n} - i\epsilon} \mathbf{k}\cdot\mathbf{d}_{1n}\delta(p-p^0). \quad (208)$$

For any finite N, the diagonal transition (208) is negligible as this term is proportional to Ω^{-1}.

In Appendix J we present the result of integration over $\mathbf{k}$ in (206), using a short-range Gaussian repulsive interaction (see (J8) and (J12)). We see that the effect of the interaction for particles n in (206) remains finite for $|\mathbf{q}_1^0 - \mathbf{q}_n^0| \to \infty$ (see (J15)). This results from the resonance singularity at $\mathbf{k}\cdot\mathbf{g}_{1n}^0 = 0$ in (206). Similar to the discussion in Section 8 the resonance effect leads to the long-range correlations between the particle 1 and n whatever their distance. Hence the order of this contribution is $O(\lambda N)$. Similarly one can show that the order of (207) from the binary correlations is $\lambda^2 N$, and from the ternary correlations in λ^2 contribution is $O(\lambda^2 N^2)$, and so on (see the discussion below). As the result, if the number of particles $N \to \infty$, then (206) generally diverges. In order for (206) to be an invariant of motion, N should be finite. Even if N is finite, but too large, then the series expansion in λ may not converge.

We can easily extend the above estimations for the diagonal transition and the off-diagonal transitions to all orders of λ. Indeed, by increasing λ in the off-diagonal transition, we multiply by the factor $\Omega^{-1}\sum_{\mathbf{k}}$ (see (28)). This factor does not lead to any extra volume factor in the limit of $\Omega \to \infty$ (see (20)). A new particle may or may not participate in the interaction. On the other hand, the diagonal transition is a point transition in the summation over $\mathbf{k}$, so that it leads to a factor Ω^{-1} without any summation over the wave vector. Hence this vanishes in the limit $\Omega \to \infty$. As the consequence, all diagonal transitions are negligible for 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 $\mathbf{k}' = 0$ in (207) is of order $(\epsilon\Omega)^{-1}$ and can be neglected by the condition (B2).

Extension of these estimations to more general observables in equation (196) is straightforward. Applying these results to NLLS (171), we see that they reduce to the linear Lippmann–Schwinger equation (178).

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 non-integrable situations which cannot be described by Newtonian trajectory theory.

11. PERSISTENT INTERACTIONS AND SINGULAR DISTRIBUTION FUNCTIONS

In the previous sections we have constructed the invariants of motion (203) for systems with a finite number of particles and described by regular distribution functions. We now show that the new momenta defined in (200) are no longer invariants of motion when they are associated to singular distribution functions.

Let us integrate (200) over the coordinate q,

$$I(p, t) = \int \mathrm{d}q \mathbf{P}_1^D(q, p, t). \tag{209}$$

The diagonal transition in (208) now gives a finite contribution, while the off-diagonal transitions in (206) and (207) vanish because of the restriction by $Q^{(0)}$ in the $\mathbf{D}^{(0)}$ operator. Therefore we obtain from (208) (e.g. $N = 1$, and dropping the index of particle 1)

$$\frac{\mathrm{d}}{\mathrm{d}t} I(\mathbf{p}, t) = \lambda^2 \int \mathrm{d}\mathbf{k} \int \mathrm{d}\mathbf{p}' \mathbf{p}' |V_k|^2 \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}'} \pi \delta(\mathbf{k} \cdot \mathbf{v}') \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}'} \delta(\mathbf{p}' - \mathbf{p}) + \mathrm{O}(\lambda^3). \tag{210}$$

We see that $I(\mathbf{p}, t)$ evolves in time.

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

$$\rho_{\mathbf{k}}(0) = \rho_0^d(\mathbf{p}, 0) \delta_\Omega(\mathbf{k}) + \rho_{\mathbf{k}}'(\mathbf{p}, 0), \tag{211}$$

where we assume that ρ_0^d and $\rho_{\mathbf{k}}'$ do not depend on Ω in the limit of large volumes. Because of this singularity, the effect of the diagonal transitions are amplified Ω times. As the result, $I(\mathbf{p}, t)$ evolves in time.‡

However, we note that the normalization of this singular distribution function diverges,

$$\int \mathrm{d}\mathbf{q} \int \mathrm{d}\mathbf{p} \rho(\mathbf{q}, \mathbf{p}, 0) = \int \mathrm{d}\mathbf{p} [\Omega \rho_0^{\mathrm{d}}(1\mathbf{p}, 0) + \rho_0'(\mathbf{p}, 0)] \to \infty. \tag{212}$$

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 (210), we obtain for the ensemble (211),

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle\langle \tilde{\mathbf{p}}^D(t) | \rho(0) \rangle\rangle = \lambda^2 \int \mathrm{d}\mathbf{k} \int \mathrm{d}\mathbf{p} \mathbf{p} |V_k|^2 \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \pi \delta(\mathbf{k} \cdot \mathbf{v}) \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}} \rho_0^d(\mathbf{p}, 0) + \mathrm{O}(\lambda^3). \tag{213}$$

Therefore $\langle\langle \tilde{\mathbf{p}}^D(t) | \rho(0) \rangle\rangle$ evolves in time when associated to the singular distribution function (211). In the right-hand side of (213) we recognize the Fokker–Planck operator (see (95)). Dissipative processes are enhanced by the delta function singularity in (211).

‡For this case non-negligible diagonal transitions appear only in the vacuum of correlation. Hence, the analytic continuation for the diagonal operators is also uniquely determined by the complex distribution, as in the case of the thermodynamic limit discussed in (97).

The system is non-integrable for persistent interaction described by the singular distribution functions.

In the evolution of $\langle\langle \tilde{\mathbf{p}}^D(t)|\rho(0)\rangle\rangle$ there appear generally higher order contributions in time, as $(-i\theta_a^{(0)}t)^n$ with $n \geq 2$ (see (141)). However, as one can easily see, a repetition of diagonal transitions always leads to extra volume factor Ω^{-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 $\tilde{\mathbf{p}}^D(t)$ is strictly linear in time. In previous papers we have investigated in detail this situation and performed numerical simulations [1, 2, 16]. The agreement is excellent.

Because of the linear time dependence of $\langle\langle \tilde{\mathbf{p}}^D(t)|\rho(0)\rangle\rangle$ in (213), 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 such as (45) in the thermodynamic limit.

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 (211). This is generally true for all contributions in the $\Pi^{(0)}$ subspace, whenever the contributions involve the effect of the interaction λL_V. However, there is an exceptional component which leads to a divergence in the Λ transformations. That is the contribution coming from the free motion. For example, the unperturbed component of $\langle\langle \tilde{\mathbf{p}}^D(t)|\rho(0)\rangle\rangle$ diverges when it is associated to the singular function (211), in spite of the fact that its time derivative gives the finite contribution (213). The integration of the momentum $\mathbf{p}_1^0$ in (206) 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.

12. SINGULAR DISTRIBUTION FUNCTIONS AND THE THERMODYNAMIC LIMIT

We now consider the singular distribution functions of class (45) 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 non-equilibrium statistical mechanics (NESM). Its time dependence has been already investigated in our earlier work [17–19]. All results obtained from the 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. 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 $t \to \infty$ [17]. 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 non-unitary transformation Λ. To illustrate this, let us evaluate the transformed momentum $\tilde{\mathbf{p}}_1^D(0)$ on the ensemble (45). As in (206), we have to first order in λ:

$$\langle\langle \tilde{\mathbf{p}}_1^D(0)|\rho(0)\rangle\rangle = \int d p \mathbf{p}_1 \rho_0(|p, 0)$$

$$- \lim_{\Omega\to\infty} \frac{\lambda}{\Omega^2} \sum_{n=2}^{N} \sum_{\mathbf{k}} \int d p \mathbf{p}_1 \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{p}_1} \frac{V_k}{\mathbf{k}\cdot\mathbf{g}_{1n} - i\epsilon} \rho_{\mathbf{k},-\mathbf{k}}(\mathbf{p}_1, \mathbf{p}_n|p^{N-2}, 0) + O(\lambda^2). \quad (214)$$

Note that the difference in the volume dependence between (214) and (206). Now the transformed momentum has a well-defined value of order c in the thermodynamic limit (2).

One can easily verify that (214) is well-defined to the arbitrary order of λ, as follows. In the second order contribution λ^2, there are three possible contributions; the first is the diagonal transition coming from the vacuum of correlation $\rho_0(|p)$, the second from the binary correlations $\rho_{\mathbf{k}'-\mathbf{k}'}(\mathbf{p}_1, \mathbf{p}_n|)$, and the third from the ternary correlations $\rho_{\mathbf{k},\mathbf{k}',-\mathbf{k}-\mathbf{k}'}(\mathbf{p}_1, \mathbf{p}_j, \mathbf{p}_n|)$. 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 (206)). In all the three cases there appears an extra volwme factor Ω^{-1} through the new interaction (see (28)) as compared with the first order contribution in (214).

However, for the first case with ρ_0 we have an extra factor Ω as compared to $\rho_{\mathbf{k},-\mathbf{k}}$ in (214), which compensates the factor Ω^{-1} coming from the interaction. Hence, the first contribution is also of order c. In the second case with $\rho_{\mathbf{k}',-\mathbf{k}'}$ we have an extra summation over $\mathbf{k}'$. This summation, together with the factor Ω^{-1} from the interaction, leads to well-defined result in the thermodynamic limit. Hence, the second contribution is also order c. Similarly, one can easily show that any order terms in λ from binary correlations give the contribution of order c. In the third case with $\rho_{\mathbf{k},\mathbf{k}',-\mathbf{k}-\mathbf{k}'}$ we obtain a contribution which is of order c^2. Similarly, one can show that any order terms in λ from ternary correlations give contribution of order c^2, as the summation over the third particle gives a contribution of order N which compensates the factor Ω^{-1}. One can in this way verify that all terms coming from nth order correlations lead to contributions of order c^{n-1}. Therefore, assuming convergence of the series[‖] the transformed momentum $\tilde{\mathbf{p}}_1^D(0)$ in (214) is well-defined to the arbitrary order in λ. Similarly, the transformed observables (193) are finite in the thermodynamic limit. Ensembles described by the distribution function in (45) are in the domain of the non-unitary transformations Λ.

In order to compare the behaviour of $\tilde{\mathbf{p}}_1^D(t)$ in association with the ensembles (45) to the results in the previous section, let us evaluate its time evolution. As mentioned before, $\tilde{\mathbf{p}}_1^D(t)$ is in the $\Pi^{(0)}$ subspace. Hence, we can apply the formula (141). Then, we obtain

$$\frac{d}{dt}\langle\langle \tilde{\mathbf{p}}_1^D(t)|\rho(0)\rangle\rangle = \int d p \mathbf{p}_1 \frac{\partial}{\partial t}\rho_0(p, t) + O(\lambda^3), \quad (215)$$

where $\rho_0(p, t)$ satisfies (under the integration over the momentum in (215)) the Fokker–Planck equation,

$$\frac{\partial}{\partial t}\rho_0(p, t) = \lim_{\Omega\to\infty} \frac{\lambda^2}{\Omega^2} \sum_{n=2}^{N} \sum_{\mathbf{k}} |V_k|^2 \mathbf{k}\cdot\mathbf{d}_{1n} \pi\delta(\mathbf{k}\cdot\mathbf{g}_{1n})\mathbf{k}\cdot\mathbf{d}_{1n}\rho_0(p, t) + O(\lambda^3). \quad (216)$$

In the thermodynamic limit, the right-hand side of (216) gives a finite contribution of order c.

In this equation we can neglect the contribution of $\partial/\partial\mathbf{p}_n$ in the derivative operator $\mathbf{d}_{1n}$ at the left because of the boundary condition (5). This is possible, because we understand (216) together with the inner product together with the observable $\tilde{\mathbf{p}}_1^D$ that leads to the integration over the momentum in (215).

The result (215) is quite similar to (213), but there is an interesting difference. The

[‖]This may involve resummations.

right-hand side of (216) depends on time, while it does not in (213). 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 the higher contribution of t^n with $n \geq 2$ (see the discussion around (213)). Because of this non-linear contribution in time, the system approaches equilibrium in a finite time scale $t_r \sim (\lambda^2 c)^{-1}$.

We shall not try to summarize the results we obtain starting from the singular distribution functions (45) and applying our complex spectral decomposition. This would involve a summary of most of non-equilibrium statistical mechanics [17]. 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 (45) 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.

13. THE THERMODYNAMIC LIMIT AND THE COLLAPSE OF THE TRAJECTORIES

We now start with the initial condition (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 (45). 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 Λ. For this class, time going on, trajectories are destroyed by the Poincaré resonances and the distribution function approaches the class of (45).

Let us consider the time evolution of momentum $\mathbf{p}_1$ with the initial condition (4) corresponding to a trajectory. The evolution operator $\mathcal{U}(t)$ satisfies the integro-differential equation,

$$\mathcal{U}(t) = \mathrm{e}^{-iL_0 t} - i\int_0^t \mathrm{d}t'\, \mathrm{e}^{-iL_0(t-t')}\lambda L_V \mathcal{U}(t'). \tag{217}$$

The iteration of this equation leads to a perturbation expansion of $\mathcal{U}(t)$. Applying the expansion to the momentum in (52) for $j = 1$, we obtain the first order contribution of λ,

$$\begin{aligned}\mathbf{p}_1(t) &\approx \mathbf{p}_1^0 + \lim_{\Omega\to\infty} \lambda \int \mathrm{d}p\mathbf{p}_1 \sum_k (L_V)_{0,p;k,p^0} \frac{1}{\mathbf{k}\cdot v^0 - i\epsilon}(\mathrm{e}^{-ik\cdot v^0 t} - 1)\,\mathrm{e}^{-ik\cdot q^0} \\ &= \mathbf{p}_1^0 + \lim_{\Omega\to\infty} \frac{\lambda}{\Omega}\sum_{\mathbf{k}}\sum_{n=2}^{N}(-\mathbf{k})\frac{V_k}{\mathbf{k}\cdot\mathbf{g}_{1n}^0 - i\epsilon}(\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{g}_{1n}^0 t} - 1)\,\mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{q}_1^0 - \mathbf{q}_n^0)},\end{aligned} \tag{218}$$

where we have added $-i\epsilon$ with the positive infinitesimal ϵ in the denominator. This addition does not change the value of the right-hand side, since $k\cdot v^0 = 0$ is not the singular point of the integrand in (218).

Let us first consider the case where N is finite. With non-vanishing 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 $\mathbf{p}_1(t)$ reaches asymptotically a constant. Indeed, for $t \to +\infty$ the time dependent term in (218) vanishes, as the pole at $\mathbf{k}\cdot\mathbf{g}_{1n}^0 = +i\epsilon$ in this term does not contribute for $t > 0$. In Appendix J we show this explicitly for a specific interaction. Then we obtain (for $t \to +\infty$)

$$\mathbf{p}_1(t) \to \mathbf{p}_1^0 + \lambda \sum_{n=2}^{N} \int d\mathbf{k} \frac{V_k}{\mathbf{k} \cdot \mathbf{g}_{1n}^0 - i\epsilon} \mathbf{k}\, e^{-i\mathbf{k}\cdot(\mathbf{q}_1^0 - \mathbf{q}_n^0)} + O(\lambda^2) = \mathbf{P}_1^D(q^0, p^0). \tag{219}$$

This corresponds to $\mathbf{P}_1^D(q^0, p^0)$ in (206). Recall that the contributions to the invariant come only from the space $\Pi^{(0)}$. In contrast, the time dependent term in (218) is the contribution from the creation operator $\lambda \mathbf{C}_1^{(2)}$ in the $\Pi^{(2)}$ subspace associated to the binary correlations $P^{(2)}$. Hence, the asymptotic contribution comes only from the $\Pi^{(0)}$ subspace.

As mentioned (see after (208)), the resonance singularity at $\mathbf{k} \cdot \mathbf{g}_{1n}^0 = 0$ in the denominator in (219) leads to a non-vanishing contribution in the limit of $|\mathbf{q}_1^0 - \mathbf{q}_n^0| \to \infty$, even for the short-range interaction. Due to the collisions, long-range correlations are build up. As the result, (219) may diverge in the limit $N \to \infty$. Then, trajectories do not belong to the domain of $\mathbf{D}^{(0)}$, and neither to the domain of Λ. As the thermodynamic limit implies the existence of 'intensive variables', this limit does not exist when $\mathbf{p}_1(t)$ diverges for $N \to \infty$.*

However, there are classes of initial conditions that give a finite contribution to $\mathbf{p}_1(t)$ as well as to $\mathbf{P}_1^D(q^0, p^0)$, even in the limit $N \to \infty$. For example, let us suppose that the initial positions of the particles $\mathbf{q}_n^0$ are chosen randomly. Here, random means that the algorithm to write the sequence $\mathbf{q}_1^0, \mathbf{q}_2^0, \mathbf{q}_3^0, \ldots$ is 'incompressible' [40]. Then, in the thermodynamic limit, the summation over n and $\mathbf{k}$ in (218) gives a contribution of order,

$$\frac{1}{\Omega} \sum_{\mathbf{k}} \sum_{n}^{N} f_{\mathbf{k}}\, e^{-i\mathbf{k}\cdot(\mathbf{q}_1^0 - \mathbf{q}_n^0)} \sim \frac{\sqrt{(NL^3)}}{L^3}. \tag{220}$$

As a consequence, the right-hand side of (218) 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 (220) over $\mathbf{q}_n^0$ with the assumption of an uniform distribution of $\mathbf{q}_n^0$ 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 $\mathbf{q}_1^0, \mathbf{q}_2^0, \mathbf{q}_3^0, \ldots$, the value of the summation (220) may change significantly. However, the interest of this estimate is that it guarantees a finite value of (220) for almost all choice of the initial condition $\mathbf{q}_1^0, \mathbf{q}_2^0, \mathbf{q}_3^0, \ldots$ 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 [40].

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 (218) (such as has been done in (219)), 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 $\mathbf{k}$ simultaneously. This difference between two limiting procedures is essential to understand the origin of dissipative processes. We have therefore tested the two different estimates for a simple example by numerical simulations. We present the results in Appendix M. The results confirm our expectation and are in agreement with (220).

As a result of a random initial condition, the destruction operator in (206), as well as in (207), gives a finite contribution for the trajectory in the thermodynamic limit. Moreover, the collision operator θ_2 (which corresponds to a diagonal transition) in (208) also gives a finite contribution in the thermodynamic limit, which is of order c regardless of the random

*The above argument holds in any order of λ whenever the $\mathcal{T}$-matrix exists, as the long-range correlation is the result of the resonance at $k \cdot v^0 = 0$ in the denominator of (203). In quantum mechanics there are many examples whose explicit form of the $\mathcal{T}$-matrix are known, such as the delta-shell potential, separable potential etc.

or coherent choice of the initial values $\mathbf{q}_n^0$, as θ_2 does not depend on $\mathbf{q}_n^0$. One can easily see that for every order in λ the destruction operator gives finite contribution. Moreover, one can extend these estimates for the reduced observables (50) depending on a finite number of particles. This shows that this class of initial conditions belongs to the domain of the non-unitary transformations.

It is interesting to compare the trajectory in the thermodynamic limit $N \to \infty$ with the one with a random distribution of $\mathbf{q}_n^0$ but for a finite number N of particles. If N is large but finite, then (220) vanishes as $L^{-3/2}$ in the large volume limit. As a result, the effect of the interactions in (219) vanishes. Hence, the value of $\mathbf{p}_1(t)$ approaches its initial value (for $t \to \infty$)

$$\mathbf{p}_1(t) \to \mathbf{p}_1^0, \qquad \text{(in the average)}. \tag{221}$$

This contrasts with the situation in the thermodynamic limit.

As in the thermodynamic limit the collision operator leads to diffusion processes, the trajectory is not maintained in time. The trajectory 'collapses' due to the Poincaré resonances. In Appendix F we illustrate the collapse of trajectory, using as a simple example the 'perfect Lorentz gas' [1, 18]. There, we evaluate $\langle \mathbf{p}_1(t) \rangle$ as well as $\langle [\mathbf{p}_1(t)]^2 \rangle$ for a given initial condition of a single trajectory for the system in terms of the $\lambda(\lambda^2 t)^n$-approximation (see the remark in Section 8). We have, of course, $\langle \mathbf{p}_1(0) \rangle^2 = \langle [\mathbf{p}_1(0)]^2 \rangle$. But we shall show that $\langle \mathbf{p}_1(t) \rangle^2 \neq \langle [\mathbf{p}_1(t)]^2 \rangle$ for $t > 0$ (see (F21)). $\mathbf{p}_1(t)$ becomes a stochastic variable and obeys a Langevin type of stochastic equation. The usual meaning of a trajectory is thus destroyed.

In Appendix F we shall also show that all effects of initial correlations in $\Pi^{(\nu)}$ subspace except for $\Pi^{(0)}$ in equation (F10) vanish asymptotically. In the $\Pi^{(0)}$ subspace the correlation is generated from the vacuum of correlation $P^{(0)}$ through the creation operator $\mathbf{C}^{(0)}$ (see (93)). As illustrated in (48) the interaction λL_V (hence the creation operator) introduces an extra volume factor Ω^{-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 (45). Therefore, the delta function singularity in Fourier space emerges as time goes on, even if we start from a non-singular distribution function. The class of singular distribution functions (45) acts again as an attractor.

In conclusion the maintainance of the volume dependence of the trajectory (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 (45) in the sense of distributions.

14. CONCLUDING REMARKS

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 transformations (Sections 4 and 5). 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 Θ. Non-Newtonian contributions appear in this representation. They would 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 [17–19, 23–25]. The main difference is that at this time we assumed that we had to limit ourselves to the Hilbert

space. To obtain a semi-group representation (including complex eigenvalues) we had to introduce a non-unitary transformation from the distribution function ρ to a new distribution function $\tilde{\rho} = \Lambda\rho$ (the so-called 'physical' representation). Now irreversibility appears already in ρ. The non-unitary transformation theory appears naturally as the result of the intertwining relation between L_H and Θ (see Section 6).

This non-unitary transformation is necessary to formulate $\mathcal{H}$-quantities which decrease with time until equilibrium is reached. The existence of $\mathcal{H}$-functions have 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 $\mathcal{H}$-function depends on the deviation from equilibrium. It is natural to assume the existence of an entropy barrier. Only states which lead to finite values of $\mathcal{H}$ may be found in nature (or can be prepared, see Section 8). In more anthropomorphic terms that means that only systems involving a 'finite information' exist in nature. From the mathematical point of view, this means that only distribution functions which are in the domain of the non-unitary transformation $\wedge$ are realized in nature. For a finite number of particles, this includes simple trajectories. 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 (see Section 8). As shown in Section 13, 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. 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 to deterministic chaos [14]. But the nature of the function space is quite different. There the extension is introduced to avoid the difficulties associated to 'sensitivity to initial conditions'. Here the main new element is the role of resonances associated to 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. It would be interesting to consider also the effect of attractive forces. Also we have used formal expressions in the coupling constant λ without studying their radius of convergence. In concrete situations we may need partial resummations. Incomplete as this work is, it shows 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.

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APPENDIX A. COMPLEX EIGENVALUES OF THE LIOUVILLIAN

In this appendix we shall show that the imaginary part of the eigenvalue of the Liouvillian associated to the future $t > 0$ is non-positive. We shall use the resolvent formalism. The advantage of this method is that we can derive some general properties, such as the sign of the imaginary part of the eigenvalues, without going into detailed calculations. However, to solve the eigenvalue problem the formulation presented in Sections 4 and 5 is much more straightforward.

In terms of the resolvent operator $R(z) \equiv (z - L_H)^{-1}$ associated to the Liouvillian, the evolution operator in (7) is written by (for $t > 0$)

$$\mathcal{U}(t) = \frac{1}{2\pi}\int_{C^+} dz\, e^{-izt} R(z), \tag{A1}$$

where the contour C^+ lies in the upper-half plane of z running from $+\infty$ to $-\infty$. We have the resolvent identities,

$$R(z) = \frac{1}{z - L_0} + \frac{1}{z - L_0}\lambda L_V R(z), \tag{A2}$$

and

$$R(z') - R(z) = (z - z')R(z)R(z'). \tag{A3}$$

Equation (A2) leads to the expansion in powers of the coupling constant,

$$R(z) = \sum_{n=0}^{\infty}\left[\frac{1}{z - L_0}\lambda L_V\right]^n \frac{1}{z - L_0}. \tag{A4}$$

We consider the matrix element together with observables M (see (50)) and the distribution function ρ,

$$R_{M,\rho}(z) = \langle\langle M|R(z)|\rho\rangle\rangle. \tag{A5}$$

Because of the hermiticity of L_H in the Hilbert space, each term of $R_{M,\rho}(z)$ in (A4) is holomorphic in z for $\mathrm{Im}\, z \neq 0$. Let us recall that throughout this article we are considering the situations where the perturbation expansions, such as (72) and (A4), converge. Hence, $R_{M,\rho}(z)$ itself is holomorphic for $\mathrm{Im}\, z \neq 0$.* For the continuous spectrum limit, each terms of $R_{M,\rho}(z)$ in (A4) are represented by Cauchy integrals which have a discontinuity on the real axis of z approaching from above and from below [18]. The discontinuity of $R_{M,\rho}(z)$ spreads over the whole real axis, as the Liouvillian is not bounded from below [18]. Because the contour lies in the upper-half plane for $t > 0$, we are interested in the resolvent operator defined in the upper-half plane. Let us analytically continue the function $R_{M,\rho}(z)$ to the lower-half plane, and denote the analytically continued function as $R^+_{M,\rho}(z)$. Then, $R^+_{M,\rho}(z)$ has singularities in the lower-half plane or on the real axis.

In the simplest case the singularities are simple poles located at Z_α with $\mathrm{Im}\, Z_\alpha \leq 0$ (including the case $\mathrm{Im}\, Z_\alpha < 0$). An example is the perfect Lorentz gas presented in Appendix F. We then consider the 'residue' of a state $R(z)|\rho\rangle\rangle$ with arbitrary $|\rho\rangle\rangle$ at this pole,

$$|F_\alpha\rangle\rangle \equiv \lim_{z \to Z_\alpha} (z - Z_\alpha)R(z)|\rho\rangle\rangle. \tag{A6}$$

We now show that $|F_\alpha\rangle\rangle$ is the eigenstate of the Liouvillian with the eigenvalue Z_α, i.e.

$$L_H|F_\alpha\rangle\rangle = Z_\alpha|F_\alpha\rangle\rangle. \tag{A7}$$

Using the resolvent formula (A3), we have

$$|F_\alpha\rangle\rangle = \lim_{z' \to Z_\alpha} (z' - Z_\alpha)[R(z') - R(z)]|\rho\rangle\rangle = (z - Z_\alpha)R(z) \lim_{z' \to Z_\alpha} (z' - Z_\alpha)R(z')|\rho\rangle\rangle = (z - Z_\alpha)R(z)|F_\alpha\rangle\rangle. \tag{A8}$$

This gives a state $R^+(z)|F_\alpha\rangle\rangle$ which is regular in the upper-half plane,

$$R^+(z)|F_\alpha\rangle\rangle = \frac{1}{z - Z_\alpha}|F_\alpha\rangle\rangle. \tag{A9}$$

Hence, we obtain the desired result,

$$L_H|F_\alpha\rangle\rangle = \lim_{t \to 0+} \frac{1}{2\pi}\int_{C^+} dz\, e^{-izt}\frac{z}{z - L_H}|F_\alpha\rangle\rangle = Z_\alpha|F_\alpha\rangle\rangle. \tag{A10}$$

This show that the imaginary part of eigenvalues of the Liouvillian which is associated to the future $t > 0$ is indeed non-positive.

However, the above argument specifies only the sign of the imaginary part of eigenvalues. In order to solve the eigenvalue problem explicitly, we have to know in detail the analytic properties of the resolvent operator. This can be done, for example, by the series expansion of $R(z)$ in (A4). In each term of this expansion we have to specify the branch of analytic continuation. This is precisely what is achieved through the rule of time ordering corresponding to the $i\epsilon$-rule presented in the earlier works [26, 29].

*See [41, 42] for a similar statement for the resolvent of the Hamiltonian for quantum N-body systems.

APPENDIX B. ON THE LIMIT OF $\epsilon \to 0+$

For the continuous spectrum limit $\Omega \to \infty$ the propagator in (74) becomes the distribution,

$$\frac{1}{l_\mu - l_\nu \mp i\epsilon} \to \mathcal{P}\frac{1}{l_\mu - l_\nu} \pm i\pi\delta(l_\mu - l_\nu), \tag{B1}$$

where $\mathcal{P}$ stands for the principal part. The use of the δ function $\delta(l_\mu - l_\nu)$ is possible only because we consider the wave vectors $\mathbf{k}$ as a continuous variable. For finite ϵ the delta function $\pi\delta(l_\nu)$ are approximated by the Lorentzian distribution $\epsilon/(l_\nu^2 + \epsilon^2)$. To obtain a consistent evaluation for the delta function in terms of the box normalization formalism, there should be enough discrete states around the peak of the Lorentzian. Therefore, our expressions have to be understood in the continuous limit $\Delta k = 2\pi/L \to 0$ and $\epsilon \to 0+$ with the condition (see (19))

$$\frac{|\mathrm{d}l_\nu/\mathrm{d}k|\Delta k}{\epsilon} \to 0. \tag{B2}$$

APPENDIX C. COMPLEX DISTRIBUTIONS

Let us define the 'complex delta function' by (with a suitable test function $f(z)$)

$$\int_{\mathbf{R}} \mathrm{d}w f(w)\delta_c(w - z) = f(z). \tag{C1}$$

Then the complex distribution in (79) can be written as (for $Z_\alpha^{(\nu)} = w' - i\gamma$ with real w' and γ with $\gamma \geqslant 0$)

$$\int_{\mathbf{R}} \mathrm{d}w \frac{f(w)}{[w - z]^+_{Z_\alpha^{(\nu)}}} = \int_{\mathbf{R}} \mathrm{d}w \left[\frac{1}{w - Z_\alpha^{(\nu)}} + 2\pi i\delta_c(w - Z_\alpha^{(\nu)})\right] f(w). \tag{C2}$$

The most striking consequence of the analytic continuations (76) is that the transformed state $|\rho_B\rangle\rangle$ in (130) does not preserve the positivity of distribution functions. This is the result of the complex distribution (76a) which leads to an exponentially growing contribution in space. Let us consider a one-dimensional integration over l with a suitable test function $f(l)$ and with $v > 0$ and $x > 0$:

$$I(x) = \int_{-\infty}^{+\infty} \frac{f(l)}{[lv - z]^+_{Z_\alpha^{(\nu)}}} \mathrm{e}^{ilx}\,\mathrm{d}l. \tag{C3}$$

Then, the residue $\mathrm{Res}[I]$ of this integration at the pole $l = Z_\alpha^{(\nu)}/v$ is given by

$$\mathrm{Res}[I] = \frac{2\pi i}{v} f(Z_\alpha^{(\nu)}/v)\,\mathrm{e}^{iZ_\alpha^{(\nu)}x/v}. \tag{C4}$$

This gives the exponentially growing contribution in x for decay modes with $\mathrm{Im}\, Z_\alpha^{(\nu)} < 0$.

This type of contribution in space is necessary to ensure the causal evolution of the decay modes, as the damping factor $\exp(-iZ_\alpha^{(\nu)}t)$ in time necessary requires a space dependence given by $\exp[iZ_\alpha^{(\nu)}(x - vt)/v]$. For $v > 0$ with finite time t, this diverges in the limit of $x \to +\infty$. However, the bi-completeness relation of the eigenstates ensures that the contribution from $x > vt$ in the distribution function vanishes. As the result, some components of the transformed states should have negative values for $x > vt$ (see Fig. 2). This question will be more fully discussed in a separate paper [43].

Note that the causal evolution in the frame of the complex spectral representation has been already verified for a quantum unstable system, i.e. the Friedrichs modes, which is a model for the spontaneous emission of photons by an excited atom [44]. The reader should consult the original article for more details.

APPENDIX D. BI-ORTHONORMALITY AND THE ANALYTIC CONTINUATION

In this appendix we shall prove that the analytic continuations (76) for the right eigenstates and (102) for the left eigenstates are sufficient to lead to a bi-orthonormal set of the eigenstates of L_H.

Let us consider the inner products

$$\langle\langle \tilde{F}_\alpha^{(\nu)}|F_\beta^{(\mu)}\rangle\rangle = (N_\alpha^{(\nu)}N_\beta^{(\mu)})^{1/2}[\langle\langle \tilde{v}_\alpha^{(\nu)}|u_\beta^{(\mu)}\rangle\rangle + \langle\langle \tilde{v}_\alpha^{(\nu)}|\mathcal{D}^{(\nu)}(Z_\beta^{(\nu)})\mathcal{C}^{(\mu)}(Z_\alpha^{(\mu)})|u_\beta^{(\mu)}\rangle\rangle]. \tag{D1}$$

As far as $Z_\alpha^{(\nu)}$ and $Z_\beta^{(\mu)}$ which have non-vanishing finite imaginary parts, or the off-diagonal transitions are concerned, these inner products are well defined. The danger of divergence for the inner products occurs in the diagonal transitions with $\nu = \mu$ and $\beta = \alpha$ (recall that we consider here only the non-degenerate case), when the imaginary part of the eigenvalue becomes infinitesimal. As discussed in Appendix F (see also Appendix K) infinitesimal imaginary parts appear in the diffusion modes for macroscopic scales in space, such as the hydrodynamic scale. However, even for diagonal transitions, (D1) is well defined, as the analytic continuations (76) and (102) lead to the product of the propagators (see (82), (101) and the discussion of the analytic continuation in (97))

$$\langle\langle \tilde{v}_\alpha^{(\nu)}|\mathcal{D}^{(\nu)}(Z_\alpha^{(\nu)})\mathcal{C}^{(\nu)}(Z_\alpha^{(\nu)})|u_\alpha^{(\nu)}\rangle\rangle \sim \frac{1}{([z - L_0]^+_{Z_\alpha^{(\nu)}})^2}. \tag{D2}$$

This is in contrast with the situation corresponding to the 'velocity inversion experiment' discussed in Appendix K. There appears the square of the absolute value of the propagator (see (K7)), instead of its square as in (D2). As the result, there appear singularities in the inner products which lead to an infinite 'entropy barrier' in the asymptotic time scale.

As (D2) are well defined for all ν and α we can now prove that our analytic continuations lead to the bi-orthgonal relation of the eigenstates. As usual, let us consider the relation

$$\langle\langle \tilde{F}_\alpha^{(\nu)}|L_H|F_\beta^{(\nu)}\rangle\rangle = Z_\alpha^{(\nu)}\langle\langle \tilde{F}_\alpha^{(\nu)}|F_\beta^{(\nu)}\rangle\rangle = Z_\beta^{(\nu)}\langle\langle \tilde{F}_\alpha^{(\nu)}|F_\beta^{(\nu)}\rangle\rangle. \tag{D3}$$

As the inner products are well defined, and we consider the non-degenerate case, we have the bi-orthogonality for $\alpha \neq \beta$,

$$\langle\langle \tilde{F}_\alpha^{(\nu)}|F_\beta^{(\nu)}\rangle\rangle = 0. \tag{D4}$$

Moreover, the eigenstates are bi-normalizable.

We note that if we would use a simple analytic continuation with a single sign of $i\epsilon$, such as the Möller scattering states in (184), we would obtain diverging products of order ϵ^{-1}, such as (191) without the factor Ω^{-1}, for the non-integrable systems (see also (K8)). Our analytic continuations (76) remove this difficulty. The existence of well-defined inner products is essential to obtain a consistent description of non-integrable LPS in the thermodynamic limit.

Let us recall that the analytic continuation (75) leads to the non-linear Lippmann–Schwinger equations (171). By acting with $L_0 - l_\nu$ on (171), we recover the intertwining relations (127). This shows that $|F_\alpha^{(\nu)}\rangle\rangle$ and $\langle\langle \tilde{F}_\alpha^{(\nu)}|$ with our analytic continuations are indeed eigenstates of L_H. The bi-completeness of the eigenstates should be verified for each specific Hamiltonian.

APPENDIX E. THE BRILLOUIN–WIGNER PERTURBATION METHOD

Let us consider the lowest order contribution (i.e. to λ^2 order) of the collision operators. To this order ψ_C and ψ_D are identical. Denoting them by ψ_2, we have (see (97) and (121))

$$L_0 P^{(\nu)} + \lambda^2 \psi_2^{(\nu)} = L_0 P^{(\nu)} + \lambda^2 \theta_2^{(\nu)}. \tag{E1}$$

The intermediate states have a higher order of correlation than the initial and final states in (E1) (see the discussion of (97)). This determines the analytic continuation of the denominator as in (97). Let us then denote the eigenstates of ψ_2 by

$$(L_0 P^{(\nu)} + \lambda^2 \psi_2^{(\nu)})|g_\alpha^{(\nu)}\rangle\rangle = \xi_\alpha^{(\nu)}|g_\alpha^{(\nu)}\rangle\rangle, \qquad \langle\langle \tilde{g}_\alpha^{(\nu)}|(L_0 P^{(\nu)} + \lambda^2 \psi_2^{(\nu)}) = \langle\langle \tilde{g}_\alpha^{(\nu)}|\xi_\alpha^{(\nu)}. \tag{E2}$$

They also satisfy

$$L_0|g_\alpha^{(\nu)}\rangle\rangle = l_\nu|g_\alpha^{(\nu)}\rangle\rangle, \qquad \langle\langle \tilde{g}_\alpha^{(\nu)}|L_0 = \langle\langle \tilde{g}_\alpha^{(\nu)}|l_\nu, \tag{E3}$$

as well as

$$\langle\langle \tilde{g}_\alpha^{(\nu)}|g_\beta^{(\nu)}\rangle\rangle = \delta_{\alpha,\beta}, \qquad \sum_\alpha |g_\alpha^{(\nu)}\rangle\rangle\langle\langle \tilde{g}_\alpha^{(\nu)}| = P^{(\nu)}. \tag{E4}$$

The classical version of the Brillouin–Wigner equations are then given by [4]

$$|F_\alpha^{(\nu)}\rangle\rangle = |g_\alpha^{(\nu)}\rangle\rangle + Q_\alpha^{(\nu)} \sum_\mu \frac{-1}{(l_\mu - Z_\alpha^{(\nu)})_{C_{\nu\mu}}} P^{(\mu)} \lambda L_V |F_\alpha^{(\nu)}\rangle\rangle, \tag{E5a}$$

$$\langle\langle \tilde{F}_\alpha^{(\nu)}| = \langle\langle \tilde{g}_\alpha^{(\nu)}| + \sum_\mu \langle\langle \tilde{F}_\alpha^{(\nu)}|\lambda L_V P^{(\mu)} \frac{1}{(Z_\alpha^{(\nu)} - l_\mu)_{D_{\nu\mu}}} Q_\alpha^{(\nu)}, \tag{E5b}$$

where

$$Z_\alpha^{(\nu)} = \langle\langle \tilde{g}_\alpha^{(\nu)}|L_H|F_\alpha^{(\nu)}\rangle\rangle = \langle\langle \tilde{F}_\alpha^{(\nu)}|L_H|g_\alpha^{(\nu)}\rangle\rangle, \tag{E6}$$

and

$$Q_\alpha^{(\nu)} \equiv 1 - |g_\alpha^{(\nu)}\rangle\rangle\langle\langle \tilde{g}_\alpha^{(\nu)}|. \tag{E7}$$

The iterative use of these equations leads to the Brillouin–Wigner perturbation expansion of the eigenstates of the Liouvillian.

APPENDIX F. THE PERFECT LORENTZ GAS AND THE COLLAPSE OF THE TRAJECTORY

In this appendix we shall illustrate the 'collapse' of the trajectory using a simple model; the so-called perfect Lorentz gas [18]. We have already used this model in a previous paper to illustrate the complex spectral representation [1]. We shall first present a brief summary of the results (for more detail, see the original paper [1], as well as [43]). This model corresponds to the motion of a light particle of mass m_1 scattered by infinitely many

heavy particles of mass $m_n (m_1 \ll m_n$ for $n \geq 2)$. The Hamiltonian is given by (1) with a short-range repulsive interaction $V(|\mathbf{q}_j - \mathbf{q}_n|)$. Moreover, we improve the condition,

$$V(|\mathbf{q}_j - \mathbf{q}_n|) = \begin{cases} V(|\mathbf{q}_1 - \mathbf{q}_n|), & \text{for } j = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{F1}$$

The perfect Lorentz gas is defined as follows:

(i) We assume $m_1/m_n \ll 1$ for $n \geq 2$. Therefore, we can drop the terms proportional to m_n^{-1} in (26).
(ii) Because of their large mass, the average velocity of the heavy particles is much smaller than the average velocity of the test particle. The distribution function for the velocities of the heavy particles is replaced by a product of delta functions, $\delta_1(v) \equiv \prod_{r=2}^{N} \delta(\mathbf{v}_r)$.

We shall consider a weakly coupled system $\lambda \ll 1$. Then, the results we have obtained can be summarized as follows.

(1) $\Pi^{(0)}$ *subspace*

In the λ^2 order approximation, the collision operators $\theta_C^{(0)}$ and $\theta_D^{(0)}$ are the same (see (97)). Let us denote them by $\lambda^2\theta_2^{(0)}$. Then, the matrix element of $\lambda^2\theta_2^{(0)}$ is given by

$$\lambda^2 \langle\langle 0, v|\theta_2^{(0)}|0, u\rangle\rangle = \lambda^2 \theta_0 \delta(v - u), \tag{F2}$$

where (c as the concentration of the heavy particles, and with the unit $m_1 = 1$)

$$\lambda^2\theta_0 \equiv i(2\pi)^2\lambda^2 c \int \mathbf{dl} |V_l|^2 \mathbf{l} \cdot \frac{\partial}{\partial \mathbf{v}_1} \delta(\mathbf{l} \cdot \mathbf{v}_1) \mathbf{l} \cdot \frac{\partial}{\partial \mathbf{v}_1}. \tag{F3}$$

This is a linear (anti-hermitian) operator acting on the velocity of the light particle. Hence, in the eigenvalue problem

$$\lambda^2 \theta_0 f_\alpha(\mathbf{v}_1) = Z_\alpha f_\alpha(\mathbf{v}_1; \alpha), \tag{F4}$$

the eigenvalues Z_α are purely imaginary and the left-eigenstates of the collision are hermitian conjugates of the right-eigenstates. The linearity is a characteristic feature of the perfect Lorentz model, and thanks to it, we can solve explicitly the eigenvalue problem for the collision operator. It is well known that the Fokker–Planck operator for the perfect Lorentz gas can be written in terms of the 'orbital angular momentum' operator (see [18]). Therefore, the solutions of the eigenvalue problem are given by (with the index $\alpha = (w, l, m)$) [1]

$$f_\alpha(\mathbf{v}_1) = w^{-1} \delta(|\mathbf{v}_1| - w) Y_l^m(\theta, \phi), \tag{F5}$$

where $Y_l^m(\theta, \phi)$ is the spherical harmonics, where θ and ϕ are angles in the polar coordinates of $\mathbf{v}$ in an arbitrary reference system. The eigenvalues are given by

$$Z_\alpha = -i\lambda^2 A w^{-3} l(l + 1), \tag{F6}$$

where

$$A = 4c\pi^5 \int_0^\infty \mathrm{d}q q^3 |V_q|^2. \tag{F7}$$

The equilibrium mode corresponding to the zero eigenvalue of the Liouvillian belongs to the $\Pi^{(0)}$ subspace, and all non-vanishing eigenvalues in this subspace satisfy $\mathrm{Im}\, Z_\alpha^{(0)} < 0$ with $\mathrm{Im}\, Z_\alpha^{(0)} \sim \lambda^2 c$.

(2) $\Pi^{(\nu)}$ *subspace with* $\nu \neq 0$

In the same approximation, the collision operators with non-vanishing wave vector $k \neq 0$ for $\nu = (k, v)$ are complex operators, and are given by (see (97))

$$\langle\langle k, v|\theta_C^{(\nu)}|k, u\rangle\rangle \approx \langle\langle k, v|\theta_D^{(\nu)}|k, u\rangle\rangle \approx \theta_k \delta(v - u), \tag{F8}$$

where

$$\theta_k = (\mathbf{k} \cdot \mathbf{v}_1) + \lambda^2 \theta_0. \tag{F9}$$

The eigenvalues of θ_k depend on the wave vector $\mathbf{k}$, and are generally complex numbers. Hence, the left-eigenstates of the collision are not hermitian conjugates of the right-eigenstates. There are no steady eigenstates with zero eigenvalue for θ_k. For small $|\mathbf{k}|$ (which corresponds to large scale in space in the Fourier analysis) eigenvalues are purely imaginary number and proportional to $|\mathbf{k}|^2$. They correspond to the diffusion modes in space. For large $|\mathbf{k}|$, there are critical values k_c, thereafter, the eigenvalues are complex numbers. For large $|\mathbf{k}|$, the real part of the eigenvalue approaches $\mathbf{k} \cdot \mathbf{v}_1$. Hence, for small scales in space there appears a convection flow [41]. The diffusion modes with small non-vanishing k are the slowest damped modes. All other modes decay with a relaxation time of order $t_r \sim (\lambda^2 c)^{-1}$. The time scale t_d of damping for the diffusion modes depends as usual on the wave vector as $t_d \sim (\lambda^2 c|\mathbf{k}|^2)^{-1}$: the larger the scale in space (i.e. the smaller the $|\mathbf{k}|$), the slower the damping. Hence in any finite time scale, the effect of the diffusion modes does not vanish for sufficiently small $|\mathbf{k}|$ [1, 41].

Let us now discuss the collapse of the trajectory. We consider as the initial condition the trajectory (4)

$$\rho(q, v, 0) = \frac{1}{L^{3N}} \sum_k e^{ik\cdot(q-q^0)} \delta(\mathbf{v} - \mathbf{v}^0) \prod_{r=2}^{N} \delta(\mathbf{v}_r), \tag{F10}$$

where we have dropped the index 1 of the light particle to simplify the notations. The correlation components with $k \neq 0$ have the same volume dependence as the vacuum of correlation component with $k = 0$. There is no delta function singularity for the wave vectors for the trajectory. We assume that the initial conditions q^0 are chosen in such a way that we are in the domain of the non-unitary transformation. This means that the spatial distribution of the heavy particles is random (see Section 13). Therefore, we can apply the subdynamics (141) to evaluate the evolution of the velocity $\mathbf{v}$ of the test particle.

As mentioned, we shall consider weak coupling, $\lambda \ll 1$. The traditional approximation for weakly coupled system in kinetic theory is the $\lambda^2 t$-approximation [17]. Then we only retain contributions of order $(\lambda^2 t)^n$ with $n \geq 0$. We shall go beyond this approximation and keep terms in the order of $\lambda(\lambda^2 t)^n$ in subdynamics (141). In this approximation, we use the completeness relation of the spectral decomposition by adding the contributions from other subspaces than $\Pi^{(0)}$ (see also the related remark in Section 11). Therefore, our approximation is applicable to all time scales, and is no longer an asymptotic approximation such as the $\lambda^2 t$-approximation. It is easy to extend this procedure to higher order approximations.

In the $\lambda(\lambda^2 t)^n$-approximation we have to retain the contribution to $\mathbf{v}$ in the binary correlation subspaces $\Pi^{(2)}$, in addition of the contribution from the vacuum of the correlation subspace $\Pi^{(0)}$. The contribution from all other subspaces are negligible. Then we have (see (141))

$$\langle \mathbf{v}_t \rangle = \langle \mathbf{v}_t \rangle_0 + \langle \mathbf{v}_t \rangle_2, \tag{F11}$$

where

$$\begin{aligned} \langle \mathbf{v}_t \rangle_0 &\equiv \int d\upsilon \mathbf{v} \langle\langle 0, \upsilon | e^{-i\theta^{(0)}t} [P^{(0)} + \lambda \mathbf{D}_1^{(0)}] | \rho(0) \rangle\rangle \\ &= \int d\mathbf{v}\mathbf{v}\, e^{-i\theta_0 t} \delta(\mathbf{v} - \mathbf{v}^0) \\ &\quad + \frac{\lambda}{\Omega} \sum_{n=2}^{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{q}^0 - \mathbf{q}_n^0)} \int d\mathbf{v}\mathbf{v}\, e^{-i\theta_0 t} \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{v}} \frac{-V_k}{\mathbf{k}\cdot\mathbf{v} - i\epsilon} \delta(\mathbf{v} - \mathbf{v}^0), \end{aligned} \tag{F12}$$

and

$$\begin{aligned} \langle \mathbf{v}_t \rangle_2 &\equiv \lambda \int d\upsilon \mathbf{v} \langle\langle 0, \upsilon | \mathbf{C}_1^{(2)} e^{-i\theta^{(2)}t} | \rho(0) \rangle\rangle \\ &= \frac{\lambda}{\Omega} \sum_{n=2}^{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{q}^0 - \mathbf{q}_r^0)} \int d\mathbf{v}\mathbf{v}\mathbf{k} \cdot \frac{\partial}{\partial \mathbf{v}} \frac{V_k}{\mathbf{k}\cdot\mathbf{v} - i\epsilon} e^{-i\theta_k t} \delta(\mathbf{v} - \mathbf{v}^0). \end{aligned} \tag{F13}$$

where θ_0 and θ_k are given in (F3) and (F9). For $t = 0$ in (F11) we recover the initial condition $\langle \mathbf{v}_0 \rangle = \mathbf{v}^0$.

Because θ_0 and θ_k are finite in the thermodynamic limit, the diagonal transitions associated with the collision operators give finite contribution in (F12) and (F13). In contrast, if we do not introduce any restriction in the initial condition in (F10), then the perturbation series of $\langle \mathbf{v}_t \rangle$ diverge for asymptotic time scales due to the off-diagonal transition associated to the destruction operator (see (219), (J3) and (J15)). The assumption of the random distribution of $\mathbf{q}_r^0$ for the heavy particles leads to a finite contribution of the off-diagonal transitions (see Section 13). As a result, the effect of the diagonal transition is enhanced as compared with the effect of off-diagonal transitions. One can then isolate the contribution of the diagonal transitions from the contribution of off-diagonal transitions.

Because of the relation,

$$\begin{aligned} \mathbf{v} &= (\upsilon \sin\theta \cos\phi,\ \upsilon \sin\theta \sin\phi,\ \upsilon \cos\theta) \\ &= \left(\frac{\upsilon}{2}(Y_1^1 + Y_1^{-1}),\ \frac{\upsilon}{2i}(Y_1^1 - Y_1^{-1}),\ \upsilon Y_1^0 \right), \end{aligned} \tag{F14}$$

all components of $\mathbf{v}$ are represented by the spherical hermonics with the index $l = 1$. Hence, $\mathbf{v}$ belongs the decay mode of θ_0 with the eigenvalue $-i\lambda^2\gamma_1$ (see (F6)), where

$$\gamma_1(w) \equiv 2Aw^{-3}. \tag{F15}$$

Then we obtain (with $\upsilon^0 \equiv |\mathbf{v}^0|$)

$$\langle \mathbf{v}_t \rangle_0 = \mathbf{v}^0 e^{-\lambda^2 \gamma_1(\upsilon^0)t} + \frac{\lambda}{\Omega} \sum_{n=2}^{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{q}^0 - \mathbf{q}_n^0)} \int d\mathbf{v}\mathbf{v}\, e^{-\lambda^2\gamma_1(\upsilon)t} \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{v}} \frac{-V_k}{\mathbf{k}\cdot\mathbf{v} - i\epsilon} \delta(\mathbf{v} - \mathbf{v}^0). \tag{F16}$$

Similarly we can follow the time evolution of $\mathbf{v}^2$. We note $\mathbf{v}^2 \sim Y_0^0(\theta, \phi)$. Hence, $\mathbf{v}^2$ is the eigenfunction of θ_0 with zero eigenvalue,

$$\theta_0 \mathbf{v}^2 = 0. \tag{F17}$$

Then we have

$$\langle \mathbf{v}_t^2 \rangle = \langle \mathbf{v}_t^2 \rangle_0 + \langle \mathbf{v}_t^2 \rangle_2, \tag{F18}$$

where

$$\begin{aligned} \langle \mathbf{v}_t^2 \rangle_0 &= (\mathbf{v}^0)^2 + \frac{\lambda}{\Omega} \sum_{n=2}^{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{q}^0 - \mathbf{q}_n^0)} \int d\mathbf{v} v^2 \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{v}} \frac{-V_k}{\mathbf{k}\cdot\mathbf{v} - i\epsilon} \delta(\mathbf{v} - \mathbf{v}^0) \\ &= (\mathbf{v}^0)^2 + 2\lambda \sum_{r=2}^{N} V(|\mathbf{q}^0 - \mathbf{q}_r^0|), \end{aligned} \tag{F19}$$

and

$$\langle \mathbf{v}_t^2 \rangle_2 = \frac{\lambda}{\Omega} \sum_{n=2}^{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{q}^0 - \mathbf{q}_r^0)} \int d\mathbf{v} v^2 \mathbf{k} \cdot \frac{\partial}{\partial \mathbf{v}} \frac{V_k}{\mathbf{k}\cdot\mathbf{v} - i\epsilon} e^{-i\theta_k t} \delta(\mathbf{v} - \mathbf{v}^0). \tag{F20}$$

Because of the short-range interaction, only a finite number of the heavy particles can contribute to the last term of (F19). Hence, we obtain a finite non-vanishing contribution of $\langle \mathbf{v}_t^2 \rangle_0$ in the thermodynamic limit.

Let us now compare (F11) with (F18). In (F16) when we expand the exponential term in the power of t, the secular effects in the first term of (F16) start with $-\lambda^2 \gamma_1(v^0)t$, while they start with $\lambda^3 t$ in the second term in (F16). Similarly, the secular effect in (F13) starts with $\lambda^3 t$, as the imaginary part of the eigenvalues of θ_k is of order λ^2. On the other hand, for $\mathbf{v}_t^2$ there is no secular term in (F19). The secular effects come only from (F20) in the binary correlation subspace $\Pi^{(2)}$, which are of order $\lambda^3 t$.

As a consequence, secular effects of the square of (F11) start with order $\lambda^2 t$, while (F18) with order $\lambda^3 t$. This implies

$$\langle \mathbf{v}_t^2 \rangle \neq \langle \mathbf{v}_t \rangle^2. \tag{F21}$$

$\mathbf{v}_t$ becomes a stochastic variable. Hence, the usual sense of the trajectory is indeed destroyed.

We note that the effect of (F13) cannot be neglected for any time scale due to the slow processes in the diffusion modes for sufficiently small $|\mathbf{k}|$. The value of $\mathbf{v}_t$ does not vanish for any time scale, and depends on the initial condition (F10) for each individual trajectory. However, if we take the ensemble average for these randomly chosen initial conditions, then the effect of the binary correlation (F13) vanishes. In this sense we obtain (for $t \to \infty$)*

$$\langle \mathbf{v}_t \rangle \to 0. \qquad \text{(in the average)}. \tag{F22}$$

This contrasts with the situation for finite N in (221).

For finite non-vanishing $\mathbf{k}$, the spectrum of θ_k consists of decay modes with finite time scales t_r or t_d. Thus all effects of initial correlations in $\Pi^{(v)}$ subspace except for $\Pi^{(0)}$ in equation (F10) vanish asymptotically for any finite scale in space. We note that states in the $\Pi^{(0)}$ subspace satisfy the delta function singularity in (45). Therefore, the delta function singularity in Fourier space emerges as time goes on, starting from non-singular distribution functions. For this class of distribution functions, the only possible volume dependence which is stable over the time evolution is the one corresponding to (45). In this sense this class acts as an attractor.

APPENDIX G. EQUATIONS OF MOTION FOR THE PERFECT LORENTZ GAS

For non-integrable systems belonging to LPS the non-unitary transformation leads to a set of kinetic equations (132). On the other hand, the evolution of trajectories is described by the Hamilton equations of motion which correspond to a special case of the classical Heisenberg equations (14). Therefore, it is natural to inquire how the transformed equations of motion (134) look when trajectories are destroyed by resonances. In this appendix we shall give the explicit form of the transformed equations of motion for the perfect Lorentz gas. As in Appendix F, we shall put $m_1 = 1$, and we shall not distinguish the velocity from the momentum.

Let us consider the evolution of the transformed momentum for the light particle (abbreviated to particle index 1) defined by (see (130))

$$\langle\langle \hat{\mathbf{v}}_B(t)| \equiv \langle\langle \hat{\mathbf{v}}(t)|\Lambda_B^{-1}. \tag{G1}$$

To simplicity we shall consider the $\lambda^2 t$-approximation. $\langle\langle \hat{\mathbf{v}}_B(0)|$ is then identical to the unperturbed velocity $\langle\langle \hat{\mathbf{v}}|$ which is in the $P^{(0)}$ subspace. Hence, in this approximation (134) leads to

$$\langle\langle \hat{\mathbf{v}}_B(t)|P^{(0)} \approx \langle\langle \hat{\mathbf{v}}(0)|\, e^{-i\lambda^2 \theta_2^{(0)} t}. \tag{G2}$$

Recall that $\mathbf{v}$ is the eigenstates of θ_0 in (F3) with the eigenvalue $-i\lambda^2\gamma_1$ in (F15) (see (F14)). Thus, we obtain

$$\langle\langle \hat{\mathbf{v}}_B(t)|P^{(0)} \approx \langle\langle \hat{\mathbf{v}}(0)|\, e^{-\lambda^2 \gamma_1 t}. \tag{G3}$$

This leads to the equation of motion in the $\lambda^2 t$-approximation,

$$\frac{d}{dt} \langle\langle \hat{\mathbf{v}}_B(t)|P^{(0)} = -\lambda^2 \gamma_1 \langle\langle \hat{\mathbf{v}}_B(t)|P^{(0)}. \tag{G4}$$

This is a dissipative equation which breaks time-symmetry and describes the damping of the velocity.

Similarly, the transformed kinetic energy $\hat{\mathbf{v}}_B^2/2$ obeys (as $\mathbf{v}^2$ is the eigenstate of θ_0 with zero eigenvalue; see (F17)) the equation,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle \hat{\mathbf{v}}_B^2(t)/2|P^{(0)} = 0. \tag{G5}$$

One should note that these equations are identical to the equations for moments of the velocity which are generated by the Fokker–Planck equation (see (F3)),

$$\frac{\partial}{\partial t}\varphi(\mathbf{v}, t) = (2\pi)^2\lambda^2 c\int \mathrm{d}\mathbf{l}|V_l|^2\mathbf{l}\cdot\frac{\partial}{\partial \mathbf{v}}\delta(\mathbf{l}\cdot\mathbf{v})\mathbf{l}\cdot\frac{\partial}{\partial \mathbf{v}}\varphi(\mathbf{v}, t). \tag{G6}$$

APPENDIX H. STAR-UNITARY TRANSFORMATIONS

In this appendix we shall display some symmetry properties, called 'star-conjugation', of the projection operators $\Pi^{(v)}$ and of the non-unitary transformation Λ_B [14, 20, 25]. In the last part of this appendix we shall also discuss the relation between the $i\epsilon$-rule and the star-conjugation.

The projection operators $\Pi^{(v)}$ are not hermitian. They satisfy more general symmetry relation. To see this let us first observe the relation between the 'Schrödinger picture' of the evolution in (3) and the 'Heisenberg picture' in (14). By interchanging the role of the distribution functions and observables, as well as interchanging the sign of L_H, one picture leads to the other picture. The interchange operation is called the 'prime operation' [25]. For the operator $\Pi^{(v)}$ (137) this interchange operation corresponds to interchange of the left eigenstates by the right eigenstates $\tilde{F} \leftrightarrow F$. A combination of the prime operation with hermitian conjugation is called the 'star-conjugation' (or the 'Heisenberg–Schrödinger conjugation) denoted by '$*$' [4, 26].‖ Then we have

$$\begin{aligned}(\mathrm{e}^{-iL_H t}|F_\alpha^{(v)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(v)}|)^* &= (\mathrm{e}^{+iL_H t}(|F_\alpha^{(v)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(v)}|)')^\dagger \\ &= (\mathrm{e}^{+iL_H t}|\tilde{F}_\alpha^{(v)}\rangle\rangle\langle\langle F_\alpha^{(v)}|)^\dagger = |F_\alpha^{(v)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(v)}|\,\mathrm{e}^{-iL_H t},\end{aligned} \tag{H1}$$

as well as

$$(\mathrm{e}^{-iL_H t}|F_\alpha^{(v)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(v)}|)^* = (|\tilde{F}_\alpha^{(v)}\rangle\rangle\langle\langle F_\alpha^{(v)}|\,\mathrm{e}^{+iL_H t})' = |F_\alpha^{(v)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(v)}|\,\mathrm{e}^{-iL_H t}. \tag{H2}$$

Hence we obtain

$$(\mathrm{e}^{-iL_H t}|F_\alpha^{(v)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(v)}|)^* = \mathrm{e}^{-iL_H t}|F_\alpha^{(v)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(v)}|, \tag{H3}$$

and

$$\Pi^{(v)*} = \Pi^{(v)}, \qquad L_H^* = -L_H. \tag{H4}$$

$\Pi^{(v)}$ is a star-hermitian operator, while L_H is an anti-star-hermitian operator. Equation (H4) leads to

$$A^{(v)*} = A^{(v)}, \qquad \mathbf{C}^{(v)*} = \mathbf{D}^{(v)}, \tag{H5}$$

as well as

$$(|u_\alpha^{(v)}\rangle\rangle Z_\alpha^{(v)}\langle\langle \tilde{u}_\alpha^{(v)}|)^* = -|v_\alpha^{(v)}\rangle\rangle Z_\alpha^{(v)}\langle\langle \tilde{v}_\alpha^{(v)}|, \qquad \text{i.e.} \quad \theta_C^{(v)*} = -\theta_D^{(v)}. \tag{H6}$$

The collision operators $\theta_C^{(v)}$ and $\theta_D^{(v)}$ are anti-skew star-symmetric. Applying these operations to Λ_B, we have

$$\Lambda_C^* = \Lambda_D^{-1}, \qquad \Lambda_D^* = \Lambda_C^{-1}, \tag{H7}$$

that is (for $B' \neq B$ with $B, B' = C, D$)

$$\Lambda_B\Lambda_{B'}^* = \Lambda_{B'}^*\Lambda_B = 1. \tag{H8}$$

We can introduce more symmetric transformations operators [14, 20, 25]. Let us define

$$\Lambda = \sum_v A^{(v)1/2}(P^{(v)} + \mathbf{D}^{(v)}), \qquad \Lambda^{-1} = \sum_v (P^{(v)} + \mathbf{C}^{(v)})A^{(v)1/2}. \tag{H9}$$

This is a star-unitary operator,

$$\Lambda\Lambda^* = \Lambda^*\Lambda = 1. \tag{H10}$$

Then we have

$$\langle\langle \hat{M}|\mathcal{U}(t)|\rho(0)\rangle\rangle = \langle\langle \hat{M}|\Lambda^*\exp(-i\Theta t)\Lambda|\rho(0)\rangle\rangle, \tag{H11}$$

where Θ is a new collision operator defined by

$$\Theta = \Lambda L_H\Lambda^*. \tag{H12}$$

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*We thank Dr B. Misra for this remark.

‖By definition we have $(W^*)^* = W$.

This satisfies

$$\Theta = \sum_{\nu} \theta^{(\nu)}$$

with

$$\theta^{(\nu)} = (A^{(\nu)})^{-1/2}\theta_C^{(\nu)}(A^{(\nu)})^{1/2} = (A^{(\nu)})^{1/2}\theta_D^{(\nu)}(A^{(\nu)})^{-1/2}, \tag{H13}$$

as well as

$$\theta^{(\nu)*} = -\theta^{(\nu)}, \quad \text{i.e.} \quad \Theta^* = -\Theta. \tag{H14}$$

The new collision operator is an anti-star-hermitian operator. Moreover, the new transformation operator leads to the same subdynamics $\Pi^{(\nu)}$ as (137):

$$\Pi^{(\nu)} = \Lambda^* P^{(\nu)} \Lambda. \tag{H15}$$

We note that the non-unitary transformations preserve the reality of the states (see Appendix I). But the transformed states $\langle\langle q,\ p|\Lambda|\rho\rangle\rangle$, as well as $\langle\langle q,\ p|\Lambda_B\rho\rangle\rangle$, cannot be considered as probability distribution functions, as they do not preserve the positivity of the distribution function. This is a direct consequence of the causal evolution of the dynamics combined with the analytic continuation (76) and (102) involving complex distributions (see Appendix C). However, as mentioned these states play an essential role as they permit us to introduce $\mathcal{H}$-functions for dynamical systems as shown in Section 12.

The $i\epsilon$-rule and the prime operation

We shall show that the application of the prime operation to the $i\epsilon$-rule leads to (see (76))

$$(i\epsilon_{\mu\nu})' = -i\epsilon_{\mu\nu} = \begin{cases} -i\epsilon, & \text{for } d_\nu > d_\mu, \\ +i\epsilon, & \text{for } d_\nu \leqslant d_\mu. \end{cases} \tag{H16}$$

The nonlinear Lippmann–Schwinger equation (171a) leads to

$$\begin{aligned} \langle\langle \nu|\mathbf{C}^{(\nu)\dagger}|\mu\rangle\rangle &= \langle\langle \mu|\mathbf{C}^{(\nu)}|\nu\rangle\rangle^{c.c.} \\ &= \langle\langle \nu|(P^{(\nu)} + \mathbf{C}^{(\nu)\dagger})\lambda L_V|\mu\rangle\rangle \frac{1}{l_\nu - l_\mu + i\epsilon_{\mu\nu}} \\ &\quad + \langle\langle \nu|(\theta_C^{(\nu)\dagger} - L_0)|\nu\rangle\rangle\langle\langle \nu|\mathbf{C}^{(\nu)\dagger}|\mu\rangle\rangle \frac{-1}{l_\nu - l_\mu + i\epsilon_{\mu\nu}}. \end{aligned} \tag{H17}$$

On the other hand we have from (171b) that (see (H5))

$$\begin{aligned} \langle\langle \nu|\mathbf{D}^{(\nu)\prime}|\mu\rangle\rangle &= \langle\langle \nu|(\mathbf{P}^{(\nu)} + \mathbf{D}^{(\nu)\prime})(-\lambda L_V)|\mu\rangle\rangle \frac{1}{-(l_\nu - l_\mu) + (i\epsilon_{\nu\mu})'} \\ &\quad + \langle\langle \nu|(\theta_D^{(\nu)\prime} + L_0)|\nu\rangle\rangle\langle\langle \nu|\mathbf{D}^{(\nu)\prime}|\mu\rangle\rangle \frac{-1}{-(l_\nu - l_\mu) + (i\epsilon_{\nu\mu})'} \\ &= \langle\langle \nu|(P^{(\nu)} + \mathbf{C}^{(\nu)\dagger})\lambda L_V|\mu\rangle\rangle \frac{1}{l_\nu - l_\mu - (i\epsilon_{\nu\mu})'} \\ &\quad + \langle\langle \nu|(\theta_C^{(\nu)\dagger} - L_0)|\nu\rangle\rangle\langle\langle \nu|\mathbf{C}^{(\nu)\dagger}|\mu\rangle\rangle \frac{-1}{l_\nu - l_\mu - (i\epsilon_{\nu\mu})'}. \end{aligned} \tag{H18}$$

Because of (H5), equation (H17) is the same as (H18). This implies

$$(i\epsilon_{\nu\mu})' = -i\epsilon_{\mu\nu}, \tag{H19}$$

which is the desired result (H16).

Let us emphasize the difference between the 'star-conjugation' defined in this article from the one introduced in our previous paper [1]. There we defined star-conjugation through (instead of the second equation in (H4))

$$L_H^* = L_H. \tag{H20}$$

Corresponding to (H19), we have for this case

$$(i\epsilon_{\nu\mu})' = i\epsilon_{\mu\nu}. \tag{H21}$$

However, with this definition the relation between star-conjugation and Heisenberg–Schrödinger conjugation is lost. For this reason, we shall not use the definition (H20), but use the definition (H4) for the star-conjugation.

APPENDIX I. REALITY PRESERVATION BY THE NON-UNITARY TRANSFORMATIONS

In this appendix we shall proof that the non-unitary transformations (125) preserve the reality of the distribution functions $\langle\langle q,\ p|\rho\rangle\rangle$.

We verify the relations

$$(\mathbf{C}^{(-k)})^{c.c.} = \mathbf{C}^{(k)}, \quad (\mathbf{D}^{(-k)})^{c.c.} = \mathbf{D}^{(k)}, \quad (\mathbf{A}^{(-k)})^{c.c.} = A^{(k)}, \tag{I1}$$

as well as

$$(\theta_B^{(-k)})^{c.c.} = -\theta_B^{(k)}. \tag{I2}$$

Here we have specified the correlations by its value of the wave vectors k. Equation (I2) and the last equality of (I1) are the consequence of the first two equalities of (I1). As the result, $\langle\langle q, p|\Lambda_B|\rho\rangle\rangle$ are real for real distribution functions $\langle\langle q, p|\rho\rangle\rangle$.

Here we prove only the first equality of (I1). The proof of the second one is essentially the same. We start from the nonliner Lippmann–Schwinger equation (171a). In the q-representation, we have

$$\begin{aligned}\langle\langle q|\Phi_k^C\rangle\rangle = {} & \frac{1}{L^{3N/2}} e^{ik\cdot q} + \frac{1}{L^{3N}} \sum_{k',k''} e^{ik'q} \frac{-1}{l_{k'} - l_k + i\epsilon_{k',k}} \int dq' \langle\langle k'|\lambda L_V|k''\rangle\rangle e^{-ik''\cdot q'} \langle\langle q'|\Phi_k^C\rangle\rangle \\ & + \frac{1}{L^{3N}} \sum_{k',k''} \int dq' e^{ik'\cdot q} \frac{1}{l_{k'} - l_k + i\epsilon_{k',k}} e^{-ik'\cdot q'} \langle\langle q'|\Phi_k^C\rangle\rangle \int dq'' \langle\langle k''|\lambda L_V|q''\rangle\rangle \langle\langle q''|\Phi_k^C\rangle\rangle,\end{aligned} \tag{I3}$$

where we have abbreviated the momentum to save the notations. We note that

$$(iL_H)^{c.c.} = iL_H, \quad (L_H)^{c.c.} = -L_H. \tag{I4}$$

Then we take the complex conjugate of (I3). Using (26) and changing sign k as well as of the dummy variables k' and k'', we obtain by a straightforward calculation

$$\begin{aligned}\langle\langle q|\Phi_{-k}^C\rangle\rangle^{c.c.} = {} & \frac{1}{L^{3N/2}} e^{ik\cdot q} + \frac{1}{L^{3N}} \sum_{k',k''} e^{ik'q} \frac{-1}{l_{k'} - l_k + i\epsilon_{k',k}} \int dq' \langle\langle k'|\lambda L_V|k''\rangle\rangle e^{-ik''\cdot q'} \langle\langle q'|\Phi_{-k}^C\rangle\rangle^{c.c.} \\ & + \frac{1}{L^{3N}} \sum_{k',k''} \int dq' e^{ik'\cdot q} \frac{-1}{l_{k'} - l_k + i\epsilon_{k',k}} e^{-ik'\cdot q'} \langle\langle q'|\Phi_{-k}^C\rangle\rangle \int dq'' \langle\langle k''|\lambda L_V|q''\rangle\rangle \langle\langle q''|\Phi_{-k}^C\rangle\rangle^{c.c.},\end{aligned} \tag{I5}$$

where we have used the relations $l_{-k} = -l_k$ and $\epsilon_{-k',-k} = \epsilon_{k',k}$. This shows that $\langle\langle q|\Phi_{-k}^C\rangle\rangle^{c.c.}$ satisfies the same equation (I3) as $\langle\langle q|\Phi_k^C\rangle\rangle$. Moreover, we have the same boundary condition,

$$\langle\langle q|\Phi_{-k}^C\rangle\rangle^{c.c.} = \langle\langle q|\Phi_k^C\rangle\rangle = \langle\langle q|k\rangle\rangle, \quad \text{for} \quad \lambda = 0. \tag{I6}$$

Hence we obtain for any λ,

$$\langle\langle q|\Phi_{-k}^C\rangle\rangle^{c.c.} = \langle\langle q|\Phi_k^C\rangle\rangle. \tag{I7}$$

Because of the relation (see (126) and (170))

$$\langle\langle q|\Phi_k^C\rangle\rangle = \langle\langle q|(P^{(k)} + \mathbf{C}^{(k)})|k\rangle\rangle, \tag{I8}$$

we obtain the first equality of (I1). Similarly one can prove the second equality of (I1).

APPENDIX J. RESONANCE DIVERGENCE OF THE MOMENTUM

In this appendix we shall consider the time evolution of the momentum $\mathbf{p}_1(t)$ in (218). This calculation leads also to the evaluation of the invariant $\mathbf{P}_1^D(q^0, p^0)$ in (206).[§]

We assume a Gaussian potential

$$V(\mathbf{q}) = V_0 e^{-x^2/4a^2} = \frac{1}{\Omega} \sum_{\mathbf{l}} B e^{-a^2 l^2} e^{i\mathbf{l}\cdot\mathbf{q}}, \tag{J1}$$

where $B \equiv V_0 a^3/\pi^{3/2}$.

We first consider the case where N is finite. As mentioned in Section 13 the time evolution of (218) consists of the contributions from $\Pi^{(0)}$ and $\Pi^{(2)}$ subspace. Let us denote the contribution from $\Pi^{(0)}$ by $\mathbf{p}_1^{(0)}$, and the one from $\Pi^{(2)}$ by $\mathbf{p}_1^{(2)}(t)$,

$$\mathbf{p}_1(t) = \mathbf{p}_1^{(0)} + \mathbf{p}_1^{(2)}(t). \tag{J2}$$

$\mathbf{p}_1^{(0)}$ corresponds to the time independent part of (218), and we have (see also (219))

$$\mathbf{p}_1^{(0)} = \mathbf{p}_1 + \lambda B \sum_{n=2}^{N} \int d\mathbf{k} \frac{1}{\mathbf{k}\cdot\mathbf{g}_{1n} - i\epsilon} \mathbf{k} e^{-a^2k^2} e^{i\mathbf{k}\cdot\mathbf{r}_n}, \tag{J3}$$

where

$$\mathbf{r}_n \equiv \mathbf{q}_n - \mathbf{q}_1, \tag{J4}$$

[§]We thank to Mr Z. L. Zhang who has performed the integrations given in this appendix.

and we have abbreviated the superscript 0 on $\mathbf{q}$ and $\mathbf{p}$ 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 θ_n, and $\hat{\phi}_n$ in the transversal direction of $\mathbf{g}_{1n}$ parallel to the angle ϕ_n. Let us also introduce the notations,

$$r_{n1} = (\mathbf{r}_n \cdot \hat{v}_n), \qquad r_{n2} = (\mathbf{r}_n \cdot \hat{\theta}_n), \qquad r_{n3} = (\mathbf{r}_n \cdot \hat{\phi}_n), \tag{J5}$$

and

$$k_1 = (\mathbf{k} \cdot \hat{v}_n), \qquad \mathbf{k}_2 = (\mathbf{k} \cdot \hat{\theta}_n), \qquad k_3 = (\mathbf{k} \cdot \hat{\phi}_n), \tag{J6}$$

we can write (J3) as

$$\mathbf{p}_1^{(0)} = \mathbf{p}_1 + \lambda B \sum_{n=2}^{N} \int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 \int_{-\infty}^{+\infty} dk_3 \frac{1}{k_1 v_{1n} - i\epsilon} (k_1 \hat{v}_n + k_2 \hat{\theta}_n + k_3 \hat{\phi}_n) e^{-a^2(k_1^2+k_2^2+k_3^2)} e^{i(k_1 r_{n1} + k_2 r_{n2} + k_2 r_{n3})}, \tag{J7}$$

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 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 (J7), and obtain

$$\mathbf{p}_1^{(0)} = \mathbf{p}_1 + \frac{\pi^2 \lambda B}{a^3} \sum_{n=2}^{N} \frac{1}{v_{1n}} e^{-(1/4a^2)(r_{n2}^2 + r_{n3}^2)} \left(\frac{\hat{v}_n}{\sqrt{\pi}} e^{-(r_{n1}^2/4a^2)} - \frac{r_{n2}\hat{\theta}_n + r_{n3}\hat{\phi}_n}{2a} \left[1 + \operatorname{erf}\left(\frac{r_{n1}}{2a} \right) \right] \right), \tag{J8}$$

where the error function is defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \tag{J9}$$

We have

$$\operatorname{erf}(-x) = -\operatorname{erf}(x), \tag{J10}$$

and

$$\lim_{x \to +\infty} \operatorname{erf}(x) = 1. \tag{J11}$$

Similarly, $\mathbf{p}_1^{(2)}(t)$ (that corresponds to the time dependent part in (218)) is given by

$$\mathbf{p}_1^{(2)}(t) = -\frac{\pi^2 \lambda B}{a^3} \sum_{n=2}^{N} \frac{1}{v_{1n}} e^{-(1/4a^2)(r_{n2}^2 + r_{n3}^2)} \left(\frac{\hat{v}_n}{\sqrt{\pi}} e^{-(1/4a^2)(r_{n1} - v_{1n}t)^2} - \frac{r_{n2}\hat{\theta}_n + r_{n3}\hat{\phi}_n}{2a} \left[1 + \operatorname{erf}\left(\frac{r_{n1} - v_{1n}t}{2a} \right) \right] \right). \tag{J12}$$

For $t = 0$ we recover the initial condition

$$\mathbf{p}_1(0) = \mathbf{p}_1^{(0)} + \mathbf{p}_1^{(2)}(0) = \mathbf{p}_1. \tag{J13}$$

For a finite number N of particles, $\mathbf{p}_1^{(2)}(t)$ vanishes in the asymptotic time limit (see (J10) and (J11)), and the contribution comes only from $\Pi^{(0)}$ subspace, i.e. (for $t \to +\infty$)

$$\mathbf{p}_1(t) \to \mathbf{p}_1^{(0)}. \tag{J14}$$

Hence, the $\Pi^{(0)}$ subspace gives the asymptotic contribution for $\mathbf{p}_1(t)$. It is clear that the contribution from $\Pi^{(0)}$ subspace alone cannot satisfy the causality. By adding the effects in $\Pi^{(2)}$ subspace we recover the causality for $\mathbf{p}_1(t)$ in (J2).

We note that inspite 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 (J8) we have

$$\mathbf{p}_1^{(0)} \to \mathbf{p}_1 - \frac{\pi^2 \lambda B}{a^4} \sum_{n=2}^{N} \frac{1}{v_{1n}} e^{-(1/4a^2)(r_{n2}^2 + r_{n3}^2)} (r_{n2}\hat{\theta}_n + r_{n3}\hat{\phi}_n). \tag{J15}$$

For $t = 0$, $\mathbf{p}_1(t)$ was in the vacuum of correlation as it depends on only its momentum. The interaction builds up the correlations between particles 1 and n. Then the resonance effect leads to the correlation which does not vanish whatever the distance of the particles. As a result, (J15) diverges in the limit of $N \to \infty$, and the asymptotic value of $\mathbf{p}_1(t)$ is no longer analytic in λ in this limit. Only for the systems with finite number of particles do we have a meaningful estimate of the above integrals.

We note that (J15) also leads to the estimate of the invariant $\mathbf{P}_1^D$ in (206).

Let us note that in the above estimate of the integrals we have first taken the large volume limit, keeping the number N of particles finite. Therefore, the limit $N \to \infty$ in (J15) is not the thermodynamic limit. As the result, we have a different order estimate of (206) from the one in (220), when the positions of the particles are distributed randomly. For example, let us recall the relation

$$r_{n2} = r_n[\sin\theta_r \cos(\phi_r - \phi_n) - \cos\theta_r \sin\theta_n], \qquad r_{n3} = r_n \sin\theta_r \sin(\phi_r - \phi_n), \tag{J16}$$

and similar expression for r_{n1}, where r_n, θ_r, and ϕ_r are the polar coordinates of $\mathbf{r}_n$ in the reference system introduced above (see Fig. 3).

Assuming, for example, θ_r is distributed randomly, one can see that the right-hand side of (J15) increases as $\sqrt{N}$ for large N. In contrast to (220), this diverges in the limit $N \to \infty$. This result clearly shows that for randomly distributed $\mathbf{q}_n$ one cannot replace the summation over $\mathbf{k}$ in (218) by integration, but should perform the summation over the wave vector $\mathbf{k}$ and the summation over the particles n simultaneously, as we have done in (220); see also the example given in Appendix M.

APPENDIX K. VELOCITY INVERSION AND ENTROPY BARRIER

In this appendix we shall discuss the qualitative behaviour of the Lyapunov functions (or the $\mathcal{H}$-functions defined in Section 7 when we perform a velocity inversion at time t_0. We shall see that the longer we wait, a higher 'entropy barrier' is built up. In the limit $t_0 \to \infty$ the entropy barrier becomes infinity.

Let us for example prepare an initial condition with no correlations, i.e. the system is in the vacuum of correlation,

$$|\rho(0)\rangle\rangle = P^{(0)}|\rho(0)\rangle\rangle. \tag{K1}$$

By the complex spectrual representation, the evolution of the state is given by

$$|\rho(t)\rangle\rangle = \sum_{\nu}\sum_{\alpha} e^{-iZ_\alpha^{(\nu)}t}|F_\alpha^{(\nu)}\rangle\rangle\langle\langle \tilde{F}_\alpha^{(\nu)}|P^{(0)}|\rho(0)\rangle\rangle. \tag{K2}$$

The interaction then leads to the correlations among the particles. For a long time, the resonance then builds up 'long-range correlations' (see Section 8 and Appendix J). Let us then consider the contribution to the μth order correlation coming from the $\Pi^{(\nu)}$ subspace,

$$P^{(\mu)}\Pi^{(\nu)}|\rho(t)\rangle\rangle = \sum_{\alpha} e^{-iZ_\alpha^{(\nu)}t}P^{(\mu)}\mathcal{C}^{(\nu)}(Z_\alpha^{(\nu)})|u_\alpha^{(\nu)}\rangle\rangle N_\alpha^{(\nu)}\langle\langle \tilde{v}_\alpha^{(\nu)}|\mathcal{D}^{(\nu)}(Z_\alpha^{(\nu)})P^{(0)}|\rho(0)\rangle\rangle. \tag{K3}$$

At $t = t_0$, we perform the velocity inversion. Let us denote this operation by the operator $\hat{I}_v$. Then we have

$$\hat{I}_v\mathbf{q}_j = \mathbf{q}_j, \qquad \hat{I}_v\mathbf{p}_j = -\mathbf{p}_j, \tag{K4}$$

which lead to

$$\hat{I}_v L_H = -L_H. \tag{K5}$$

By an expansion in powers of λ, one can easily see that the velocity inversion for the creation and destruction operator leads to their complex conjugation.[¶] Writing only the contribution from the creation operator in (K3), we have

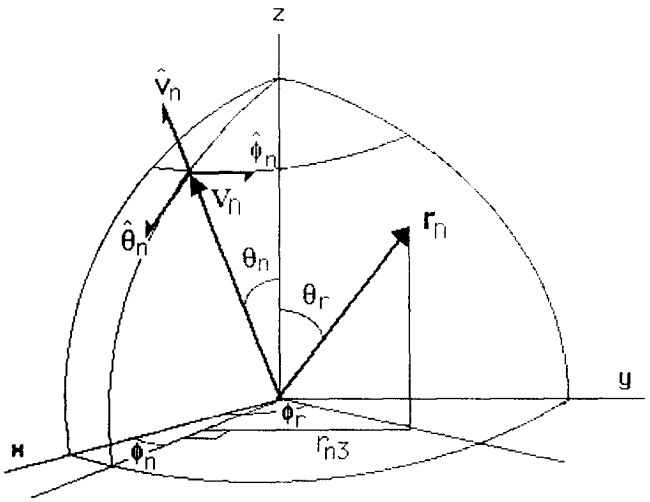

Fig. 3. In this figure we show only r_{n3} in (J16).

[¶]One can also verify that the velocity inversion changes only the sign of the real part of the collision operator, and leaves invariant its imaginary part.

$$\hat{I}_v P^{(\mu)}\Pi^{(\nu)}|\rho(t_0)\rangle\rangle \sim P^{(\mu)}[\mathscr{C}^{(\nu)}(Z_\alpha^{(\nu)})]^{c.c.}\, P^{(\nu)}. \tag{K6}$$

Starting with a certain value of Lyapunov function, its value monotonically decreases till the moment $t = t_0$ before the velocity inversion. Now let us estimate the value of the Lyapunov function coming from (K6) after the velocity inversion. To estimate this, we have to evaluate the value of the transformed state $\Lambda_B \hat{I}_v|\rho(t_0)\rangle\rangle$. Let us consider the contributions where the degree of correlation in $P^{(\mu)}$ is larger than the one in $P^{(\nu)}$, i.e. $d_\mu > d_\nu$. Then $\Lambda_B \hat{I}_v|\rho(t_0)\rangle\rangle$ involves the following contribution coming from the diagonal transition (see (81) and (100))

$$\Lambda_B \hat{I}_v \Pi^{(\nu)}|\rho(t_0)\rangle\rangle \sim P^{(\nu)}\mathscr{D}^{(\nu)}(Z_\alpha^{(\nu)})P^{(\mu)}[\mathscr{C}^{(\nu)}(Z_\alpha^{(\nu)})]^{c.c.}\, P^{(\nu)} = P^{(\nu)}\mathscr{T}_D^{(\nu)}(Z_\alpha^{(\nu)})P^{(\mu)}\frac{1}{|[z - l_\mu]^+_{Z_\alpha^{(\nu)}}|^2}P^{(\mu)}[\mathscr{T}_C^{(\nu)}(Z_\alpha^{(\nu)})]^{c.c.}\, P^{(\nu)}. \tag{K7}$$

In general, there are diffusion modes in space $\Pi^{(\nu)}$ with $\nu \neq 0$. We have illustrated this fact for the perfect Lorentz gas in Appendix F. The diffusion modes are associated to small wave vectors $\mathbf{k}$ which correspond to macroscopic scales in space, such as the hydrodynamic scale [18]. The characteristic feature of the diffusion modes is that their eigenvalues are purely imaginary and are proportional to $-i|\mathbf{k}|^2$ (see Appendix F). As mentioned, resonances lead to long-range correlations. As we wait longer, long-range correlations are built up progressively involving more particles. This implies that smaller and smaller wave vectors $\mathbf{k}$ contribute to (K7). Hence, for sufficiently large t_0, (K7) has a contribution given in the thermodynamic limit by

$$\Lambda_B \hat{I}_v|\rho(t_0)\rangle\rangle \sim \int \mathrm{d}l_\mu \frac{1}{|[z - l_\mu]^+_{-i|\mathbf{k}|^2}|^2} \sim \frac{1}{|\mathbf{k}|^2}. \tag{K8}$$

As the result, the value of the Lyapunov functions defined as the square of (K8) become larger for larger t_0. The 'entropy barrier' increases as a function of t_0, and becomes infinite for $t_0 \to +\infty$.

This divergence appears only in the diagonal transitions. For the off-diagonal transitions, the contributions are still finite even with the velocity inversion.

It is also interesting to see the behaviour of the Lyapunov functions for the integrable case discussed in Section 9 (see also Appendix L). Let us again prepare an initial condition with no correlations. As mentioned, the resonance then builds up the long-range correlations among the particles which do not vanish whatever their distance (see also Appendix J). This situation is then described by the 'retarded' states $|\Phi_\nu^+\rangle\rangle$ (see (184)). Dynamically there is no reason to exclude the opposite process which corresponds to the 'velocity inversion experiment'. The initial condition has now an infinite range of correlations which are described by the 'advanced' states $|\Phi_\nu^-\rangle\rangle$. After the collision the correlations disappear; but this situation which is possible from the dynamical point of view is not observed in nature. 'Entropy' distinguishes these two processes. To see this, let us ask if the advanced states are in the domain of Λ_B (or Λ_I in (182) for this case). For example, let us consider the normalized advanced states for the potential scattering with a single particle discussed in Appendix I. (with an abbreviation of the momentum indices in the states)

$$|\rho\rangle\rangle = L^{-3/2}|\Phi_0^-\rangle\rangle, \tag{K9}$$

where

$$\int \mathrm{d}q \int \mathrm{d}p \langle\langle q, p|\rho\rangle\rangle = 1. \tag{K10}$$

We have (see (191))

$$\langle\langle \hat{\varphi}_{\mathbf{p}_1}|\Lambda_I|\rho\rangle\rangle \sim \langle\langle \Phi_0^D|\Phi_0^-\rangle\rangle \sim \frac{1}{\Omega^2}\sum_{\mathbf{k}}\frac{1}{|\mathbf{k}\cdot\mathbf{v} - i\epsilon|^2} \sim \frac{1}{\epsilon\Omega}, \tag{K11}$$

where we have displayed only the term which is related to the 'entropy barrier' built up by the Poincaré resonances. The volume factor in (K11) comes from the volume dependence of the $\mathscr{T}$-matrix which is the same as the interaction λL_V (26). Because of the limiting procedure (B2), the resonance contribution in (K11) vanishes for $\Omega \to \infty$. Hence, the normalized advanced state is in the domain of Λ_B and still leads to a finite value of the Lyapunov function. However, the appearance of the singular factor ϵ^{-1} due to the resonances already suggests the 'difficulty' of the velocity inversion in scattering experiments even for the integrable systems. This marks the difference with retarded states.

APPENDIX L. NON-UNITARY TRANSFORMATIONS FOR AN INTEGRABLE SYSTEM

In this appendix we present the explicit form of the solutions of (178) for Φ_ν^C and Φ_ν^D for two-particle integrable systems. Observing the evolution in the center of mass system, the two-body problem reduces to potential scattering of a single particle. A similar result for the quantum potential scattering has been presented in our previous paper [1].

For potential scattering there are only two degrees of correlations; the vacuum of correlation with $d_0 = 0$, and the 'binary' correlations with $d_k = 1$. In order to simplify the notation, we shall use the plain notation for three-dimensional vectors, such as k.

The left and right eigenstates of the Liouvillian are constructed by iteration of (178). They are given by (see also (184))

$$\langle\langle \Phi^D_{0,p}| = \langle\langle \Phi^-_{0,p}| = \langle\langle 0,\, p| + \langle\langle 0,\, p|\mathcal{T}(+i\epsilon)\frac{1}{i\epsilon - L_0},$$

$$|\Phi^C_{0,p}\rangle\rangle = |\Phi^+_{0,p}\rangle\rangle = |0,\, p\rangle\rangle + \frac{1}{i\epsilon - L_0}\mathcal{T}(+i\epsilon)|0,\, p\rangle\rangle,$$

$$\langle\langle \Phi^D_{k,p}| = \langle\langle \Phi^+_{k,p}| = \langle\langle k,\, p| + \langle\langle k,\, p|\mathcal{T}(k\cdot v - i\epsilon)\frac{1}{k\cdot v - i\epsilon - L_0}, \tag{L1}$$

$$|\Phi^C_{k,p}\rangle\rangle = Q^{(0)}|\Phi^+_{k,p}\rangle\rangle + \frac{1}{k\cdot v - i\epsilon}P^{(0)}\mathcal{T}(k\cdot v + i\epsilon)|k,\, p\rangle\rangle$$
$$= |\Phi^+_{k,p}\rangle\rangle + 2\pi i\delta(k\cdot v)P^{(0)}\mathcal{T}(k\cdot v + i\epsilon)|k,\, p\rangle\rangle.$$

We have

$$L_H|\Phi^C_{0,p}\rangle\rangle = 0, \qquad \langle\langle \Phi^D_{0,p}|L_H = 0, \tag{L2}$$

as well as

$$L_H|\Phi^C_{k,p}\rangle\rangle = (k\cdot v)|\Phi^C_{k,p}\rangle\rangle, \qquad \langle\langle \Phi^D_{k,p}|L_H = \langle\langle \Phi^D_{k,p}|(k\cdot v). \tag{L3}$$

We note that the difference $|\Phi^C_{k,p}\rangle\rangle - |\Phi^+_{k,p}\rangle\rangle$ in (L1) is proportional to $\delta(k\cdot v)$. Hence, both states $\Phi^C_{k,p}$ and $\Phi^+_{k,p}$ are the eigenstates with the same eigenvalue $k\cdot v$.

APPENDIX M. NUMERICAL VALIDATION OF THE SUMMATION FORMULA (220)

In this appendix we shall give the result of numerical simulations to verify the estimate (220) in a simple example.*

Let us consider the summation (for $-L/2 \leq x_j < L/2$)

$$S(L) = \sum_{j=1}^{N}\Delta k \sum_{n=-\infty}^{+\infty}\frac{ik_n}{k_n^2 + 4\eta^2}e^{-ik_nq_j} = \sum_{j=1}^{N}\Delta k \sum_{n=-\infty}^{+\infty}\frac{k_n}{k_n^2 + 4\eta^2}\sin(k_nq_j), \tag{M1}$$

where $k_n = n\Delta k$ with $\Delta k = 2\pi/L$, and $\eta > 0$. The sum $S(L)$ is real, and its average for a uniform distribution of q_j is zero. By contour integration, one can easily perform the integration (for $L \to \infty$ with N finite)

$$S(L) \to \sum_{j=1}^{N}\int_{-\infty}^{+\infty}dk\frac{ik}{k^2 + 4\eta^2}e^{-ikq_j} = \sum_{j=1}^{N}\pi e^{-2\eta|q_j|}\,\mathrm{sgn}(q_j). \tag{M2}$$

Putting $y_j = 2q_j/L$, we obtain [45]

$$S(L) = \sum_{j=1}^{N}\sum_{n=-\infty}^{+\infty}\frac{n}{n^2 + (\eta L/\pi)^2}\sin(n\pi y_j) = \frac{\pi}{\sinh(\eta L)}\sum_{j=1}^{N}\sinh[\eta L(1 - |y_j|)]\,\mathrm{sgn}(y_j). \tag{M3}$$

For $L \to \infty$ with N finite, (M3) reduces to (M2). For $L = N/c$ we have

$$S(N/c) = \frac{\pi}{\sinh(\eta N/c)}\sum_{j=1}^{N}\sinh\left[\frac{\eta N}{c}(1 - |y_j|)\right]\mathrm{sgn}(y_j). \tag{M4}$$

We have performed numerical calculations to evaluate the sums (M3) and (M4) by using a random number generator between $-1 \leq y_j < 1$ for various values of L and N. We have chosen the value $\eta = 0.5$. We have performed the simulations with 500 different sequences of the random number y_j.

We first consider the case corresponding to the 'thermodynamic limit'. In the sum (M4) we have fixed the concentration as $c = 1$. Then we have to evaluate (M4) for various values of N between 100 to 1000. The results of the sum obtained by the numerical simulations are plotted as a function of $\sqrt{N}$ in Fig. 4. The circles represent the mean value of the sum (M4) over 500 different sequences. We have indicated the square root of the mean deviation (SRMD) by squares. By increasing the value of N, SRMD remains constant as a function of $\sqrt{N}$. This agrees with our theoretical prediction for the thermodynamic limit.

Next we consider the summation using a 'non-thermodynamic' limit. In the sum (M3) we have given to L a large value $L = 10000$. Then we have to evaluate (M3) for various values of N between 100 to 1000. The results of the sum are again plotted as a function of $\sqrt{N}$ in Fig. 5. As before, each circle corresponds to the mean value of the sum (M3) over 500 sequences. We have indicated SRMD by squares. By increasing the value of N, SRMD linearly increases as a function of $\sqrt{N}$. This again agrees with our theoretical prediction for the 'non-thermodynamic' limiting procedure.

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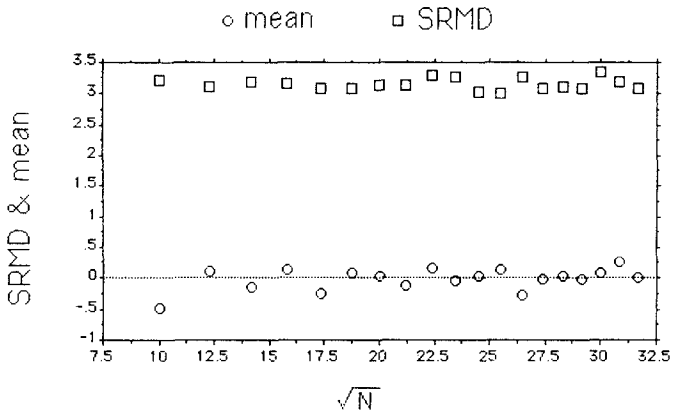

Fig. 4. The sum (M4) for the thermodynamic limit with $c = N/L = 1$ as a function of $\sqrt{N}$. We have chosen $100 \leqslant N \leqslant 1000$. Each square corresponds to the square root of the mean deviation (SRMD) represented over 500 different sequences of the random number y_i for a given N. We have also indicated the mean value of the sum by the circles. By increasing the value of N, SRMD remains constant as a function of $\sqrt{N}$.

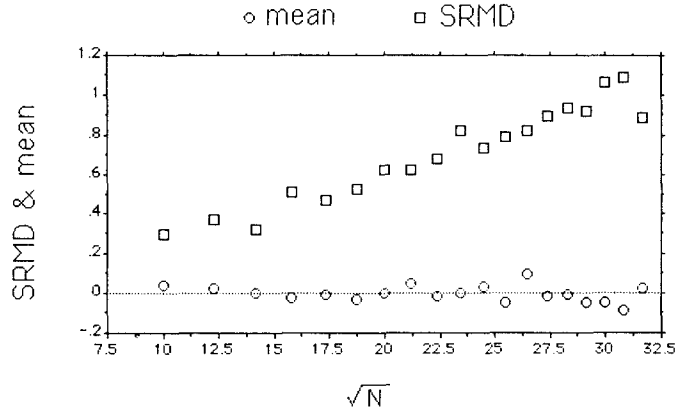

Fig. 5. The sum (M3) for the non-thermodynamic limit as a function of $\sqrt{N}$. We have chosen $L = 10^4$ and $100 \leqslant N \leqslant 1000$. Each square corresponds to the square root of the mean deviation (SRMD) represented over 500 different sequences of the random number y_i for a given N. We have also indicated the mean value of the sum by the circles. By increasing the value of N, SRMD increases linearly as a function of $\sqrt{N}$.