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Physics

Poincaré resonances and the limits of trajectory dynamics

(large Poincaré systems/singular invariants/persistent interactions/broken time symmetry/complex irreducible spectral representation)

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ABSTRACT **In previous papers we have shown that the elimination of the resonance divergences in large Poincaré systems leads to complex irreducible spectral representations for the Liouville–von Neumann operator. Complex means that time symmetry is broken and irreducibility means that this representation is implementable only by statistical ensembles and not by trajectories. We consider in this paper classical potential scattering. Our theory applies to *persistent* scattering. Numerical simulations show quantitative agreement with our predictions.**

Section 1. Introduction

A basic problem in modern physics is the elucidation of the time paradox. On all levels in nature, we find evolutionary patterns. In contrast, the traditional formulation of laws of nature does not distinguish past from future. Our goal has, therefore, been to formulate laws of physics that include time symmetry breaking. This goal has been realized for classes of dynamical systems such as chaotic maps or large Poincaré systems (LPS) (1–6). For these systems, the Brussels–Austin group derived a complex irreducible spectral representation for the operators associated to their time evolution (such as the Liouville operator or the Perron–Frobenius operator). Here, complex means that time symmetry is broken, and irreducible means that we deal with a statistical description that cannot be reduced to trajectories in classical dynamics (or to wave functions in quantum mechanics). The irreducibility of the spectral representation leading to a probabilistic theory can be considered as the *signature of chaos*. LPS (classical or quantum) are chaotic systems in this generalized sense. Here chaos is due to Poincaré resonances that lead to diffusive processes. Such a formulation is only possible in generalized function spaces in which unitary operators may admit eigenvalues of modulo different from unity. In addition, our formulation unifies fields of physics that appear quite separate in the usual presentation: dynamics (leading to the evolution of ensembles), statistical mechanics characterized by the introduction of "collision operators," and thermodynamics (microcanonical distribution).

To clarify the meaning of our approach, we consider in this paper the simple case of potential scattering. Scattering corresponds to a dynamical process. Still scattering is also the basic mechanism through which irreversibility appears in statistical mechanics (Fokker–Planck or Boltzmann equations) (7). We shall show that dissipative effects arise for *persistent* scattering, where we have to go beyond the traditional S-matrix-type approach. Classical scattering can be described in terms of Möller "states" $|\Phi^{+}_{\mathbf{k},\mathbf{v}}\rangle$ constructed in complete analogy with quantum theory [this method was introduced by Résibois (8) and extensively used by one of the authors (9)]. More precisely, we deal here with Möller operators, as they are defined here in phase space and not in the Hilbert space of quantum theory. Of special interest are the Möller states $|\Phi^{+}_{0,\mathbf{v}}\rangle$, corresponding to the value $\mathbf{k} = 0$ of the Fourier index $\mathbf{k}$. A close relation exists between $|\Phi^{+}_{0,\mathbf{v}}\rangle$ and the invariants of motion for scattering systems. We stress that these invariants are *asymptotic* invariants, valid only in the limit of large volumes $L^3 \to \infty$, where the scattering process occurs. We next consider ensemble averages of Poincaré invariants and their time derivatives. We show that the ensemble averages associated to delocalized distributions (independent of $\mathbf{x}$) decay through diffusive processes and that this decay is linear in time. These processes are not included in trajectory dynamics.

We come, therefore, to a most exciting situation, as we may test the existence of diffusive processes for LPS in the frame of classical dynamics but beyond the trajectory formulation. Numerical simulations quantitatively confirm our predictions. This result shows that classical dynamics must be reformulated on the level of ensembles when extended to LPS.

Let us first indicate the difference between "transient" and "persistent" scattering. For transient scattering the distribution function $\rho(\mathbf{x}, \mathbf{p}, t)$ is localized in the configuration space and can be normalized to one,

$$\int d\mathbf{p} \int d\mathbf{x}\, \rho(\mathbf{x}, \mathbf{p}, t) = (2\pi)^{3/2} \int d\mathbf{p} \int d\mathbf{k} \rho_{\mathbf{k}}(\mathbf{p}, t)\delta(\mathbf{k}) = 1, \quad [1]$$

where $\rho_{\mathbf{k}}(\mathbf{p})$ is the Fourier transform of $\rho(\mathbf{x}, \mathbf{p})$.

We then consider the situation where $\rho(\mathbf{x}, \mathbf{p}, t)$ has a finite limit for $|\mathbf{x}| \to \infty$. The interaction with the potential is therefore persistent. For this situation the Fourier component of the distribution function is singular function at $\mathbf{k} = 0$ with a delta function singularity (9–11).

$$\rho_{\mathbf{k}}(\mathbf{p}, t) = \rho^{d}_{0}(\mathbf{p}, t)\delta(\mathbf{k}) + \rho^{i}_{\mathbf{k}}(\mathbf{p}, t), \quad [2]$$

where $\rho^{i}_{\mathbf{k}}$ is the nonsingular part of the distribution function at $\mathbf{k} = 0$. The distribution function cannot be normalized to unity, as a square of the delta function appears in Eq. 1. For box normalization, the delta function can be understood as a weighted Kronecker symbol $\delta_{\Omega}(\mathbf{k}) \equiv \Omega\delta_{\mathbf{k},0}$, where $\Omega \equiv (L/2\pi)^3$ with volume L^3. The square of the delta function is then $\delta^{2}_{\Omega}(\mathbf{k}) = \Omega\delta_{\Omega}(\mathbf{k})$, which diverges in the limit of large volumes $\Omega \to \infty$. We shall use this interpretation in *Section 3*. The nonnormalizable situation can be realized, for example, by considering potential scattering involving many independent identical particles that interact only with a single potential. We then consider the so-called "thermodynamic limit" corresponding to a finite concentration $c = N/L^3$ with an infinite number of incident particles $N \to \infty$ and $L^3 \to \infty$ and consider a reduced distribution function.

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Abbreviations: SPI, singular Poincaré invariants; LPS, large Poincaré systems.

Note that observables such as the Hamiltonian also have a delta singularity in the Fourier representation (see Eq. 3). It is therefore natural to include distribution functions that are also singular functions. The eigenvalue problem of the Liouville operator L_H involving singular functions has quite specific features. There appears a nonunitary similitude between L_H and the "collision operator" θ (2) which has a complex spectrum. We recover in this special case the result of our general theory associated to "subdynamics" (12–15). The singular part of the eigenfunctions satisfies a closed eigenvalue problem associated to θ (in the lowest order it is precisely the well-known Fokker–Planck operator), while the regular part becomes a functional of the singular part.

The method given here can be easily extended to the problems studied in statistical mechanics. An example is the well-known Lorentz model in which a light particle interacts with an ensemble of heavy masses. We shall study this example as well as the extension of our results to quantum mechanics in subsequent papers (T.P., D. Driebe, and Z. L. Zhang, unpublished work). The aim of this paper is to give an overall view of our results. Proofs and details will be published separately.

Section 2. Classical Möller States and Singular Poincaré Invariants (SPI)

Let us consider classical potential scattering for a unit mass $m = 1$. We assume that the Hamiltonian is given by

$$H(\mathbf{x}, \mathbf{p}) = H_0(\mathbf{p}) + \lambda V(\mathbf{x}) = \int d\mathbf{k} \left(\frac{p^2}{2} \delta(\mathbf{k}) + \lambda V_{\mathbf{k}} \right) e^{i\mathbf{k}\cdot\mathbf{x}}. \quad [3]$$

The parameter λ is a dimensionless coupling constant. For simplicity we assume short-range repulsive forces (i.e., no bounded motion).

The Liouvillian is given by the Poisson bracket $L_H f \equiv i\{H, f\}$ and generates the evolution of the probability distribution function $\rho(\mathbf{x}, \mathbf{p}, t)$ of ensembles in phase space,

$$\rho(t) = e^{-iL_H t}\rho(0). \quad [4]$$

The Liouvillian is a hermitian operator in the Liouville space (9). In this space the inner product of phase functions $\langle \mathbf{x}, \mathbf{p}| g\rangle \equiv g(\mathbf{x}, \mathbf{p})$ and $\langle f|\mathbf{x}, \mathbf{p}\rangle \equiv f^{c.c.}(\mathbf{x}, \mathbf{p})$ is defined in the "bra-ket" notation (9) by $\langle f| g\rangle \equiv \int d\mathbf{x} \int d\mathbf{p}\, \langle f|\mathbf{x}, \mathbf{p}\rangle\langle \mathbf{x}, \mathbf{p}| g\rangle$.

For the unperturbed Liouvillian $L_0 \equiv L_{H_0} = -i\mathbf{p}\cdot\partial/\partial x$ the spectrum is given by ref. 9:

$$L_0|\mathbf{k}, \mathbf{v}\rangle = (\mathbf{k}\cdot\mathbf{v})|\mathbf{k}, \mathbf{v}\rangle, \quad [5]$$

where $\langle \mathbf{x}, \mathbf{p}|\mathbf{k}, \mathbf{v}\rangle = (2\pi)^{-3/2}\delta(\mathbf{p} - \mathbf{v})\exp(i\mathbf{k}\cdot\mathbf{x})$. For $\mathbf{k} = 0$ we have the invariants of motion $L_0|0, \mathbf{v}\rangle = 0$.

The completeness and orthonormality relations are

$$\int d\mathbf{v} \int d\mathbf{k} |\mathbf{k}, \mathbf{v}\rangle\langle \mathbf{k}, \mathbf{v}| = 1, \langle \mathbf{k}, \mathbf{v}|\mathbf{k}', \mathbf{v}'\rangle = \delta(\mathbf{k} - \mathbf{k}')\delta(\mathbf{v} - \mathbf{v}'). \quad [6]$$

The perturbed Liouvillian L_V is given in ref. 9;

$$\langle \mathbf{k}, \mathbf{v}|L_V|\mathbf{k}', \mathbf{v}'\rangle = V_{\mathbf{k}-\mathbf{k}'}(\mathbf{k} - \mathbf{k}')\cdot \frac{\partial\delta(\mathbf{v}' - \mathbf{v})}{\partial\mathbf{v}'}. \quad [7]$$

The matrix element is a "distribution" (as it contains a derivative of the δ-function).

Let us consider the eigenvalue problem for the total Liouvillian L_H. To this end we introduce *classical* "off-shell" Möller states in analogy with Möller's scattering states for the Hamiltonian in quantum scattering theory (16–18)

$$|\Phi_{\mathbf{k},\mathbf{v}}(z)\rangle = |\mathbf{k}, \mathbf{v}\rangle + \frac{1}{z - L_0} \mathrm{T}(z)|\mathbf{k}, \mathbf{v}\rangle, \quad [8]$$

where z is a complex number with $\mathrm{Im}z \neq 0$. The "off-shell" T-matrix is defined by

$$\mathrm{T}(z) = \lambda L_V + \lambda L_V \frac{1}{z - L_0} \mathrm{T}(z). \quad [9]$$

We also have

$$\langle \mathbf{l}, \mathbf{u}|L_H|\Phi_{\mathbf{k},\mathbf{v}}(\mathbf{k}\cdot\mathbf{v} + z)\rangle = (\mathbf{k}\cdot\mathbf{v})\langle \mathbf{l}, \mathbf{u}|\Phi_{\mathbf{k},\mathbf{v}}(\mathbf{k}\cdot\mathbf{v} + z)\rangle + \frac{z}{\mathbf{k}\cdot\mathbf{v} + z - \mathbf{l}\cdot\mathbf{u}} \mathrm{T}_{\mathbf{l},\mathbf{u},\mathbf{k},\mathbf{v}}(\mathbf{k}\cdot\mathbf{v} + z), \quad [10]$$

where $\mathrm{T}_{\mathbf{l},\mathbf{u};\mathbf{k},\mathbf{v}} \equiv \langle \mathbf{l}, \mathbf{u}|\mathrm{T}|\mathbf{k}, \mathbf{v}\rangle$.

Let us consider the "on-shell" limits $z \to \pm i0$ of the Möller states, $|\Phi^{\pm}_{\mathbf{k},\mathbf{v}}\rangle \equiv |\Phi_{\mathbf{k},\mathbf{v}}(\mathbf{k}\cdot\mathbf{v} \pm i0)\rangle$. The phase functions $\Phi^{\pm}_{\mathbf{k},\mathbf{v}}(\mathbf{x}, \mathbf{p})$ are well defined (as velocity distributions):

$$\Phi^{\pm}_{\mathbf{k},\mathbf{v}}(\mathbf{x}, \mathbf{p}) = (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{x}}\delta(\mathbf{p} - \mathbf{v}) + (2\pi)^{-3/2} \int d\mathbf{l}\, e^{i\mathbf{l}\cdot\mathbf{x}} \frac{\mathrm{T}_{\mathbf{l},\mathbf{p};\mathbf{k},\mathbf{v}}(\mathbf{k}\cdot\mathbf{v} \pm i0)}{\mathbf{k}\cdot\mathbf{v} - \mathbf{l}\cdot\mathbf{p} \pm i0}. \quad [11]$$

Then the Möller states become the *eigenstates* of the Liouvillian:

$$\langle \mathbf{x}, \mathbf{p}|L_H|\Phi^{\pm}_{\mathbf{k},\mathbf{v}}\rangle = (\mathbf{k}\cdot\mathbf{v})\langle \mathbf{x}, \mathbf{p}|\Phi^{\pm}_{\mathbf{k},\mathbf{v}}\rangle. \quad [12]$$

For this case we have also the usual completeness and orthonormality conditions for the on-shell Möller states.

Of special interest are the Möller states for $\mathbf{k} = 0$ that are related to invariants of motion. As mentioned, $\langle \Phi_{0,\mathbf{v}}(z^*)|\mathbf{x}, \mathbf{p}\rangle$ is still a distribution involving the velocity. Therefore, we consider the phase-space quantity $I_f(z)$,

$$I_f(\mathbf{x}, \mathbf{p}; z) = (2\pi)^{3/2} \int d\mathbf{v}\, f(\mathbf{v})\, \langle \Phi_{0,\mathbf{v}}(z^*)|\mathbf{x}, \mathbf{p}\rangle = f(\mathbf{p}) + \int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}} \frac{\lambda V_{\mathbf{k}}}{\mathbf{k}\cdot\mathbf{p} + z} \mathbf{k}\cdot\frac{\partial}{\partial\mathbf{p}} f(\mathbf{p}) + O(\lambda^2). \quad [13]$$

In the limit of $z \to \pm i0$, $I_f(z)$ are invariants of motion,

$$\dot{I}_f(\mathbf{x}(t), \mathbf{p}(t); \pm i0) = 0. \quad [14]$$

The standard perturbation analysis for the Hamilton– Jacobi equation using the generating function $F(\mathbf{P}, \mathbf{x})$ shows (19) that the new momenta $\mathbf{P}^{\pm}$ coincide with $I_f(\mathbf{x}, \mathbf{p}; \pm i0)$ for $f(\mathbf{p}) = \mathbf{p}$ (unpublished work). We call $I_f(\pm i0)$ "singular Poincaré invariants" (SPI), as the Fourier components of the invariants are singular at resonances $\mathbf{k}\cdot\mathbf{p} = 0$ (refs. 9 and 20; see also refs. 21 and 22).

In the above construction of SPI we have considered a scattering process that occurs in infinitely large space. We can obtain the same result, starting with the standard box normalization approach and taking the limit of large volumes $\Omega \to \infty$. It is important to stress that the invariants I_f are *asymptotic* invariants valid only in this limit.

Section 3. Limits of Trajectory Dynamics and Numerical Simulations

In the previous section we have constructed SPI through the on-shell Möller states in the phase-space representation. As

SPI are singular at the resonances, we want to see the influence of resonances on the invariants in more detail.

From Eq. **10** we have (for $\mathbf{k} = 0$)

$$\langle \mathbf{l}, \mathbf{u}|L_H|\Phi_{0,\mathbf{v}}(z)\rangle = \frac{z}{z - \mathbf{l}\cdot\mathbf{u}} T_{\mathbf{l},\mathbf{u};0,\mathbf{v}}(z). \quad [15]$$

In the $(\mathbf{l}, \mathbf{u})$ representation the on-shell Möller states are distributions in wave vectors $\mathbf{l}$, as well as in velocities. The distributions in $\mathbf{l}$ are usually handled by introducing localized test functions (the wave packets of traditional quantum scattering theory). However, we want to go here beyond the usual S-matrix theory. In Eq. **15** a *discontinuity* appears at $\mathbf{l} = 0$. For $\mathbf{l} \neq 0$ we obtain zero in the limit $z \to +i0$. On the contrary for $\mathbf{l} = 0$ we have a nonvanishing contribution for the on-shell Möller states. As this effect appears only for $\mathbf{l} = 0$, it is of the order $1/\Omega$ and can only be observed when associated to delocalized situations (see below). We verified this result by numerical simulations.

Let us consider in more detail the effect of the time variation of $\Phi_{0,\mathbf{v}}(z)$ on the Poincaré invariant $I_f(\mathbf{x}, \mathbf{p}; \pm i0)$. To do so we introduce the integral of $I_f(z)$ over the phase space with a weight function $g(\mathbf{x}, \mathbf{p})$,

$$[I_f(t; z)]_g \equiv \int d\mathbf{x}\, d\mathbf{p}\, [e^{+iL_H t} I_f(\mathbf{x}, \mathbf{p}; z)] g(\mathbf{x}, \mathbf{p}). \quad [16]$$

The application of trajectory dynamics (Eq. **14**) would lead to

$$\lim_{z \to +i0} \frac{d}{dt} [I_f(t; z)]_g = 0. \quad [17]$$

However, Eq. **17** is correct only if $g_{\mathbf{k}}(\mathbf{p})$ has no delta function singularity as in Eq. **2**; this corresponds to the situation where the function $g(\mathbf{x}, \mathbf{p})$ is a localized function in configuration space. In contrast, if g does not depend on $\mathbf{x}$, e.g., $g = g_0(\mathbf{p})$, then the time derivative (Eq. **17**) does not vanish due to the resonances. To see this, we first note that $\langle \Phi^-_{0,\mathbf{v}}| \exp(-iL_H t) L_V = \langle \Phi^-_{0,\mathbf{v}}| L_V$ because we can apply Eq. **12** for a localized interaction $V(\mathbf{x})$. Therefore, also taking into account Eq. **15**, we have for all times t

$$\begin{aligned}
&\lim_{z \to +i0} \frac{d}{dt} [I_f(t; z)]_{g_0} \\
&= -i \lim_{z \to +i0} \int d\mathbf{k} \int d\mathbf{u} \int d\mathbf{v} f(\mathbf{v}) \langle \Phi_{0,\mathbf{v}}(z^*)|L_H|\mathbf{k}, \mathbf{u}\rangle \delta(\mathbf{k}) g_0(\mathbf{u}) \\
&= -i \int d\mathbf{u} \int d\mathbf{v} f(\mathbf{v}) \langle 0, \mathbf{v}|T(+i0)|0, \mathbf{u}\rangle g_0(\mathbf{u}) \quad [18] \\
&= \lambda^2 \int d\mathbf{p} f(\mathbf{p}) \int d\mathbf{k} |V_{\mathbf{k}}|^2 \mathbf{k}\cdot \frac{\partial}{\partial \mathbf{p}} \pi\delta(\mathbf{k}\cdot\mathbf{p}) \mathbf{k}\cdot \frac{\partial}{\partial \mathbf{p}} g_0(\mathbf{p}) + O(\lambda^3).
\end{aligned}$$

We obtain a diffusion process breaking time symmetry. (The right-hand side is even in the momentum $\mathbf{p}$, the equation is therefore not invariant for $t \to -t$ and $\mathbf{p} \to -\mathbf{p}$.) [We considered here $z \to +i0$. We have a similar equation for $z \to -i0$ but with the opposite sign. This corresponds to the existence of two semi-groups. This situation has been discussed in our paper on the Friedrichs model (1)]. This effect is a *nonlocal* effect requiring therefore an extended formulation of classical dynamics involving ensembles. The origin of this effect is the role of resonances that lead to singularities.

As seen from Eq. **18**, $T_{0,\mathbf{v};0,\mathbf{u}}(+i0)$ is in the lowest approximation in λ, a second-order derivative operator in the momentum. The time evolution of $[I_f(t; z)]_{g0}$ cannot be expressed by trajectory dynamics but only as the result of diffusive processes in momentum space, as described by the Fokker–Planck operator. Following kinetic theory we shall also call this matrix the "collision operator" θ (2), which is related to the Liouvillian by

$$\begin{aligned}
\theta_{0,\mathbf{v};0,\mathbf{u}} &= T_{0,\mathbf{v};0,\mathbf{u}}(+i0) = \langle \Phi^-_{0,\mathbf{v}}|L_H|0, \mathbf{u}\rangle \\
&= \langle 0, \mathbf{v}|L_H|\Phi^+_{0,\mathbf{u}}\rangle. \quad [19]
\end{aligned}$$

The collision operator acts only on the subspace of the delocalized states with $\mathbf{k} = 0$. Eq. **19** is the basic formula which relates dynamics of LPS to nonequilibrium statistical machanics.

A close relation exists between the evolution of $[I_f(t; +i0)]_{g_0}$ in Eq. **18** and the evolution of the ensemble average $\langle f(\mathbf{p})\rangle$ of quantity $f(\mathbf{p})$ for a given initial distribution function $\rho(\mathbf{x}, \mathbf{p}, 0) = g_0(\mathbf{p})$. Indeed, they coincide in the asymptotic time limit (unpublished work). As the right-hand side of Eq. **18** is constant, the delocalized superposition of the singular invariants varies strictly linearly in time. Remarkably, the dissipative evolution associated with this linear t contribution already starts from $t = 0$ [because the singular invariants I_f belongs to $\overset{(0)}{\Pi}$ subdynamics in our complex spectral representation (unpublished data)]. In contrast, the time evolution of the ensemble average $\langle f(\mathbf{p})\rangle$ starts with t^2, as easily understood using a short time expansion.

We have done numerical simulations for potential scattering. [We thank K. H. Wen and Z. L. Zhang for the numerical simulations and will present more details about the simulations (T.P., I.P., K. H. Wen, and Z. L. Zhang, unpublished work).] We have solved the Hamilton equations of motion for trajectories and also the Liouville equation for ensembles. Thus we have calculated the evolution of the singular invariants (Eqs. **13** and **16**) both for trajectories and for delocalized ensembles. We have approximated the singular invariants to first order in λ. This leads to an error of order λ^2. Also we have approximated the Fourier integral by Fourier series, by putting the system into a large box of volume L^d with the usual periodic boundary conditions. The Fourier spectrum is therefore discrete; i.e., $\mathbf{k} = \mathbf{n}\Delta k$, where $\mathbf{n} \equiv (n_1, \ldots, n_d)$ is an integer-vector, and $\Delta k \equiv 2\pi/L$. We have also replaced the integration of the wave vectors and the Dirac delta function, respectively, by a weighted sum $\int_{\mathbf{k}} \equiv \Omega^{-1}\Sigma_{\mathbf{k}}$ and a weighted Kronecker symbol $\delta_\Omega(\mathbf{k}) \equiv \Omega\delta_{\mathbf{k},0}$ [for $\Omega \equiv L^d/(2\pi)^d$]. In the limit of large volumes the spectrum becomes continuous and they reduce respectively to the integration $\int d\mathbf{k}$ and to the delta function $\delta(\mathbf{k})$ (23).

There is a characteristic time scale $t_b \equiv (|\mathbf{v}|\Delta k)^{-1}$. We impose the condition: $t \ll t_b$. We may then consider the spectrum as continuous. We also replace the infinitesimal quantity $z = +i0$ by $z = +i\varepsilon$, where ε is a finite small positive number. As the result the delta function $\pi\delta(w_{kk'})$ is approximated by the Lorentzian distribution $\varepsilon/(w^2_{kk'} + \varepsilon^2)$. To obtain a consistent approximation of the delta function, there should have enough number of discrete states around the peak of the Lorentzian. Therefore, our expressions have to be understood in the continuous limit $\Delta k \to 0$ and $\varepsilon \to 0+$ with the condition for the small parameters: $\varepsilon \gg |\mathbf{v}|\Delta k$.

Numerical simulations for scattering in a two-dimensional configuration space, i.e., $d = 2$, were completed. We then compared the numerical results to our theoretical predictions for increasing values of the volume.

The Hamilton equations of motion have been solved by the standard fourth-order Runge–Kutta method. We have chosen a Gaussian potential given by $\lambda V(x, y) = \lambda V_0 \exp[-(x^2 + y^2)/4a^2]$ with $a = 1$. A typical time step was $\Delta t = 0.01$, and $\lambda V_0 = 10^{-3}$ was chosen for this simulation. We also chose the

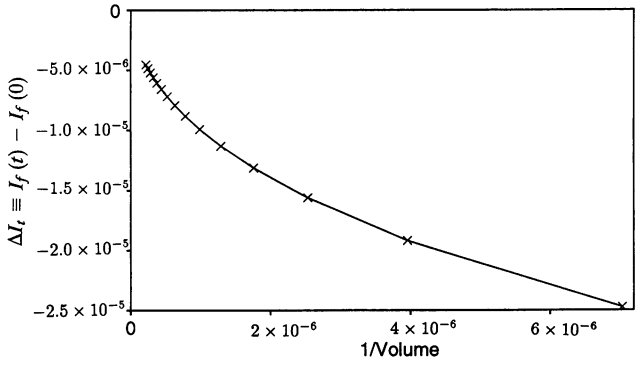

FIG. 1. Time variation of the singular invariant $\Delta I_t \equiv I_f(t) - I_f(0)$ vs. L^{-2}.

ratio $\varepsilon/(|\mathbf{v}|\Delta k) = 10$. We have verified that the energy of the system is conserved up to 12 digits.

In Fig. 1 we plot the numerical results for the time variation of the singular invariant $\Delta I_t \equiv I_f(t) - I_f(0)$ for $f(\mathbf{v}) = v_x$ in Eq. **13** vs. L^{-2}. This figure corresponds to the case of the initial condition $(x, y; p_x, p_y) = (0.4, 1.41; -0.45, -1.40)$ and to time $t = 5.0$. For small volumes the error involved in the numerical simulations exceeds the theoretically predicted error $(\lambda V_0)^2 = 10^{-6}$. By increasing the volume, the numerical error due to the volume dependence decreases, and ΔI_t reaches the predicted order of magnitude. This result shows that the singular invariant is indeed an *asymptotic* invariant.

We have next numerically solved the Liouville equation for delocalized ensembles $g_0(\mathbf{v})$ and calculated the time evolution of the ensemble average of the singular invariant in Eq. **16** in the $(\mathbf{k}, \mathbf{v})$ representation. As the Liouville equation is a partial differential equation, the numerical integration is more difficult. In the numerical integration we have to deal with four-dimensional discretized variables (k_x, k_g, v_x, v_y), which requires a large memory.

In Fig. 2 we plot the time evolution of $\Delta[I_f]_t \equiv [I_f(t)]_g - [I_f(0)]_g$ in Eq. **16** for $f(\mathbf{v}) = v_x$ and for the delocalized distribution $g = g_0(\mathbf{u})$, given by

$$g_0(\mathbf{u}) = \left(\frac{\eta}{\pi}\right)^2 \frac{1}{(u_x - u_{x0})^2 + \eta^2} \frac{1}{(u_y - u_{y0})^2 + \eta^2}. \quad [20]$$

We chose the parameters, $\eta = 0.5$, $(u_{x0}, u_{y0}) = (0.5, 0.5)$, $\lambda V_0 = 0.1$ and the volume $L^2 = (37\pi)^2$. The time step of the integration is $\Delta t = 0.001$. The numerical simulations show that it changes linearly in time. As the ensemble theory predicts, the linear dependence starts at $t = 0$.

In Fig. 3 we plot the rate of change $\Delta[I_f]_t/\Delta t$ at the first step of the iteration of the numerical integration vs. L^{-2}. By increasing the volume size, the numerical value approaches

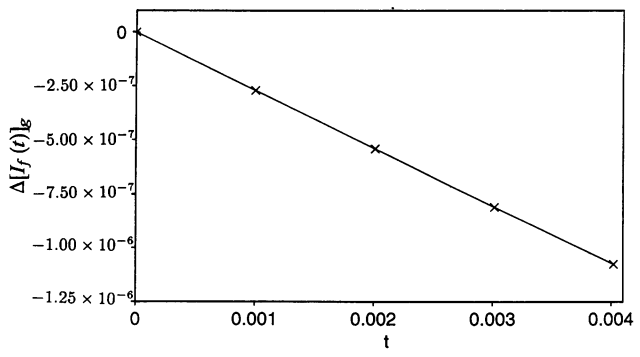

FIG. 2. Time evolution of $\Delta[I_f(t)]_g \equiv [I_f(t)]_g - [I_f(0)]_g$ in Eq. **16** for $f(\mathbf{v}) = v_x$ and the delocalized distribution (Eq. **20**).

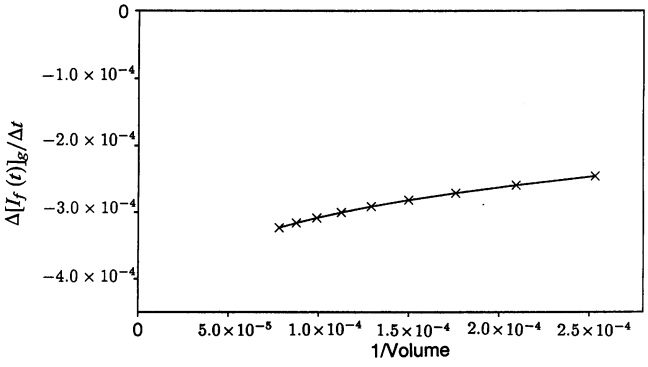

FIG. 3. Change of $\Delta[I_f(t)]_g/\Delta t$ at the first step of the iteration of the numerical integration vs. L^{-2}.

the limiting value $\approx -4.0 \times 10^{-4}$. The theoretical value of the rate of change can be estimated by the right-hand side of Eq. **18**, which gives the value $-(6.0 + 0.1) \times 10^{-4}$. Taking into account the discretization procedure, this agreement is quite satisfactory.

In conclusion these simulations prove the existence of diffusive effects in the frame of classical dynamics but which can only be observed in conjunction with delocalized ensembles.

Section 4. Complex Irreducible Spectral Representation

Our principal conclusion is that the Möller states $\Phi^{\pm}_{0,\mathbf{v}}$ are no more zero eigenstates of the Liouvillian for persistent scattering. We therefore must reconsider the eigenvalue problem

$$L_H|F(\alpha)\rangle = z_\alpha|F(\alpha)\rangle. \quad [21]$$

We sketch here only the main results; details will be forthcoming.

To solve the eigenvalue problem, let us first note the relation that can also be derived from Eq. **8**,

$$\langle\Phi_{0,\mathbf{u}}(z^*)|L_H|\Phi_{0,\mathbf{v}}(z)\rangle = \langle 0, \mathbf{u}|\mathrm{T}(z)|0, \mathbf{v}\rangle + \left\langle 0, \mathbf{u}|\mathrm{T}(z)\frac{z}{(z - L_0)^2}\mathrm{T}(z)|0, \mathbf{v}\right\rangle. \quad [22]$$

In the on-shell limit this gives (see Eq. **19**),

$$\lim_{z\to+i0} \langle\Phi_{0,\mathbf{u}}(z^*)|L_H|\Phi_{0,\mathbf{v}}(z)\rangle = \langle\Phi^-_{0,\mathbf{u}}|L_H|\Phi^+_{0,\mathbf{v}}\rangle = \langle 0, \mathbf{u}|\theta|0, \mathbf{v}\rangle. \quad [23]$$

This expression leads to a "similarity" relation between L_H and θ involving the transformation Λ,

$$\langle 0, \mathbf{u}|\Lambda^{-1}L_H\Lambda|0, \mathbf{v}\rangle = \langle 0, \mathbf{u}|\theta|0, \mathbf{v}\rangle. \quad [24]$$

Λ and its inverse operator connect the unperturbed states to the Möller states as $|\Phi^+_{0,\mathbf{v}}\rangle = \Lambda|0, \mathbf{v}\rangle$ and $\langle\Phi^-_{0,\mathbf{v}}| = \langle 0, \mathbf{v}|\Lambda^{-1}$, respectively. (To introduce Λ and the inverse operator Λ^{-1}, some care is required to deal with the resonance divergence, as well as the normalization of the Möller states.) The operator Λ is a *nonunitary* operator, as it transforms the hermitian operator L_H into the disipative operator θ, which has a complex spectrum. The nonunitarity comes from the same mechanism of the discontinuity at $\mathbf{l} = 0$ in Eq. **15** due to the resonance singularity. The relation (Eq. **24**) is in agreement with our previous approach through the subdynamics theory (2). The similitude between L_H and θ involving the nonunitary operator Λ expresses the relation between dynamics and probabilistic processes in a striking way.

We also have

$$L_H \Lambda|0, \mathbf{v}\rangle = \Lambda\theta|0, \mathbf{v}\rangle, \quad [25]$$

leading to the relation between the eigenstates $|f(\alpha)\rangle$ of the collision operator $\theta|f(\alpha)\rangle = z_\alpha|f(\alpha)\rangle$ and the eigenstates $|F(\alpha)\rangle$ of the Liouvillian (Eq. 21):

$$|f(\alpha)\rangle = \int d\mathbf{u}|0, \mathbf{u}\rangle F_0^d(\mathbf{u}; \alpha), \quad \text{and}$$

$$|F(\alpha)\rangle = \Lambda|f(\alpha)\rangle = \int d\mathbf{u}|\Phi_{0,\mathbf{u}}^+\rangle F_0^d(\mathbf{u}; \alpha), \quad [26]$$

where $F_0^d(\mathbf{u}; \alpha)$ satisfies the eigenvalue equation (with $\varepsilon_\alpha = z_\alpha\Omega$),

$$\int d\mathbf{u}\ \theta_{0,\mathbf{v};0,\mathbf{u}} F_0^d(\mathbf{u}; \alpha) = \xi_\alpha F_0^d(\mathbf{v}; \alpha). \quad [27]$$

[To obtain these relations, we have used the relation $\Lambda\theta = \Lambda \overset{(0)}{P}\theta$, where $\overset{(0)}{P} \equiv \Omega^{-1}\int d\mathbf{u}|0, \mathbf{u}\rangle\langle 0, \mathbf{u}|$ is a projection operator for the delocarized component, $(\overset{(0)}{P})^2 = \overset{(0)}{P}$, in the box normalization formalism.] As the collision operator $\theta_{0,\mathbf{v};0,\mathbf{u}}$ is well defined in the limit of large volumes, ξ_α and $F_0^d(\mathbf{v}; \alpha)$ are also well defined in this limit.

Since $|\Phi_{0,\mathbf{u}}^+\rangle$ have a delta function singularity, the eigenstates $|F(\alpha)\rangle$ also have a delta function singularity:

$$\langle \mathbf{k}, \mathbf{v}|F(\alpha)\rangle = F_0^d(\mathbf{v}; \alpha)\delta(\mathbf{k}) + F_{\mathbf{k}}^t(\mathbf{v}; \alpha). \quad [28]$$

Moreover, the nonsingular part $F_{\mathbf{k}}^t$ is a functional of the singular component F_0^d, as one can see from Eq. 26.

For weak-coupling interactions the eigenvalue problem (Eq. 27) of the collision operator reduces to the eigenvalue problem for the Fokker–Planck operator in Eq. 18. It is well know that the Fokker–Planck operator for central forces for three-dimensional case has the same structure as the orbital angular momentum operator in quantum mechanics (11). Therefore, the eigenstates of the Fokker–Planck operator are given in terms of the spherical harmonics $F_0^d(\mathbf{v}; \alpha) = \mathrm{w}^{-1}\delta(|\mathbf{v}| - \mathrm{w})Y_l^m(\theta, \phi)$ for $\alpha = (\mathrm{w}, l, m)$. The eigenvalues are then given by $\xi_\alpha = -i\lambda^2 A\mathrm{w}^{-3}l(l+1)$, where $A = 4\pi^5\int_0^\infty dq\, q^3|V_q|^2$. For $l = m = 0$, Eq. 26 leads to the microcanonical distribution for the equilibrium mode of the Liouvillian. We also see that the eigenstates of the Liouvillian break the time symmetry, as the nonvanishing eigenvalues are imaginary numbers. [The solution of our eigenvalue problem can also be tested by computer simulations. This has already been done for the quantum case which is numerically easier to handle (T.P., I.P., K. H. Wen, and Z. L. Zhang, unpublished data).]

For the class of delta singular functions the only possible invariant of the motion is the microcanonical distribution. All other invariants are destroyed due to the resonances. Therefore, potential scattering is *nonintegrable* in conjunction with persistent scattering.

As ξ_α is a well-defined finite number in the continuous limit $\Omega \to \infty$, the eigenvalue z_α is an infinitesimal quantity. We have verified the relation $z_\alpha = \Omega^{-1}\xi_\alpha$ by numerical simulation; the volume dependence corresponds to the fact that the system cannot reach equilibrium over a finite time scale because of a single scattering. We need repeated scattering. We have verified this statement for a simple model of a many-body system—i.e., the Lorentz gas. We then obtain a finite eigenvalue for the Liouvillian that is proportional to the concentration c of the scatterers (unpublished data).

Section 5. Concluding Remarks

For a long time, classical dynamics appeared a closed subject. This, however, is no more so when nonintegrable systems in the sense of Poincaré are considered. We can now go beyond Poincaré's negative statement (nonexistence of invariants analytic in the coupling constant) for classes of dynamical systems, such as LPS. For these systems, we have constructed singular Poincaré invariants (which are analytic in the coupling constant but involve distributions). They are however only *asymptotic* invariants. In conjunction with delocalized distributions they decay according to diffusive modes. That shows that there exist *nonlocal* effects in classical mechanics which can only be described on the level of *ensembles*. These effects can be studied by computer simulations. They show that a more general formulation of classical mechanics is needed when dealing with LPS. This signals the appearance of another form of chaos as we have to go beyond the trajectory description.

For persistent scattering that corresponds already to a LPS, there appear specific singularities in the distribution functions (see Eq. 2). The appearance of such singularities is quite general. They appear as well in quantum theory and in statistical mechanics, where they lead to the existence of reduced distribution functions in the thermodynamic limit (9). For this type of distribution functions we must consider other solutions of the Liouville equation that are not reducible to trajectory dynamics (or to wave functions in quantum mechanics). For this class of situations we obtain a unified formulation of laws of physics that is intrinsically statistical and irreversible. In contrast to the traditional perspective, the laws of physics express "possibilities," rather than "certitudes."

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