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# Geometric magnetism in classical transport theory

Jochen Rau
*Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany*

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The effective dynamics of a slow classical system coupled to a fast chaotic environment is described by means of a master equation. We show how this approach permits a very simple derivation of geometric magnetism. [S1063-651X(97)50108-5]

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## I. INTRODUCTION

Consider a slow classical system $S$ coupled, through its position, to a fast classical system $F$. If the fast motion is chaotic, then $F$ effectively acts as an ''environment'' [1] that induces friction [2,3] and also exerts other, nondissipative reaction forces on the slow system $S$. As for the nondissipative reaction, in the simplest ''adiabatic averaging'' approximation [4], the classical analog of the Born-Oppenheimer approximation [5], the fast motion's energy at given values of the slow coordinates serves as an external potential for the slow system; its gradient yields the ''Born-Oppenheimer force.'' In the next approximation beyond this, there is a velocity-dependent correction which has the form of a magnetic force, and for which Berry and Robbins coined the name ''geometric magnetism'' [6].

For the situation considered here, namely, a fast chaotic classical environment, there are so far two alternative derivations of geometric magnetism, both due to Berry and Robbins: (i) by taking the nonvanishing classical limit of the corresponding quantum result [7], where the appearance of geometric magnetism can be linked to the geometric phase [8] (whence its name); or (ii) in a purely classical context, by expanding the equation of motion for $S$ around the Born-Oppenheimer limit in powers of the fast-to-slow time scale ratio and identifying the first-order correction [6]. The multiple-time-scale analysis [9] used in the latter derivation appears somewhat reminiscent of the old Chapman-Enskog method to derive transport equations [10]. This is not a coincidence: After all, it should be possible to describe the evolution of any subsystem (here: $S$) coupled to an environment (here: $F$) by means of a transport (''master'') equation; and, to be consistent, such a master equation should feature a term representing geometric magnetism. It is the purpose of the present paper to show how, indeed, geometric magnetism arises naturally in a classical master equation for $S$. The derivation of geometric magnetism within this transport theory framework will turn out to be surprisingly simple.

The paper is organized as follows. First I will sketch very briefly how one obtains transport equations by means of the Nakajima-Zwanzig projection technique [11–14] (Sec. II); for more details the reader is referred to textbooks [15] and a recent review [16]. Then this projection technique is applied to the situation at hand, namely, a slow system $S$ coupled to a fast chaotic environment $F$, both taken to be classical (Sec. III). The resulting master equation for $S$ is generally non-Markovian, yet the separation of time scales and chaoticity of the fast motion permit us to take the Markovian limit. Along with the Born-Oppenheimer force, geometric magnetism then appears in a straightforward manner in the nondissipative part of the effective slow dynamics. Finally, I shall conclude with a brief summary and several additional remarks (Sec. IV).

## II. TRANSPORT EQUATIONS

A powerful tool for the derivation of transport equations is the Nakajima-Zwanzig projection technique [11–16]. Its main strength lies in the fact that by mapping the influence of irrelevant degrees of freedom onto, among other features, a nonlocal behavior in time, it opens the way to the systematic exploitation of separated time scales and hence serves as a good starting point for powerful approximations such as the Markovian and quasistationary limits; furthermore, it permits one to discern easily the dissipative and nondissipative parts of the effective dynamics.

When studying the dynamics of a complex system away from equilibrium one typically monitors the evolution of the expectation values

$$g_a(t) := (\rho(t)|G_a) \tag{1}$$

of only a very small set of selected (''relevant'') observables $\{G_a\}$, which change according to

$$\dot{g}_a(t) = i(\rho(t)|\mathcal{L}G_a). \tag{2}$$

Here the meanings of $\rho(t)$, $G_a$, and the inner product $(\,|\,)$, as well as of another scalar product $\langle ; \rangle_\rho$ which we shall use later, depend on whether the system under consideration is quantum or classical; they are summarized in Table I. The ''Liouvillian'' $\mathcal{L}$ takes the commutator with the Hamilton operator $\hat{H}$,

$$i\mathcal{L} = (i/\hbar)[\hat{H}, *], \tag{3}$$

for a quantum system, or generates a Lie dragging in the direction of the Hamiltonian vector $X_H$,

$$i\mathcal{L} = \pounds_{X_H}, \tag{4}$$

for a classical system [17], respectively. For simplicity we assume that the Hamiltonian and hence the Liouvillian, as well as the relevant observables, are not explicitly time dependent.

 

TABLE I. Various symbols used in transport theory.

| Generic symbol | Quantum | Classical |
|---|---|---|
| state $\rho$ | statistical op. $\hat{\rho}$ | phase space dist. $\rho(\pi)$ |
| observable $G_a$ | Hermitian op. $\hat{G}_a$ | real function $G_a(\pi)$ |
| $(A\|B)$ | $\mathrm{tr}(\hat{A}^\dagger \hat{B})$ | $\int d\pi A^*(\pi)B(\pi)$ |
| $\langle \mathbf{A};\mathbf{B}\rangle_\rho$ | $\int_0^1 d\mu\ \mathrm{tr}[\hat{\rho}^\mu \hat{A}^\dagger \hat{\rho}^{1-\mu}\hat{B}]$ | $\int d\pi \rho(\pi)A^*(\pi)B(\pi)$ |

The right-hand side of the equation of motion (2) will generally depend not just on the selected, but also on all other (''irrelevant'') degrees of freedom. In order to eliminate these and hence obtain a closed ''transport equation'' for the $\{g_a(t)\}$, one employs a suitable projection operator which projects arbitrary observables onto the subspace spanned by 1 and the relevant observables $\{G_a\}$. The projector may depend on the current expectation values of the relevant observables and thus vary in time, $\mathcal{P}(t)\equiv\mathcal{P}[g_a(t)]$, and is assumed to have the three properties: (i) $\mathcal{P}(t)^2=\mathcal{P}(t)$, (ii) $\mathcal{P}(t)A=A$ if and only if $A\in\mathrm{span}\{1,G_a\}$, and (iii)

$$(\rho(t)|[d\mathcal{P}(t)/dt]A)=0 \quad \forall \rho(t),A\,. \tag{5}$$

Its complement is denoted by $\mathcal{Q}(t):=1-\mathcal{P}(t)$. One further defines an operator $\mathcal{T}(t',t)$ (again in the space of observables) by

$$(\partial/\partial t')\mathcal{T}(t',t)=-i\mathcal{Q}(t')\mathcal{L}\mathcal{Q}(t')\mathcal{T}(t',t) \tag{6}$$

and the initial condition $\mathcal{T}(t,t)=1$, which may be pictured as describing the evolution of the system's *irrelevant* degrees of freedom. The equation of motion for the selected expectation values $\{g_a(t)\}$ can then be cast into the (still exact) form

$$\begin{aligned}\dot{g}_a(t)=&\,i(\rho(t)|\mathcal{P}(t)\mathcal{L}G_a)\\&-\int_0^t dt'(\rho(t')|\mathcal{P}(t')\mathcal{L}\mathcal{Q}(t')\mathcal{T}(t',t)\mathcal{Q}(t)\mathcal{L}G_a)\\&+i(\rho(0)|\mathcal{Q}(0)\mathcal{T}(0,t)\mathcal{Q}(t)\mathcal{L}G_a),\end{aligned} \tag{7}$$

for any time $t\geqslant 0$. This constitutes the desired closed system of (possibly nonlinear) coupled integro-differential equations for the selected expectation values $\{g_a(t)\}$, provided $(\rho(0)|\mathcal{Q}(0)$ and with it the last (''residual force'') term vanishes.

In many practical applications the initial state $\rho(0)$ is not known exactly but characterized solely by the initial expectation values $\{g_a(0)\}$ of the relevant observables. From this insufficient information one generally constructs that distribution which maximizes the entropy $S[\rho]:=-k(\rho|\ln\rho)$ and hence can be considered ''least biased'' or ''maximally noncommittal'' with regard to the unmonitored degrees of freedom: It is the generalized canonical state

$$\rho(0)=Z(0)^{-1}\exp[-\lambda^a(0)G_a]\,, \tag{8}$$

with summation over $a$ implied (Einstein convention), partition function

$$Z(0):=(1|\exp[-\lambda^a(0)G_a]) \tag{9}$$

and the Lagrange parameters $\{\lambda^a(0)\}$ adjusted such as to yield the correct $\{g_a(0)\}$.

In an analogous fashion one defines a ''relevant part''

$$\rho_{\mathrm{rel}}(t):=Z(t)^{-1}\exp[-\lambda^a(t)G_a] \tag{10}$$

of the exact state $\rho(t)$ at *all* times $t$, where $\rho_{\mathrm{rel}}(0)=\rho(0)$ but generally $\rho_{\mathrm{rel}}(t)\neq\rho(t)$ for $t>0$. There exists a unique time-dependent projector $\mathcal{P}_{\mathrm{R}}(t)$, namely, the projector orthogonal with respect to the time-dependent scalar product $\langle;\rangle_{\rho_{\mathrm{rel}}(t)}$, which has all required properties (i)–(iii) and, moreover, yields

$$(\rho(t)|\mathcal{P}_{\mathrm{R}}(t)=(\rho_{\mathrm{rel}}(t)| \tag{11}$$

at all times. This special choice, originally proposed by Robertson [14,18], has the important advantage that for initial states of the form (8) it ensures $(\rho(0)|\mathcal{Q}_{\mathrm{R}}(0)=0$ and so renders the transport equation (7) closed. We shall use the Robertson projector throughout the remainder of the paper (and, for brevity, immediately drop the subscript $R$).

One principal feature of the transport equation (7) is that it is non-Markovian: Future expectation values of the selected observables are predicted on the basis of both their present values and their past history. There are two distinct time scales: (i) the scale $\tau_{\mathrm{rel}}$—or several scales $\{\tau^i_{\mathrm{rel}}\}$—on which the selected expectation values $\{g_a(t)\}$ evolve; and (ii) the ''memory time'' $\tau_{\mathrm{mem}}$ which characterizes the length of the time interval that contributes significantly to the memory integral. Only if this memory time is small compared to the typical time scale on which the selected observables evolve, $\tau_{\mathrm{mem}}\ll\tau_{\mathrm{rel}}$, can memory effects be neglected and predictions for the selected observables be based solely on their present values. One may then assume that in the memory term $g_a(t')\approx g_a(t)$ and hence replace

$$\begin{aligned}&\mathcal{P}[g_a(t')]\to\mathcal{P}[g_a(t)],\quad (\rho(t')|\mathcal{P}(t')\to(\rho(t)|\mathcal{P}(t),\\&\mathcal{T}(t',t)\to\exp[i(t-t')\mathcal{Q}(t)\mathcal{L}\mathcal{Q}(t)]\end{aligned} \tag{12}$$

(Markovian limit). Furthermore, at times $t\gg\tau_{\mathrm{mem}}$ it no longer matters for the dynamics when exactly the evolution started, and hence in Eq. (7) the integration over the system's history may just as well extend from $-\infty$ to $t$, rather than from 0 to $t$ (quasistationary limit) [19].

In the Markovian and quasistationary limits the equation of motion simplifies to

$$\begin{aligned}\dot{g}_a(t)=&\,i(\rho(t)|\mathcal{L}_{\mathrm{rel}}(t)G_a)\\&-\pi(\rho(t)|\mathcal{P}(t)\mathcal{L}\mathcal{Q}(t)\delta(\mathcal{Q}(t)\mathcal{L}\mathcal{Q}(t))\mathcal{Q}(t)\mathcal{L}G_a)\end{aligned} \tag{13}$$

modulo residual force, where

$$\begin{aligned}\mathcal{L}_{\mathrm{rel}}(t)=&\,\mathcal{P}(t)\mathcal{L}\mathcal{P}(t)+\frac{i}{2}\int_0^\infty d\tau\mathcal{P}(t)\mathcal{L}[\mathcal{L}(t;\tau)\\&-\mathcal{L}(t;-\tau)]\mathcal{P}(t)\end{aligned} \tag{14}$$

with

$$\mathcal{L}(t;\tau):=\exp[i\tau\mathcal{Q}(t)\mathcal{L}\mathcal{Q}(t)]\mathcal{L} \tag{15}$$

denotes a (possibly time-dependent) effective Liouvillian for the relevant observables. Provided the evolution operator $\mathcal{T}$ is unitary with respect to the scalar product $\langle;\rangle_{\rho_{\rm rel}(t)}$ then the first term in the Markovian transport equation (13) is nondissipative. In this case dissipation stems entirely from the second term, which yields a non-negative entropy growth rate

$$\dot{S}[\rho_{\rm rel}(t)]=k\lambda^a(t)\dot{g}_a(t)$$
$$=k\pi\langle\mathcal{QL}\lambda^b G_b;\delta(\mathcal{QLQ})\mathcal{QL}\lambda^a G_a\rangle_{\rho_{\rm rel}}\geqslant 0 \tag{16}$$

($H$ theorem).

## III. EFFECTIVE FORCE CAUSED BY A FAST CHAOTIC ENVIRONMENT

We now apply the above general results to a slow system $S$ coupled to a fast chaotic, but not necessarily macroscopic, environment $F$. Both $S$ and $F$ are treated classically, and their state is described in a phase space with canonical coordinates $Z=\{\mathbf{Q},\mathbf{P}\}$ pertaining to $S$ and $z=\{\mathbf{q},\mathbf{p}\}$ pertaining to $F$, respectively. The full Hamilton function for the combined system $S\times F$ is taken to be of the form

$$H(Z,z)=H_{\rm S}(Z)+h(\mathbf{Q},z), \tag{17}$$

where $H_{\rm S}$ governs the free dynamics of the system $S$ and $h$ describes both the coupling (through the slow position $\mathbf{Q}$) of $S$ to the environment and the internal dynamics of the latter. Associated with the Hamilton function is a Liouvillian (4) which we decompose,

$$\pounds_{X_H}=\pounds_{X_{H,Z}}+\pounds_{X_{H,z}}, \tag{18}$$

into a part dragging along the slow coordinates,

$$X_{H,Z}=\sum_i [V^i(\partial/\partial Q^i)-(\partial_i H_S+\partial_i h)(\partial/\partial P_i)] \tag{19}$$

with slow velocity $V^i=\partial H_S/\partial P_i$ and $\partial_i:=\partial/\partial Q^i$, and a part dragging along the fast coordinates,

$$X_{H,z}=\sum_k\left(\frac{\partial h}{\partial p_k}\frac{\partial}{\partial q^k}-\frac{\partial h}{\partial q^k}\frac{\partial}{\partial p_k}\right). \tag{20}$$

At $t=0$ and hence, due to energy conservation, at all times the combined system $S\times F$ is assumed to have a sharp total energy $E$. For the purposes of the Nakajima-Zwanzig projection technique all observables pertaining to $S$, as well as the total energy which is a constant of the motion, are taken to be relevant; while the internal degrees of freedom of the environment and system-environment correlations are deemed irrelevant. This gives rise to a time-independent representation of the Robertson projector,

$$\mathcal{P}A=\frac{1}{\partial_E\Omega}\int dz\,\delta(H-E)A=:\langle A\rangle_E \tag{21}$$

for any observable $A$. Here $\partial_E:=\partial/\partial E$ and

$$\Omega:=\int dz\,\theta(H-E); \tag{22}$$

its derivative $\partial_E\Omega$ may be interpreted as the surface of the microcanonical energy shell.

The slow system's effective dynamics must be described with a transport equation of the form (7), which in general is non-Markovian and includes a residual force. Only if we take the initial state of the environment to be microcanonical, i.e.,

$$\rho(0)=\rho_S(0)\times(1/\partial_E\Omega)\,\delta(H-E), \tag{23}$$

where $\rho_S(0)$ denotes the (arbitrary) initial state of $S$, then the residual force term vanishes [20]. This assumption of a microcanonical distribution and the resultant omission of the residual force term amount to averaging over an entire ensemble of fast chaotic systems. However, even if the slow system is coupled to a single fast chaotic system the transport equation without residual force will describe the main global feature of the slow dynamics; the residual force causes only fluctuations around the average trajectory [21].

The separation of time scales and chaoticity of the fast motion permit us to take the Markovian and quasistationary limits. Moreover, we focus on the nondissipative part of the slow dynamics. The latter is governed by the effective Liouvillian (14), which immediately yields the (Heisenberg-picture) equation of motion

$$\dot{G}=\langle\pounds_{X_{H,Z}}G\rangle_E+\frac{1}{2}\int_0^\infty d\tau\langle\pounds_{X_{H,Z}}[\pounds_{X_{H,Z}(\tau)}-\pounds_{X_{H,Z}(-\tau)}]G\rangle_E \tag{24}$$

for an arbitrary slow observable $G(Z)$ [22]. Here we have used $\pounds_{X_{H,z}}\mathcal{P}=\mathcal{P}\pounds_{X_{H,z}}=0$ to replace $\pounds_{X_H}$ by $\pounds_{X_{H,Z}}$, and defined the "rotated" Hamiltonian vector $X_{H,Z}(\tau)$ as in Eq. (19) but with components dragged along the fast coordinates,

$$\partial_i h\rightarrow(\partial_i h)_\tau:=\exp[\tau\pounds_{X_{H,z}}](\partial_i h). \tag{25}$$

Upon choosing $G=\mathbf{P}$ we obtain an effective force, with components

$$\dot{P}_i=-\langle\partial_i H\rangle_E-\frac{1}{2}\sum_j V^j\int_0^\infty d\tau\langle\partial_j[(\partial_i h)_\tau-(\partial_i h)_{-\tau}]\rangle_E$$
$$=F_i^{\rm BO}+F_i^{\rm geo}. \tag{26}$$

The first term constitutes the usual Born-Oppenheimer force; while the second (integral) term gives rise to geometric magnetism: For an arbitrary function $A(Z,z)$ it is

$$\langle\partial_j A\rangle_E=\partial_j\langle A\rangle_E+\langle\partial_j H\rangle_E\partial_E\langle A\rangle_E$$
$$+(1/\partial_E\Omega)\partial_E[\partial_E\Omega\langle A\tilde{\partial}_j H\rangle_E], \tag{27}$$

where $\tilde{\partial}_j H:=\partial_j H-\langle\partial_j H\rangle_E$. This identity, together with $\tilde{\partial}_j H=\tilde{\partial}_j h$,

$$\langle(\partial_i h)_\tau\rangle_E=\langle(\partial_i h)_{-\tau}\rangle_E \tag{28}$$

and

$$\langle(\tilde{\partial}_i h)_{-\tau}\tilde{\partial}_j h\rangle_E=\langle(\tilde{\partial}_j h)_\tau\tilde{\partial}_i h\rangle_E, \tag{29}$$

yields

$$F_i^{\mathrm{geo}}=\sum_j B_{ij}V^j \tag{30}$$

with an antisymmetric matrix (''magnetic field'')

$$B_{ij}=-\frac{1}{2\partial_E\Omega}\partial_E\left[\partial_E\Omega\int_0^\infty d\tau\langle(\tilde{\partial}_i h)_\tau\tilde{\partial}_j h-(\tilde{\partial}_j h)_\tau\tilde{\partial}_i h\rangle_E\right] \tag{31}$$

in agreement with the result by Berry and Robbins [6,7].

## IV. CONCLUSION

We have succeeded in deriving geometric magnetism within the framework of classical transport theory: Starting from the general formula (14) for the effective Liouvillian, the derivation turned out to be surprisingly simple. This means that treating the fast chaotic system as an ''environment'' for the slow system and describing the dynamics of the latter with a master equation is a consistent and useful physical picture. More generally, it shows that methods from transport theory are not limited to the description of macroscopic systems but apply as well to low-dimensional chaos.

As a by-product we have obtained the nondissipative equation of motion (24) for arbitrary slow observables, which is coordinate-free and applies to any form of the microscopic Hamilton function: It could serve as the starting point for interesting generalizations of the model Hamiltonian considered here. Higher-order corrections to the Born-Oppenheimer force and geometric magnetism will presumably have to take into account memory effects; an example for this is Jarzynski's force [23]. Here, too, transport theory with its non-Markovian evolution equation (7) will furnish a good starting point for the systematic study of non-Markovian corrections.

Finally, transport theory adds a somewhat new perspective to Berry and Robbins' observation that geometric magnetism is the ''antisymmetric cousin of friction'' [6]. In our formulation the memory term in Eq. (7) gives rise, upon taking the Markovian and quasistationary limits, to both dissipative and nondissipative parts of the dynamics; they appear as the parts symmetrized and antisymmetrized, respectively, with respect to the history integration variable $\tau=(t-t')$. When evaluated for our model Hamiltonian and the special choice $G=\mathbf{P}$ these two parts translate into effective forces proportional to the slow velocity, one with a symmetric matrix of coefficients (friction: not considered in this paper), the other with an antisymmetric matrix [geometric magnetism: Eq. (31)].

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