Geometric magnetism in classical transport theory

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I. INTRODUCTION

Consider a slow classical system $S$ coupled to a fast chaotic environment $F$. If the fast motion is chaotic then $F$ effectively acts as an “environment” which induces friction and also exerts other, non-dissipative reaction forces on the slow system $S$. As for the non-dissipative reaction, in the simplest “adiabatic averaging” approximation—the classical analogue of the Born-Oppenheimer approximation—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”.

For the situation considered here, namely a fast chaotic environment, there are so far two alternative derivations of geometric magnetism, both due to Berry and Robbins: (i) by taking the (non-vanishing) classical limit of the corresponding quantum result, where the appearance of geometric magnetism can be linked to the geometric phase (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/slow time scale ratio, and identifying the first-order correction.

The multiple-time-scale analysis used in the classical derivation of geometric magnetism appears somewhat reminiscent of the old Chapman-Enskog method to derive transport equations. This is not a mere 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

II. TRANSPORT EQUATIONS

A powerful tool for the derivation of transport equations is the Nakajima-Zwanzig projection technique. Its main strength lies in the fact that by mapping the influence of irrelevant degrees of freedom onto—among other features—a non-local 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 non-dissipative 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

$$g_a(t) := \langle \rho(t) | G_a \rangle$$  \hspace{1cm} (1)

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

$$g_a(t) = i (\rho(t) | \mathcal{L} G_a \rangle \hspace{1cm} (2)$$

Here the meanings of $\rho(t)$, $G_a$ and $(\cdot | (\cdot)$, as well as of the scalar product $(\cdot | (\cdot)_\rho$ 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 $\hat{H}$,

$$i \mathcal{L} = (i/\hbar) [\hat{H}, (\cdot) | (\cdot)$$  \hspace{1cm} (3)

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

$$i\mathcal{L} = \mathcal{L}_{X_H},$$

(4)

for a classical system \cite{17}, respectively. For simplicity we assume that the Hamiltonian and hence the Liouvil-
lian, as well as the relevant observables, are not explicitly
time-dependent.

The right-hand side of the equation of motion (8) 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 closed 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, $P(t) = P[g_a(t)]$, and is assumed to have the three
properties (i) $P(t)^2 = P(t)$; (ii) $P(t)A = A$ if and only if
$A \in \text{span}\{1, G_a\}$; and (iii):

$$\left(\rho(t) \frac{dP(t)}{dt} A\right) = 0 \quad \forall \rho(t), A.$$

(5)

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

$$\frac{\partial}{\partial t'} T(t', t) = -iQ(t')LQ(t')T(t', t)$$

(6)

with initial condition $T(t, t) = 1$, 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

$$\dot{g}_a(t) = i(\rho(t)|P(t)LG_a)$$

\begin{equation}
- \int dt' (\rho(t')|P(t')LQ(t')T(t', t)Q(t)LG_a) + i(\rho(0)|Q(0)T(0, t)Q(t)LG_a),
\end{equation}

(7)

for any time $t \geq 0$. This constitutes the desired closed system of (possibly nonlinear) coupled integro-
differential equations for the selected expectation values $\{g_a(t)\}$ if and only if $\rho(0)|Q(0)$ 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 non-committal” with regard to the
unmonitored degrees of freedom: It is the generalized
canonical state

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

(8)

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

$$Z(0) := \langle 1|\exp[-\lambda^a(0)G_a]\rangle$$

(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”

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

(10)

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

$$(\rho(t)|P_R(t) = (\rho_{\text{rel}}(t))$$

(11)

at all times. This special choice, originally proposed by
Robertson \cite{14,18}, has the important advantage that for
initial states of the form (8) it ensures $\langle \rho(0)|Q_R(0) = 0$
and so renders the transport equation (8) closed. We
shall use the Robertson projector throughout the remain-
der of the paper (and, for brevity, immediately drop the
subscript ‘R’).

One principal feature of the transport equation (8) 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 $\tau_{\text{rel}}$ –or several scales
$\{\tau_{rel}^k\}$– on which the selected expectation values $\{g_a(t)\}$
evolve; and (ii) the “memory time” $\tau_{\text{mem}}$ which char-
acterizes 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, $\tau_{\text{mem}} \ll \tau_{\text{rel}}$, can mem-
ory 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

$$P[g_a(t')] \rightarrow P[g_a(t)]$$

$$\langle \rho(t')|P(t') \rightarrow (\rho(t)|P(t)$$

$$T(t', t) \rightarrow \exp[iQ(t)LQ(t)\cdot(t-t')]$$

(12)

(Markovian limit). Furthermore, at times $t \gg \tau_{\text{mem}}$ it no
longer matters for the dynamics when exactly the evolution
started, and hence in Eq. (8) the integration over the system’s history may just as well extend from $-\infty$ to $t$, rather than from 0 to $t$ (quasistationary limit) \cite{19}. In the Markovian and quasistationary limits the equation of motion simplifies to

$$\dot{g}_a(t) = i(\rho(t)|L_{\text{rel}}(t)G_a)$$

\begin{equation}
- \pi(\rho(t)|P(t)LQ(t)\delta(Q(t)LQ(t))Q(t)LG_a)
\end{equation}

(13)

modulo residual force, where
\[ \mathcal{L}_{\text{rel}}(t) = \mathcal{P}(t) \mathcal{L} \mathcal{P}(t) \]
\[ + \frac{i}{2} \int_0^\infty d\tau \mathcal{P}(t) \mathcal{L}(t; \tau) - \mathcal{L}(t; -\tau) ] \mathcal{P}(t) \]  

with

\[ \mathcal{L}(t; \tau) := \exp[\mathcal{L}(t)\Delta(t)\tau] \mathcal{L} \]

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 \( \langle \cdot \rangle_{\mathcal{P}(t)} \), then the first term in the Markovian transport equation (13) is non-dissipative. In this case dissipation stems entirely from the second term, which yields a non-negative entropy growth rate

\[ \dot{S}[\rho_{\text{rel}}(t)] = k \chi^a(t) \dot{g}_a(t) \]
\[ = k \pi(\mathcal{Q}\mathcal{L}\lambda^0 \mathcal{G}_0; \delta(\mathcal{Q}\mathcal{L}\mathcal{Q}) \mathcal{Q}\mathcal{L} \lambda^0 \mathcal{G}_0)_{\rho_{\text{rel}}} \geq 0 \]  

(\( H \)-theorem).

### III. EFFECTIVE 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 described in a phase space with canonical coordinates \( Z = \{Q, P\} \) pertaining to \( S \) and \( z = \{q, p\} \) pertaining to \( F \), respectively. The full Hamiltonian function for the combined system \( S \times F \) is taken to be of the form

\[ H(Z, z) = H_S(Z) + h(Q, z) \],

where \( H_S \) governs the free dynamics of the system \( S \), and \( h \) describes both the coupling through the slow position \( Q \) of \( S \) to the environment and the internal dynamics of the latter. Associated with the Hamilton function is a Liouvillian (14) which we decompose

\[ \mathcal{L}_S = \mathcal{L}_{S \times F} + \mathcal{L}_{S \times z} \]

into a part dragging along the slow coordinates,

\[ X_{S, Z} = \sum_i \left( V^i \frac{\partial}{\partial Q^i} - (\partial_i H_S + \partial_i h) \frac{\partial}{\partial P^i} \right) \]

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,

\[ X_{S, z} = \sum_k \left( \frac{\partial h}{\partial P_k} \frac{\partial}{\partial q^k} - \frac{\partial h}{\partial q^k} \frac{\partial}{\partial P_k} \right) \].

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,

\[ \mathcal{P}A = \frac{1}{\partial E} \int dz \delta(H - E) A \]
\[ =: \langle A \rangle_E \]  

for any observable \( A \). Here \( \partial E := \partial / \partial E \) and

\[ \Omega := \int dz \theta(H - E) \]

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 (16), 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.,

\[ \rho(0) = \rho_S(0) \times \frac{1}{\partial E} \delta(H - E) \]

where \( \rho_S(0) \) denotes the (arbitrary) initial state of \( S \), then the residual force term vanishes (22). 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 (22).

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

\[ \dot{G} = \langle \mathcal{L}_{S \times z} G \rangle_E \]
\[ + 1 \int_0^t d\tau \langle \mathcal{L}_{S \times z} \mathcal{L}_{S \times z} \rangle \mathcal{L}_{S \times z} G \]  

for an arbitrary slow observable \( G(Z) \). Here we have used \( \mathcal{L}_{S \times z} \mathcal{P} \mathcal{L}_{S \times z} = 0 \) to replace \( \mathcal{L}_{S \times z} \) by \( \mathcal{L}_{S \times z} \), and defined the “rotated” Hamiltonian vector \( X_{S, Z}(t) \) as in (20) but with components dragged along the fast coordinates:

\[ \partial_i h \rightarrow (\partial_i h)_z := \exp[\tau \mathcal{L}_{S \times z}] (\partial_i h) \].

Upon choosing \( G = P \) we obtain an effective force, with components
\[ \dot{P}_i = -\langle \partial_i H \rangle_E - \frac{1}{2} \sum_j V^j \int_0^\infty \! dt \, \langle \partial_j [(\partial_i h)_r - (\partial_i h)_{-r}] \rangle_E \]
\[ = F_i^{BO} + F_i^{geo} . \]  

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
\[ \langle \partial_j A \rangle_E = \partial_j \langle A \rangle_E + \langle \partial_j H \rangle_E \partial_E \langle A \rangle_E \]
\[ + \frac{1}{\partial E \Omega} \partial_E \left[ \partial_E \Omega \cdot \langle A \partial_j H \rangle_E \right] , \]

where \( \partial_j H := \partial_j H - \langle \partial_j H \rangle_E \). This identity, together with \( \partial_j H = \tilde{\partial}_j h \)
\[ \langle (\tilde{\partial}_j h)_r \rangle_E = \langle (\tilde{\partial}_j h)_{-r} \rangle_E \]

and
\[ \langle (\tilde{\partial}_j h)_{-r} \tilde{\partial}_j h \rangle_E = \langle (\tilde{\partial}_j h)_r \tilde{\partial}_j h \rangle_E , \]

yields
\[ F_i^{geo} = \sum_j B_{ij} V^j \]

with an antisymmetric matrix (“magnetic field”)
\[ B_{ij} = -\frac{1}{2} \partial E \Omega \left[ \partial E \Omega \int_0^\infty \! dt \langle (\tilde{\partial}_j h)_r \tilde{\partial}_j h - (\tilde{\partial}_j h)_r \tilde{\partial}_j h \rangle_E \right] , \]

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

IV. CONCLUSION

We have succeeded in deriving geometric magnetism within the framework of classical transport theory: Starting from the general formula (23), 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 an equation of motion for arbitrary slow observables (Eq. (24)) 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 [24]. Here, too, transport theory with its non-Markovian evolution equation (17) 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” [4]. In our formulation the memory term in Eq. (6) gives rise, upon taking the Markovian and quasistationary limits, to both dissipative and non-dissipative parts of the dynamics; they appear as the parts symmetrized and antisymmetrized, resp., with respect to the history integration variable \( \tau = (t - t') \). When evaluated for our model Hamiltonian and the special choice \( G = P \) 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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sometimes also called Kawasaki-Gunton projector; cf. K. Kawasaki and J. D. Gunton, Phys. Rev. A 8, 2048 (1973).

[19] The quasistationary limit is not justified if the system exhibits a finite recurrence time \( \tau_{\text{rec}} \), as is the case for a finite quantum system with discrete spectrum. The history integration in Eq. (6) must then remain limited to a time interval much shorter than \( \tau_{\text{rec}} \), and the resultant transport equation will only be valid at intermediate times \( \tau_{\text{mem}} \ll t \ll \tau_{\text{rec}} \). Taking the quasistationary limit would lead to paradoxical results such as the disappearance of friction upon quantization of a finite system. For a discussion of this apparent “quantum/classical discordance” and a consideration of the time scales involved, see Ref. [6].

[20] The residual force should not be confused with the stochastic force that enters into the fluctuation-dissipation theorem [3], so a vanishing residual force does not imply that there is no friction. Friction stems from the second term in Eq. (13).

[21] That geometric magnetism (which will eventually emerge from our transport equation) captures the main global feature of the slow dynamics even if coupled to a single fast chaotic system has been illustrated with examples in M. V. Berry and E. C. Sinclair, J. Phys. A 30, 2853 (1997).

[22] The effective dynamics need not necessarily be hamiltonian: There need not exist \( H_{\text{rel}} \) such that \( i\mathcal{L}_{\text{rel}} = \mathcal{L}_{\mathcal{H}_{\text{rel}}} \).

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| TABLE I. Various symbols used in transport theory |
|----------------------------------------|----------------|----------------|
| **generic symbol** | **quantum** | **classical** |
| state \( \rho \) | statistical op. \( \hat{\rho} \) | phase space dist. \( \rho(\pi) \) |
| observable \( G_\alpha \) | Hermitian op. \( \hat{G}_\alpha \) | real function \( G_\alpha(\pi) \) |
| \( \langle A; B \rangle \) | \( \text{tr}(\hat{A}^\dagger \hat{B}) \) | \( \int d\pi A^*(\pi)B(\pi) \) |
| \( \langle A; B \rangle_\rho \) | \( \int_0^\rho d\mu \text{tr}[\hat{\rho}^\mu \hat{A}^\dagger \hat{B}^{1-\mu}] \) | \( \int d\tau \rho(\pi)A^*(\pi)B(\pi) \) |