

Memory Matrix Formalism for Parity-violating Transport

Xiaodong Hu*

Department of Physics, Boston College

(Dated: September 4, 2020)

We review the memory matrix formalism with the example of parity-preserving transport, then switching to the parity-violating case (time-reversal symmetry is preserved) where anomalous Hall effect is expected to emerge. Such terms have already been revealed from pure hydrodynamic analysis in high energy physics. As another independent tool, memory matrix formalism is believed to provide the same result for the overlapping regime with hydrodynamics. In this letter, we will show the accordance of them.

流成笔下春风瓣，吹散弦上秋草声。

—— 雨楼清歌「一瓣河川」

Contents

I. Memory Matrix Formalism	1
A. Basic Properties of Kubo Pair	1
B. Memory Matrix Theory	2
C. Momentum Relaxation and Drude Formula	4
D. Magnetotransport	5
II. Parity-violating Transport	5
References	5

I. MEMORY MATRIX FORMALISM

A. Basic Properties of Kubo Pair

Definition 1. (Kubo Pair) The *Kubo pair*, or *canonical correlation function* [1] of two operators A and B is defined as (with $k_B = \hbar \equiv 1$)

$$C_{AB} := \frac{1}{\beta} \int_0^\beta d\lambda \langle A^\dagger(t) B(i\lambda) \rangle_T \equiv T \int_0^{1/T} d\lambda \langle A e^{-iLt} B(i\lambda) \rangle_T, \quad (1)$$

where $\langle \cdots \rangle_T$ is the finite-temperature statistical average, $A(t) \equiv e^{iHt} A e^{-iHt}$ and $L \equiv [H, \circ]$ is the Liouville operator (so that $A(t) \equiv e^{iLt} A$).

Claim 1.

$$\partial_t C_{AB}(t) = -iT \langle [A(t), B] \rangle_T \quad (2)$$

▷ Expressing $B(i\lambda)$ in terms of Liouville operator as well, we have

$$\partial_t C_{AB}(t) = -iT \int_0^{1/T} d\lambda \langle A L e^{-iLt} B(i\lambda) \rangle_T = -iT \int_0^{1/T} d\lambda \langle A e^{-iLt} L \cdot e^{-L\lambda} B \cdot e^{-H/T} \rangle.$$

After the integration over λ , we obtain

$$\partial_t C_{AB}(t) = -iT \langle A e^{-iLt} L \cdot (-L)^{-1} (e^{-Lt} - 1) B \cdot e^{-H/T} \rangle$$

*Electronic address: xiaodong.hu@bc.edu

$$\begin{aligned}
&= iT \left\langle Ae^{-iLt} e^{-Lt} B \cdot e^{-H/T} \right\rangle - iT \left\langle Ae^{iLt} \cdot B \cdot e^{-H/T} \right\rangle \\
&= iT \left\langle Ae^{-Lt} \cdot e^{-iLt} B \cdot e^{-H/T} \right\rangle - iT \left\langle A \cdot e^{-iLt} B \cdot e^{-H/T} \right\rangle \\
&= iT \left\langle A \cdot e^{-Lt} B(-t) \cdot e^{-H/T} \right\rangle - iT \left\langle AB(-t) e^{-H/T} \right\rangle \\
&\equiv iT \left\langle A \cdot e^{-H/T} B(-t) e^{H/T} \cdot e^{-H/T} \right\rangle - iT \langle AB(-t) \rangle_T \\
&= iT \left(\langle B(-t) A \rangle_T - \langle AB(-t) \rangle \right) \equiv -iT \langle [A, B(-t)] \rangle_T = -iT \langle [A(t), B] \rangle,
\end{aligned}$$

where in the line next to the last we explicitly write out the Liouville operator and cycle the trace. \square

This result connects Kubo pair with the retarded Green function. By definition $iG_{AB}^R(t) := \theta(t) \langle [A(t), B] \rangle$, so we have

$$\theta(t) \partial_t C_{AB}(t) \equiv -TG_{AB}^R(t). \quad (3)$$

Integrating (3) over time, we get

$$\frac{1}{T} \left(C_{AB}(t = \infty) - C_{AB}(t = 0) \right) = - \int_{-\infty}^{\infty} dt G_{AB}^R(t) \equiv - \int_{-\infty}^{\infty} dt G_{AB}^R(t) e^{-i\omega t} \big|_{\omega=0} \equiv G_{AB}^R(\omega = 0) \equiv \chi_{AB}.$$

Assuming operators A and B decay at late time $t \rightarrow \infty$, we then come to a somewhat counterintuitive result,

$$\frac{1}{T} C_{AB}(t = 0) = G_{AB}^R(\omega = 0) \equiv \chi_{AB}, \quad (4)$$

connecting a fixed time ($t = 0$) quantity on the LHS to a fixed frequency (integral over time axis) quantity on the RHS.

B. Memory Matrix Theory

The essence of memory matrix theory is to

- **assign (freely) a selective set of long-lived operators (as hydrodynamic degree of freedom);**
- **perform a series of manipulation on $C_{AB}(z)$ to extract the dominating contribution to conductivities ($\sigma_{AB}(z) \equiv \frac{1}{T} C_{AB}(z)$).**

Since perturbation theory for quantum mechanics is well-established, defining a ‘‘Hilbert space for operators’’ will be helpful. To achieve this, we need to assign a *complete inner product* ($\circ \mid \circ$) on the linear space of operators. A natural choice is the Kubo pair we defined above

$$(A(t) \mid B) := C_{AB}(t), \quad (5)$$

so from equation (4)

$$(A \mid B) \equiv (A(0) \mid B) \equiv C_{AB}(t = 0) = TG_{AB}^R(\omega = 0) = T\chi_{AB}. \quad (6)$$

Note 1. The *bilinearity* of ($\circ \mid \circ$) is obvious. But to show (5) indeed define an inner product, we also have to prove the *complex conjugation* $(A(t) \mid B)^* \equiv (B \mid A(t))$ and *positive-definiteness* $(A \mid A) \geq 0$. They can all be checked as properties of Kubo pairs [1, 2]. Besides this, we can even show that such inner product is actually *real* and *symmetric*. Time-translation symmetry also gives $(A(-t) \mid B) \equiv (e^{-iLt} A, B) = (A \mid B(t)) \equiv (A, e^{iLt} B)$, indicating $(iL)^{\text{adj}} = -iL$ in the operator Hilbert space. But one must be aware that, **under the basis of long-lived operators (rather than the basis of complete eigenstates), Liouville operator does not appear as a matrix. So the ‘‘adjoint’’ of one operator should not be simply taken as the ‘‘conjugate transpose’’ as in usual Quantum Mechanics.** In fact, by moving the position of H and cycling the trace,

$$(A \mid L \mid B) \equiv \frac{1}{\beta} \int_0^\beta \frac{1}{\mathcal{Z}} \text{tr} \left\{ e^{-\beta H} A e^{-\lambda H} (HB - BH) e^{\lambda H} \right\}$$

$$= \frac{1}{\beta} \int_0^\beta \frac{1}{\mathcal{Z}} \text{tr} \left\{ e^{-\beta H} (AH - HA) e^{-\lambda H} B e^{\lambda H} \right\} \equiv -(LA, B) \equiv -(A|L^{\text{adj}}|B),$$

we get $L^{\text{adj}} = -L$ (and clearly $i^{\text{adj}} = i$). For the full proof of the properties, please refer to my Xournal++ writing notes.

Note 2. Strickly speaking, to define a useful Hilbert space, we also demand such inner product to be *complete* and the Hilbert space to be *separable*¹. But they have little to do with our main derivation so we just assume they are true and leave the work to mathematicians.

With the help of this inner product, the laplace transformation of Kubo pair $C_{AB}(t)$ can now be written as

$$C_{AB}(z) \equiv \int_0^\infty dt e^{izt} C_{AB}(t) \equiv \int_0^\infty dt e^{izt} (A|e^{-iLt}|B) = (A|i(z-L)^{-1}|B).$$

In quantum mechanics, perturbation theory is done by splitting the ground state and excited states, or splitting the Hilbert space into low-energy and high-energy sectors. In the same spirit, we can split the operator Hilbert space into fast-decaying and long-lived sectors by introducing the projection operator

$$q \equiv \mathbb{1} - p \equiv \mathbb{1} - \sum_{A,B} |A\rangle (|A\rangle\langle B|)^{-1} \langle B| \equiv \mathbb{1} - \frac{1}{T} \sum_{AB} |A\rangle \chi_{AB}^{-1} \langle B|.$$

Using the operator identity

$$(U - V)^{-1} \equiv U^{-1} + U^{-1}V(U - V)^{-1}, \quad (7)$$

we have

$$(z - L)^{-1} \equiv ((z - Lq) - Lp)^{-1} \equiv (z - Lq)^{-1} + (z - Lq)^{-1}Lp(z - L)^{-1}$$

and the correlation function can be evaluated through

$$C_{AB}(z) = i(A|(z - Lq)^{-1}|B) + i \sum_C (A|(z - Lq)^{-1}L|C)(C|p(z - L)^{-1}|B).$$

Note that by definition $q|A\rangle \equiv 0$ for all long-lived operators A , so

$$(A|(z - Lq)^{-1}|B) \equiv \left(A \left| \frac{1}{z} + \frac{Lq}{z^2} + \dots \right| B \right) = \frac{1}{z} (A|B) \equiv \frac{T}{z} \chi_{AB}.$$

For the other part, inputing the definition of p ,

$$p(z - L)^{-1}|B\rangle \equiv \frac{1}{T} \sum_{CD} |C\rangle \chi_{CD}^{-1} (D|(z - L)^{-1}|B) \equiv \frac{1}{iT} \sum_{CD} |C\rangle \chi_{CD}^{-1} C_{DB}(z).$$

Thus we have

$$\begin{aligned} C_{AB}(z) - \frac{iT}{z} \chi_{AB} &= \frac{1}{T} \sum_{CD} (A|(z - Lq)^{-1}|C) \chi_{CD}^{-1} C_{DB}(z) \\ &= \frac{1}{T} \sum_{CD} \left(A \left| \left(z^{-1} + z^{-1}Lq(z - Lq)^{-1} \right) L \right| C \right) \chi_{CD}^{-1} C_{DB}(z), \end{aligned}$$

where identity (7) is again utilized. Expanding the parenthesis and using the property of projection operator $q^2 \equiv q$ such that

$$q(z - Lq)^{-1} \equiv \frac{q}{z} + \frac{qLq}{z^2} + \frac{qLqLq}{z^3} + \dots = \frac{q}{z} + \frac{q(qLq)q}{z^2} + \frac{q(qLq)(qLq)q}{z^3} + \dots = q(z - qLq)^{-1}q,$$

¹ As a reminder, a Hilbert space is separable provided it contains a dense countable subset. Along with Zorn's lemma, this means a Hilbert space is *separable* if and only if it admits a countable orthonormal basis.

we get

$$C_{AB}(z) - \frac{iT}{z} \chi_{AB} = \frac{1}{Tz} \sum_{CD} (A|L|C) \chi_{CD}^{-1} C_{DB}(z) + \frac{1}{Tz} \sum_{CD} (A|Lq(z - qLq)^{-1}L|C) \chi_{CD}^{-1} C_{DB}(t).$$

Denoting $iL|A) \equiv |\dot{A})$ (since $|A(t)) \equiv e^{iLt}|A)$), and introducing the *memory function*²

$$\begin{cases} M_{AC}(z) := \frac{i}{T} (\dot{A}|q(z - qLq)^{-1}q|\dot{C}), \\ N_{AB} := \frac{1}{T} (A|L|B) \equiv \frac{1}{T} (A|\dot{B}) = \chi_{AB} \equiv \frac{-1}{T} (\dot{A}|B) = -\chi_{AB}, \end{cases} \quad (8)$$

we then arrive at the close equation for correlation function

$$C_{AB}(z) \equiv \frac{1}{z} \left\{ iT\chi_{AB} - i \sum_{CD} N_{AC} \chi_{CD}^{-1} C_{DB}(z) - i \sum_{CD} M_{AC}(z) \chi_{CD}^{-1} C_{DB}(z) \right\},$$

or in a long-lived-operator-basis-independent form

$$C \equiv \frac{1}{z} \left(iT\chi - i(M + N)\chi^{-1}C \right) \implies C \equiv \chi \frac{1}{M(z) + N - iz\chi} \chi. \quad (9)$$

So the generalized conductivities for operators A and B reads

$$\sigma_{AB}(\omega) \equiv \frac{1}{T} C_{AB}(\omega) \sum_{CD} \chi_{AC} \left(\frac{1}{M(\omega) + N - i\omega\chi} \right)_{CD} \chi_{DB}. \quad (10)$$

Namely, σ_{AB} is know as we have evaluated all static susceptibilities and memory matrices for long-lived operators.

C. Momentum Relaxation and Drude Formula

As an appetizer, we will focus on the *isotropic* system whose translation invariance is slightly broken so the (total) momentum operator \mathbf{P} is long-lived. Another two long-lived operators are charge current \mathbf{J} and heat current \mathbf{Q} . They are *believed* to have a significant overlap (in the sense of static susceptibilities like $(J_x|P_x)$) simply because in the picture of normal phase (like Fermi Liquid), the motion of quasiparticles usually indicate the flow of both charge and heat. But one must be aware that the validity of such guess may be questionable. Unlike integrable systems, in general it is hard to determine the correct set of long-lived operators.

In the first case, our system is supposed to have both *time-reversal* and *parity symmetry*³. Under time-reversal transformation, the retarded Green function is known to satisfy the *Onsager reciprocal relation* [3] (in the presence of time-reversal-breaking magnetic fields)

$$G_{\alpha\beta}^R(\omega; B) = \varepsilon_\alpha \varepsilon_\beta G_{\beta\alpha}^R(\omega; -B). \quad (11)$$

For the simplest case here $\sigma_{xy} = \sigma_{yx}$. On the other hand, the rotation symmetry demands $\sigma_{xy} = -\sigma_{yx}$. So the interplay of them requires the charge conductivity matrix to be diagonal $\sigma_{xx} = \sigma_{yy}$, and we are left to calculate

$$\sigma_{xx} \equiv \sigma_{J_x J_x} = \sum_{A, B \in \{\mathbf{J}, \mathbf{Q}, \mathbf{P}\}} \chi_{J_x A} \left(\frac{1}{M - i\omega\chi} \right)_{AB} \chi_{B J_x}. \quad (12)$$

Here matrix $N = 0$ because all three long-lived operators are time-reversal odd (which is usually the case). Similarly since $\chi_{AB} \equiv G_{AB}^R(\omega = 0)$, the above argument can also be applied, giving $\chi_{J_x J_y} = \chi_{P_x P_y} = \chi_{Q_x Q_y} = 0$.

² **Matrix N is always antisymmetric** from the property we have proven in **Note 1**.

$$(A|L|B) = -(A, L^{\text{adj}} B) = -(B|L|A).$$

So clearly **it vanishes in a time-reversal invariant theory** (since the “operator state” $|\dot{A})$ switch its sign under $t \mapsto -t$). In fact, any expression with an even number of Liouville operator will vanishes under time-reversal transformation. So **in general we cannot tell any symmetric information about the memory function $M(z)$, but it must be symmetric in a time-reversal invariant theory**.

³ In 2D the parity symmetry is just mirror symmetry $x \mapsto y, y \mapsto -x$ (with magnetic field B reversed, if exists).

D. Magnetotransport

II. PARITY-VIOLATING TRANSPORT

-
- [1] R. Kubo, Journal of the Physical Society of Japan **12**, 570 (1957).
 - [2] D. Forster, *Hydrodynamic fluctuations, broken symmetry, and correlation functions* (CRC Press, 2018).
 - [3] L. Onsager, Physical review **37**, 405 (1931).