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Time-reversal symmetry for systems in a constant external magnetic field

Sara Bonella*
CECAM Centre Européen de Calcul Atomique et Moléculaire, École Polytechnique Fédérale de Lausanne, Batochime, Avenue Forel 2, 1015 Lausanne, Suisse

Alessandro Coretti†
CECAM Centre Européen de Calcul Atomique et Moléculaire, École Polytechnique Fédérale de Lausanne, Batochime, Avenue Forel 2, 1015 Lausanne, Suisse and Department of Physics, Università di Roma La Sapienza, Ple. A. Moro 5, 00185 Roma, Italy

Lamberto Rondoni‡
INFN, Sezione di Torino, Via P. Giuria 1, 10125 Torino, Italy and Dipartimento di Scienze Matematiche and Graphene@Polito Lab Politecnico di Torino, Corso Duca degli Abruzzi 24, 10125 Torino, Italy

Giovanni Ciccotti§
Institute for Applied Computing "Mauro Picone" (IAC), CNR, Via dei Taurini 19, 00185 Rome, Italy; School of Physics, University College of Dublin UCD–Belfield, Dublin 4, Ireland; and Università di Roma La Sapienza, Ple. A. Moro 5, 00185 Roma, Italy

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The time-reversal properties of charged systems in a constant external magnetic field are reconsidered in this paper. We show that the evolution equations of the system are invariant under a new symmetry operation that implies a new signature property for time-correlation functions under time reversal. We then show how these findings can be combined with a previously identified symmetry to determine, for example, null components of the correlation functions of velocities and currents and of the associated transport coefficients. These theoretical predictions are illustrated by molecular dynamics simulations of superionic AgI.

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I. INTRODUCTION

The common view on charged systems in an external magnetic field is that the symmetry properties of their correlation functions require special treatment because the equations of motion violate standard time-reversal invariance. Indeed, given the observables Φ and Ψ (functions of phase space) and the symmetry operation $\mathcal{T}_B(\mathbf{r},\mathbf{p},t;\mathbf{B}) = (\mathbf{r},-\mathbf{p},-t;-\mathbf{B})$, the work by Kubo [1–3] in the context of linear response theory in the 1950s, established that in the stationary state

$$\langle \Phi(0)\Psi(t)\rangle_{\mathbf{B}} = \epsilon_\Phi\epsilon_\Psi\langle \Phi(0)\Psi(-t)\rangle_{-\mathbf{B}} = \epsilon_\Phi\epsilon_\Psi\langle \Phi(t)\Psi(0)\rangle_{-\mathbf{B}}. \tag{1}$$

Above, the angular brackets indicate an average with respect to the equilibrium probability distribution and, when it exists, $\epsilon_{\Phi,\Psi}$ is the signature of the observable with respect to $\mathcal{T}_B$. Note that, since the magnetic field in Eq. (1) appears with opposite sign in the first and in the subsequent terms, this relationship involves two distinct physical systems subject to different magnetic fields. This limits, to some extent, its conceptual interest and hinders its usefulness in interpreting the results of experiments and computer simulations, which usually occur in a single magnetic field. The symmetry operation $\mathcal{T}_B$ is used frequently, for example to derive fluctuation relations for particles in a magnetic field [4–7].

In this paper, we note that the evolution equations for a system in constant magnetic field are invariant under a new generalized time-reversal operation. As discussed in Sec. II, combining this new symmetry with a previously identified time-reversal operation [8], makes it possible to predict analytically symmetry properties of physical observables such as the diffusion or conductivity tensor. In Sec. III, we verify that these predictions are indeed verified by molecular dynamics simulations of an interesting condensed phase system, AgI in the superionic phase.

II. THEORY

In the following, we shall consider N point particles of charge q_i and mass m_i interacting via the potential V, and in the presence of an external magnetic field $\mathbf{B}$, of constant intensity B_0 and directed along the z axis. This setup is often adopted to discuss the unusual behavior of systems in external magnetic field under time reversal (see, for example, [7,9,10]), and it has both theoretical and experimental interest. We also note that, since the wavelength of magnetic fields of practical interest are several orders of magnitude larger than the typical dimensions of simulation boxes, the assumption of a, spatially, uniform field is usually well justified in simulations [11]. Finally, although generalizing our considerations to a spatially uniform but time-dependent field may be possible, the notion of time-reversal invariance for nonautonomous equations of

*sara.bonella@epfl.ch
†alessandro.coretti@epfl.ch
‡lamberto.rondoni@polito.it
§giovanni.ciccotti@roma1.infn.it

motion is nontrivial and requires a treatment beyond the scope of this work.

Indicating with $\Gamma \equiv \{\mathbf{r}_i,\mathbf{p}_i\}_{i=1,\ldots,N}$ a point in phase space, the Hamiltonian of the system is

$$\mathcal{H}(\Gamma) = \sum_{i=1}^{N} \frac{[\mathbf{p}_i - q_i\mathbf{A}(\mathbf{r}_i)]^2}{2m_i} + \frac{1}{2}\sum_{i\neq j} V(r_{ij}), \tag{2}$$

where $\mathbf{A}(\mathbf{r})^T \equiv B_0(-y,x,0)/2$ is the vector potential, and the interaction between the particles is assumed pairwise and dependent only on $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, the magnitude of the distance between the pairs of particles. The evolution equations for this system are

$$\begin{aligned}
\dot{x}_i &= \frac{p_i^x}{m_i} + \omega_i y_i,\\
\dot{y}_i &= \frac{p_i^y}{m_i} - \omega_i x_i,\\
\dot{z}_i &= \frac{p_i^z}{m_i},\\
\dot{p}_i^x &= F_i^x + \omega_i(p_i^y - m_i\omega_i x_i),\\
\dot{p}_i^y &= F_i^y - \omega_i(p_i^x + m_i\omega_i y_i),\\
\dot{p}_i^z &= F_i^z,
\end{aligned} \tag{3}$$

where $i = 1,\ldots,N$, $\omega_i = q_i B_0/2m_i$ is the cyclotron frequency, and F_i^α is the force on particle i and direction α due to the pairwise potential. Direct inspection of the equations above shows that they are not invariant under standard time reversal, $\mathcal{T}(\mathbf{r},\mathbf{p},t) = (\mathbf{r},-\mathbf{p},-t)$, and that the additional inversion of the magnetic field in $\mathcal{T}_B$ is necessary to restore invariance. This originates the opposite signs of the field in Eq. (1).

Direct inspection of the evolution equations, however, also shows that the dynamics is invariant under the time-reversal transformation

$$\widetilde{\mathcal{M}}(x,y,z,p^x,p^y,p^z,t;\mathbf{B}) = (-x,y,z,p^x,-p^y,-p^z,-t;\mathbf{B}) \tag{4}$$

which (see Sec. II A) implies

$$\langle\Phi(0)\Psi(t)\rangle_{\mathbf{B}} = \tilde{\eta}_\Phi\tilde{\eta}_\Psi\langle\Phi(0)\Psi(-t)\rangle_{\mathbf{B}} = \tilde{\eta}_\Phi\tilde{\eta}_\Psi\langle\Phi(t)\Psi(0)\rangle_{\mathbf{B}}, \tag{5}$$

where, for example, $\tilde{\eta}_\Phi$ is the signature of Φ under $\widetilde{\mathcal{M}}$.

Exploiting the analogy of the magnetic dynamical system, Eqs. (3), with the so-called Sllod equations for a system subject to shear [12,13], in [8] we also noted that the time-reversal transformation

$$\mathcal{M}(x,y,z,p^x,p^y,p^z,t;\mathbf{B}) = (x,-y,z,-p^x,p^y,-p^z,-t;\mathbf{B}) \tag{6}$$

preserves the Hamiltonian and hence the evolution equations (3). This symmetry leads to the following property for equilibrium time-correlation functions

$$\langle\Phi(0)\Psi(t)\rangle_{\mathbf{B}} = \eta_\Phi\eta_\Psi\langle\Phi(0)\Psi(-t)\rangle_{\mathbf{B}} = \eta_\Phi\eta_\Psi\langle\Phi(t)\Psi(0)\rangle_{\mathbf{B}}, \tag{7}$$

where η_Φ and η_Ψ denote the signature of observable Φ and Ψ, respectively, under $\mathcal{M}$.

At variance with the Kubo relation, Eq. (1), the relationships in Eqs. (5) and (7) refer to a single value of the constant magnetic field, and therefore to the statistics of a single physical system. The symmetry of the system under the transformations defined in Eqs. (4) and (6) is a direct consequence of the form of the Lorentz force for the geometry considered in this work and reflect the essential equivalence of the x and y directions on the plane perpendicular to the magnetic field.

A. Proof of Eqs. (5) and (7)

The time-reversal properties of the correlation functions defined in Eqs. (5) and (7) can be proved using two different points of view. The first, adopted in [8], focuses on the effect of the generalized time-reversal symmetries on the evolution of the phase-space points, i.e. on the microscopic state of the system (see, for example, Ref. [14]). The second, considers as the fundamental object of interest in statistical mechanics the functions of phase space associated with the physical observables, and identifies the properties of their evolution under the symmetry operations. In the following, we summarize the proof of the time-reversal symmetry of the correlation function using the second perspective. To simplify the notation, we refer to the symmetry $\mathcal{M}$.

We start by discussing some general properties of the time evolution of the observables. We shall restrict our considerations to the properties of the dynamical system described by Eqs. (3), but the discussion can be generalized to the time-reversal properties of other systems. Let us indicate with U_t the time evolution operator on the space of the functions of Γ endowed with the scalar product

$$\langle\Phi,\Psi\rangle = \int d\Gamma\, \rho(\Gamma)\Phi^*(\Gamma)\Psi(\Gamma), \tag{8}$$

where $\rho(\Gamma)$ is the equilibrium probability density of the system and $*$ indicates the complex conjugate. We have [15]

$$U_t\Psi(\Gamma) \doteq \Psi(\mathcal{U}_t\Gamma), \tag{9}$$

where $\mathcal{U}_t$ is the evolution operator corresponding to Eqs. (3). Similarly, we define

$$M_\Gamma\Psi(\Gamma) \doteq \Psi(\mathcal{M}_\Gamma\Gamma) \tag{10}$$

with $\mathcal{M}_\Gamma(x,y,z,p^x,p^y,p^z) = (x,-y,z,-p^x,p^y,-p^z)$. Given that $M_\Gamma^2 = 1$, we have trivially $M_\Gamma^{-1} = M_\Gamma$. This operator is also Hermitian, i.e., $\langle\Phi,M_\Gamma\Psi\rangle = \langle M_\Gamma\Phi,\Psi\rangle$. To prove it, let us consider

$$\begin{aligned}
\langle\Phi,M_\Gamma\Psi\rangle &= \int d\Gamma\, \rho(\Gamma)\Phi^*(\Gamma)[M_\Gamma\Psi(\Gamma)]\\
&= \int d\Gamma\, \rho(\Gamma)\Phi^*(\Gamma)\Psi(\mathcal{M}_\Gamma\Gamma).
\end{aligned} \tag{11}$$

We now perform the change of variables $X = \mathcal{M}_\Gamma\Gamma$, so $\Gamma = \mathcal{M}_\Gamma^{-1}X = \mathcal{M}_\Gamma X$ to obtain

$$\begin{aligned}
\langle\Phi,M_\Gamma\Psi\rangle &= \int dX\, \rho(X)\Phi^*(\mathcal{M}_\Gamma^{-1}X)\Psi(X)\\
&= \int dX\, \rho(X)[M_\Gamma^{-1}\Phi^*(X)]\Psi(X)
\end{aligned}$$

$$= \int dX\, \rho(X)[M_\Gamma \Phi^*(X)]\Psi(X)$$
$$= \langle M_\Gamma \Phi, \Psi \rangle \tag{12}$$

which completes the proof, noting that

$$M_\Gamma \rho(X) = \rho(X) \tag{13}$$

since the Hamiltonian, as defined in Eq. (2), is invariant under this transformation, $M_\Gamma \mathcal{H}(X) = \mathcal{H}(X)$, and the probability density is a function of the Hamiltonian.

We define as time-reversal invariance the situation in which the evolution backwards in time of any observable

$$\frac{d\Psi}{d(-t)} = i\mathcal{L}\Psi, \tag{14}$$

where $i\mathcal{L} = \{\cdot, \mathcal{H}\}$ is the Poisson bracket of a function with the Hamiltonian, is identical to the forward evolution of the observable transformed under the symmetry operation M_Γ,

$$\frac{d[M_\Gamma \Psi]}{dt} = i\mathcal{L}[M_\Gamma \Psi]. \tag{15}$$

Multiplying both sides of the equation by $M_\Gamma^{-1} = M_\Gamma$,

$$\frac{d\Psi}{dt} = M_\Gamma i\mathcal{L} M_\Gamma \Psi \tag{16}$$

and comparing Eq. (14) and Eq. (16), we obtain the following relation for the generator of the dynamics

$$M_\Gamma i\mathcal{L} M_\Gamma = -i\mathcal{L}. \tag{17}$$

Given that the operators on the observables act through changes on the underlying phase space, we prove the relationship above operating on the phase-space substrate. To that end, we apply the operators on the right and on the left of Eq. (17) to $\Gamma = (x,y,z,p^x,p^y,p^z)$. Acting with the operator on the right, we have

$$-i\mathcal{L}\Gamma = -\dot{\Gamma}(\Gamma), \tag{18}$$

where $\dot{\Gamma}$ is the vector of the time derivatives of positions and momenta. The effect of the three operators on the left-hand side of Eq. (17) can be obtained applying them from left to right:

$$\mathcal{M}_\Gamma i\mathcal{L}\mathcal{M}_\Gamma \Gamma = i\mathcal{L}(\Gamma')\mathcal{M}_{\Gamma'}\Gamma' = \mathcal{M}_{\dot{\Gamma}'}\dot{\Gamma}'(\Gamma') = \dot{\Gamma}''(\Gamma'). \tag{19}$$

In the equation above, $\Gamma' = (x,-y,z,-p^x,p^y,-p^z)$, and $\dot{\Gamma}'' = [\dot{x}(\Gamma'),-\dot{y}(\Gamma'),\dot{z}(\Gamma'),-\dot{p}^x(\Gamma'),\dot{p}^y(\Gamma'),-\dot{p}^z(\Gamma')]$.

The equality of the results in Eqs. (18) and (19) under the evolution induced by Eqs. (3) is verified by direct inspection. Applying, for example, the left-hand side of Eq. (17) to p_i^y we get

$$M_\Gamma i\mathcal{L} M_\Gamma p_i^y = \dot{p}_i^y(x,-y,z,-p^x,p^y,-p^z) \tag{20}$$

and, from Eqs. (3), we have

$$\dot{p}_i^y(x,-y,z,-p^x,p^y,-p^z)$$
$$= F_i^{-y} - \omega_i\left[-p_i^x + m_i\omega_i(-y_i)\right]$$
$$= -\left[F_i^y - \omega_i\left(p_i^x + m_i\omega_i y_i\right)\right], \tag{21}$$

where we have used the fact that the force, given by the derivative of the (even) potential with respect to y, is an odd function under the symmetry. On the other hand, applying the right-hand side of Eq. (17), we have

$$-i\mathcal{L}p_i^y = -\dot{p}_i^y(x,y,z,p^x,p^y,p^z) \tag{22}$$

and, using again Eqs. (3),

$$-\dot{p}_i^y(x,y,z,p^x,p^y,p^z) = -\left[F_i^y - \omega_i\left(p_i^x + m_i\omega_i y_i\right)\right]. \tag{23}$$

Comparing Eqs. (21) and (23), we see that Eq. (17) is indeed verified.

Note that, repeating the steps above for

$$\widetilde{\mathcal{M}}_\Gamma i\mathcal{L}\widetilde{\mathcal{M}}_\Gamma = -i\mathcal{L}, \tag{24}$$

where $\widetilde{\mathcal{M}}_\Gamma(x,y,z,p^x,p^y,p^z) = (-x,y,z,p^x,-p^y,-p^z)$ shows that $\widetilde{\mathcal{M}}$ is also a time-reversal symmetry for the dynamical system, Eqs. (3). Using the same procedure, it can also be verified that, when $B_0 \neq 0$, the standard time-reversal transformation $\mathcal{T}_\Gamma(x,y,z,p^x,p^y,p^z) = (x,y,z,-p^x,-p^y,-p^z)$ is not a time-reversal symmetry for the system.

From Eq. (17), it also follows

$$M_\Gamma U_t M_\Gamma = U_{-t}. \tag{25}$$

The relation above can be inverted to give

$$U_t = M_\Gamma U_{-t} M_\Gamma. \tag{26}$$

We can now make use of this result to prove the time-reversal properties stated in Eq. (7). The time-correlation function is defined as

$$\langle \Phi(0)\Psi(t)\rangle_{\mathbf{B}} = \int d\Gamma\, \rho(\Gamma)\Phi^*(\Gamma)[U_t\Psi(\Gamma)].$$

Using Eq. (26), we can write

$$\langle \Phi(0)\Psi(t)\rangle_{\mathbf{B}} = \int d\Gamma\, \rho(\Gamma)\Phi^*(\Gamma)[M_\Gamma U_{-t} M_\Gamma \Psi(\Gamma)].$$

Using the definition of the adjoint operator, the expression above can be written as

$$\langle \Phi(0)\Psi(t)\rangle_{\mathbf{B}} = \int d\Gamma [M_\Gamma \rho(\Gamma)\Phi^*(\Gamma)][U_{-t} M_\Gamma \Psi(\Gamma)]$$
$$= \int d\Gamma\, \rho(\Gamma)[M_\Gamma \Phi^*(\Gamma)][U_{-t} M_\Gamma \Psi(\Gamma)]$$
$$= \eta_\Phi \eta_\Psi \int d\Gamma\, \rho(\Gamma)\Phi^*(\Gamma)[U_{-t}\Psi(\Gamma)]$$
$$= \eta_\Phi \eta_\Psi \langle \Phi(0)\Psi(-t)\rangle_{\mathbf{B}} = \eta_\Phi \eta_\Psi \langle \Phi(t)\Psi(0)\rangle_{\mathbf{B}}, \tag{27}$$

where, in going from the first to the second line we have used the invariance of the probability density under M_Γ, and in the third line we have recognized, for example, that $M_\Gamma \Phi(\Gamma) = \Phi(\mathcal{M}_\Gamma \Gamma) = \eta_\Phi \Phi(\Gamma)$. Finally, the last equality follows from time translational invariance.

Repeating the steps above with $\widetilde{\mathcal{M}}_\Gamma$ proves the relationships in Eq. (5).

B. Consequences of Eqs. (5) and (7)

The simultaneous existence of the two generalized time-reversal symmetries has a rather interesting implication. Indeed, in order to fulfill simultaneously both relations at any given time, the correlation functions must either have the same overall signature with respect to $\mathcal{M}$ and $\widetilde{\mathcal{M}}$ or be zero. This translates immediately, via linear response theory, into properties of the transport coefficients for the system.

Let us consider, as an example, the correlation function of different components of the particle velocities. Equations (3) show that $v_i^x = \dot{x}_i$ is odd (i.e., $\eta_{\dot{x}_i} = -1$), $v_i^y = \dot{y}_i$ is even (i.e., $\eta_{\dot{y}_i} = 1$), and $v_i^z = \dot{z}_i$ is odd (i.e., $\eta_{\dot{z}_i} = -1$) under $\mathcal{M}$. This implies the following relations for the time-correlation functions of the components of the velocities

$$\begin{aligned}\langle v_i^x(t)v_i^y(0)\rangle &= -\langle v_i^x(0)v_i^y(t)\rangle,\\ \langle v_i^x(t)v_i^z(0)\rangle &= \langle v_i^x(0)v_i^z(t)\rangle,\\ \langle v_i^y(t)v_i^z(0)\rangle &= -\langle v_i^y(0)v_i^z(t)\rangle. \end{aligned} \tag{28}$$

On the other hand, see again Eqs. (3), $v_i^x = \dot{x}_i$ is even (i.e., $\tilde{\eta}_{\dot{x}_i} = 1$), $v_i^y = \dot{y}_i$ is odd (i.e., $\tilde{\eta}_{\dot{y}_i} = -1$), and $v_i^z = \dot{z}_i$ is odd (i.e., $\tilde{\eta}_{\dot{z}_i} = -1$) under $\widetilde{\mathcal{M}}$ so the relations

$$\begin{aligned}\langle v_i^x(t)v_i^y(0)\rangle &= -\langle v_i^x(0)v_i^y(t)\rangle,\\ \langle v_i^x(t)v_i^z(0)\rangle &= -\langle v_i^x(0)v_i^z(t)\rangle,\\ \langle v_i^y(t)v_i^z(0)\rangle &= \langle v_i^y(0)v_i^z(t)\rangle \end{aligned} \tag{29}$$

hold too. Comparing the right-hand sides of the second and third lines of Eqs. (28) and (29) shows that these correlation functions must be zero for all times. Considering the time integrals of the correlation functions, this immediately implies that some components of the diffusion tensor must be zero. In particular, $D_{xz} = D_{zx} = D_{yz} = D_{zy} = 0$. Note that, since the first lines of Eqs. (28) and (29) are equal, we can only make the (weaker) statement that these correlation must be zero at zero time, and that $D_{xy} = -D_{yx}$. Similarly, for the diagonal components of the velocity correlation functions, all even under both symmetries, no specific prediction can be made.

The observations above can be trivially extended to the correlation functions of the components of the current $\mathbf{J} = \sum_{i=1}^N q_i \mathbf{v}_i$. This, in turn, means that the only off-diagonal components of the conductivity tensor that can be different from zero are $\sigma_{xy} = -\sigma_{yx}$. In fact, a nonzero value of these components of the conductivity tensor signals the onset of the Hall effect in the system [16,17].

III. A NUMERICAL EXAMPLE

In this section, we illustrate the validity of the properties of the time-correlation functions discussed above for an interesting condensed phase system: the prototypical superionic conductor, AgI. Superionic conductors have attracted considerable interest [18–24], most recently due to their potential applications in clean batteries production [25,26]. They are characterized by a solid phase with a conductivity comparable to that of the melt. In this phase, the dominant charge transport is due to the motion of an ionic species diffusing almost freely in the lattice formed by the counterions. Superionic AgI exists at ambient pressures between 420 and 831 K. In this system, the conductivity is due primarily to the motion of Ag^+, while the I^- form a bcc lattice. The unit cell accommodates two Ag^+ that are located preferentially at the tetrahedral sites in the anion lattice and diffuse through a hopping mechanism between them [19,27–29]. In [17], the charge transport of AgI in the presence of an external magnetic field was studied for the first time via molecular dynamics. In that paper, it was shown in particular that the Hall mobility of the system can indeed be computed and is in good agreement with experiments over a significant range of temperatures. Simulations also showed that the system exhibits ionic magnetoresistence (i.e., a decrease of the diagonal components of the conductivity tensor compared to the case of the isolated system). Here, we reconsider the data to illustrate the symmetry properties of the time correlations discussed in the previous section.

The simulation setup adopted in this paper is similar to that in Ref. [30]. AgI is modeled via the pair potential introduced by Shimojo and Kobayashi [31]. The simulation box contains 250 Ag^+ and 250 I^-, and the number density is $\rho = 0.0306$ Å^{-3}. Trajectories for nonzero magnetic field are obtained using the algorithm, derived in the Liouvillian formalism, described in [16]. The field intensity is set to $B_0 = 100$ u (see below for units) based on the results in [17] showing that, for this value, the Lorentz force is comparable to the interatomic interactions, and that magnetic effects on the correlation functions and transport coefficients are significant. The correlation functions are calculated from a simulation at constant (N,V,E) from initial conditions obtained from an equilibrated constant (N,V,T) run employing a generalized Nose-Hoover thermostat [16], with temperature $T = 573$ K. Long-range forces are treated via direct implementation of the Ewald method [32]. The value of the thermostat mass during equilibration is $Q = 0.1$ and the equilibration time is

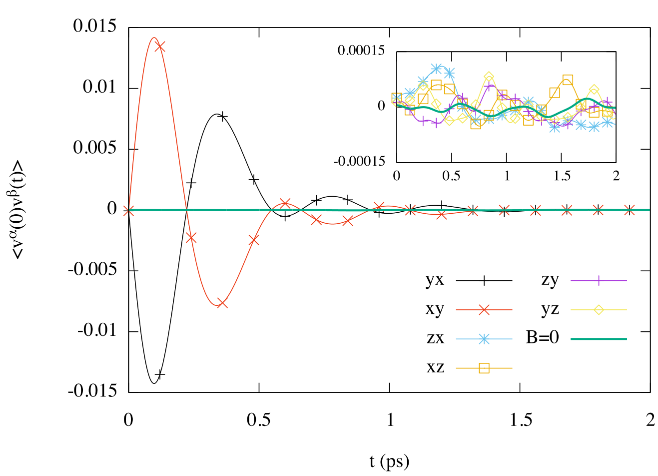

FIG. 1. Time-correlation functions of the cross components of the velocity of Ag in superionic AgI. Labels and symbols in the figure are as indicated in the legend with, for example, xy referring to $\langle v^x(0)v^y(t)\rangle = \frac{1}{N_{\rm Ag}}\sum_{i=1}^{N_{\rm Ag}} \frac{1}{\mathcal{T}}\int_0^{\mathcal{T}} d\tau\, v_i^x(\tau)v_i^y(\tau+t)$. The main plot shows the nonzero components of the time-correlation function. In the inset, we show the null components. Note that the scale of the vertical axis in the inset is two orders of magnitude smaller than in the main figure. All results are for $B_0 = 100$ u except for those reported in the green curve, which were obtained at $B_0 = 0$ as a reference for noise.

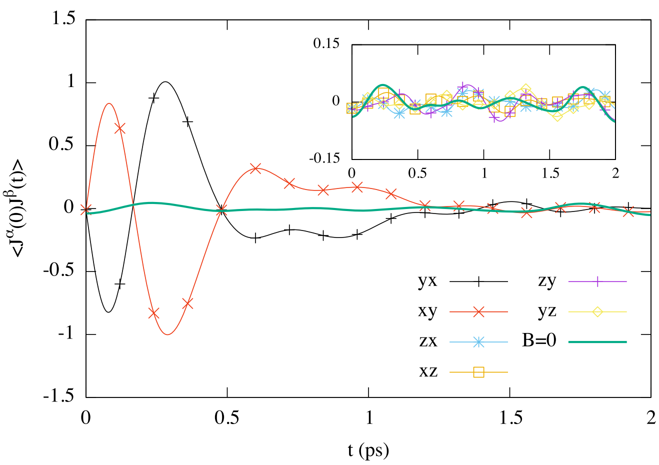

FIG. 2. Time-correlation functions of the cross components of the current. Labels and colors are as in Fig. 1. Also as in Fig. 1, the main plot shows the nonzero components of the time-correlation function. In the inset, we show the null components. In this case, the scale of the vertical axis in the inset is one order of magnitude smaller than in the main figure. The higher level of noise in the zero components derives from the fact that the current is a collective (as opposed to single particle) property.

20 ps, with a time step of 0.2 fs. Production runs for AgI are 800 ps and 120 ns long, for computing the velocity and current time-correlation functions, respectively. In the system of units adopted in this work, distances are measured in angstroms, charges in units of the electron charge e, masses in atomic mass unit, and energies in kJ/mol. The derived unit for the magnetic field is 1.04 u $= 10^4$ T.

Figures 1 and 2 show the cross correlation functions of the velocities and currents, respectively. The green curve shows the value of the average of these quantities in the absence of magnetic field to provide a reference on the noise of the signals. Both figures show a clear difference between the $x - y$ cross correlations and the others. The correlation between components on the plane orthogonal to the magnetic field are zero at zero time, and opposite for finite t. The other components are indistinguishable from zero based on the comparison with the value at $B_0 = 0$. Thus, the data verifies the symmetries derived in the previous section.

IV. CONCLUSIONS

A new time-reversal symmetry operation that preserves the evolution equations of a system of charged particles in a constant external magnetic field was introduced. This time-reversal symmetry entails a new signature property of time-correlation functions. The simultaneous validity of the symmetries $\widetilde{\mathcal{M}}$ and $\mathcal{M}$ presented in this paper makes it possible to identify null time-correlation functions of some relevant physical observables and the corresponding transport coefficients. As an interesting numerical illustration, we have shown that these symmetry predictions are indeed verified by the velocity and current correlations of superionic AgI under strong external magnetic field.

Note that the evolution equations in Eqs. (3) are formally identical to those describing a system subject to constant shear in the so-called Sllod evolution [33] (indeed, the generalized time-reversal introduced in [8] was inspired by work on this system), provided that the intensity of the magnetic field is substituted by the viscosity. They are also formally identical to the evolution equations of a body rotating uniformly around a fixed axis, where the angular velocity plays the role of the magnetic field. These observations indicate that the work presented in this paper has broader applicability than that of the specific case of the magnetic system considered here.

As a final remark, we point out that the results discussed in this paper assume that the observables whose correlation is measured have a definite signature under the transformations $\mathcal{M}$ and/or $\widetilde{\mathcal{M}}$. Interestingly, not all observables that have a signature under standard time reversal maintain this property under the new symmetries. For example, in contrast with the case of standard time reversal, the intermediate scattering function, $F(\mathbf{k},t) = \langle e^{-i\mathbf{k}\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}(t)} \rangle / N$, does not have a signature when $B_0 \neq 0$, since the components of the coordinates transform with different signs under the new symmetries. Future work will investigate measurable effects of this observation on physical observables.

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