

# Master equation approach to the conjugate pairing rule of Lyapunov spectra for many-particle thermostated systems

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The master equation approach to Lyapunov spectra for many-particle systems is applied to nonequilibrium thermostated systems to discuss the conjugate pairing rule. We consider iso-kinetic thermostated systems with a shear flow sustained by an external restriction, in which particle interactions are expressed as a Gaussian white randomness. Positive Lyapunov exponents are calculated by using the Fokker-Planck equation to describe the tangent vector dynamics. We introduce another Fokker-Planck equation to describe the time-reversed tangent vector dynamics, which leads to the calculation of the negative Lyapunov exponents. Using the Lyapunov exponents provided by these two Fokker-Planck equations we show the conjugate pairing rule is satisfied for thermostated systems with a shear flow in the thermodynamic limit which allow us to replace the friction coefficient with a constant number. We also give an explicit form to connect the Lyapunov exponents with the time correlation of the interaction matrix in a thermostated system with a color field.

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## I. INTRODUCTION

The Lyapunov exponent is an essential concept to express the instability of orbits and the amount of the information in a dynamical system. It is introduced as an exponential expansion (or contraction) rate of an infinitesimal perturbation of orbits, and its positivity implies that the system is chaotic. In general there is a Lyapunov exponent for each independent direction of the infinitesimal perturbation of the orbit, and the sorted set of such Lyapunov exponents is called the Lyapunov spectrum, and has been the subject of study in many-particle systems. For example, the existence of its thermodynamic limit [1–3], an effect of the rotational degrees of freedom of molecules [4], its stepwise structure and the Lyapunov modes (a wavelike structure in the tangent space) [5], and a tracer particle effect [6] have been observed and discussed in the Lyapunov spectra of many-particle chaotic systems.

Some algorithms for numerical computations of Lyapunov spectra are well known (e.g., the algorithm due to Benettin *et al.* [7,8] and the constraint method [9]), and so far full Lyapunov spectra have been calculated mainly using numerical approaches. On the other hand, analytical calculations of the full Lyapunov spectra for many-particle systems still remain as a difficult task at present. The master equation approach, which was recently proposed, is one of the methods that can be used to calculate the full Lyapunov spectra for many-particle systems [10]. This method is applied to systems with random particle interactions, and uses a master equation to describe the tangent space dynamics, which allows the calculation of all individual positive Lyapunov exponents through the average of the magnitude of the tangent vector.

The master equation approach is characterized by using random particle interactions, like in the other random matrix approaches [11–15] to the Lyapunov spectrum, and this characteristic distinguishes this approach from approaches using deterministic many-particle models. Especially, models in

the master equation approach are specified by the form of time correlation functions of the matrix expressing the particle interactions, whereas models in the deterministic Hamiltonian dynamics are specified by the form of a potential function, or more generally, of the Hamiltonian. In this sense, using the master equation approach we move away from considering particular Hamiltonian model systems. Under the assumption that the random particle interactions are expressed by a Gaussian white randomness, the master equation is simply attributed to a Fokker-Planck equation, and leads to a direct connection between the Lyapunov exponents and the time correlation of the particle interaction matrix. Systematic investigations to justify the Gaussian white random assumption for particle interactions using a deterministic many-particle Hamiltonian model have not been done yet [16], but it is expected that a Gaussian behavior of the interaction matrix may be justified by the central limit theorem as the number of particles goes to infinity, namely, in the thermodynamic limit. In order to justify the white random property of the time-correlations of the interaction matrix, (that is their  $\delta$ -function relaxations), as a description of a deterministic chaotic system whose characteristic correlation time scale is not infinitesimal, it may be necessary to modify the time scale. Such a change of the time scale multiplies the Lyapunov exponents by a factor, but if we only consider ratios of Lyapunov exponents, for example the Lyapunov exponents divided by the largest Lyapunov exponent, then the problem of the time scale no longer appears explicitly. Under the assumption of this Gaussian white random interaction, the master equation approach reproduced the stepwise structure of the Lyapunov spectrum and the Lyapunov mode, which were actually observed in the numerical simulation of a deterministic many-hard-disk system.

A characteristic of the Lyapunov spectrum that is known in Hamiltonian systems, is that the Lyapunov exponents appear as a pair, namely, any positive Lyapunov exponent accompanies a negative Lyapunov exponent with its opposite sign [17]. This characteristic, which is based on the symplectic structure of the Hamiltonian mechanics, is not correct in

non-Hamiltonian systems, but it is interesting to know how it is modified in quasi-Hamiltonian systems such as a Hamiltonian system coupled to a thermodynamic reservoir. This problem has been considered in some thermostated dynamics where a term to extract the heat produced in the system by external force fields is included, and led to the proposal of the *conjugate pairing rule* for thermostated systems, which claims that the sum of any Lyapunov exponent pair (excluding zero exponents) is not zero but a constant regardless of the exponent number [18,19]. This conjecture was confirmed by many following numerical calculations [20–22]. This also led to the discovery that some thermostated systems contain hidden Hamiltonian structure [23,24]. The pairing rule is not only interesting as a mathematical structure of the thermostated system but is also valuable for a practical use; the conjugate pairing rule for the thermostated system allows us to calculate non-equilibrium transport coefficients (e.g., conductivity and viscosity) from only one pair of the Lyapunov exponents, such as the largest and smallest Lyapunov exponents only [19,22,25,26].

A problem is that the necessary and the sufficient conditions for the conjugate pairing rule to hold for thermostated systems is not clearly known. The conjugate pairing rule for the iso-kinetic thermostated system with a color field was proved for the soft core interaction potential [27] and the hard core interaction potential [24,28], regardless of the number of particles. A similar discussion was done in Nosé Hamiltonian dynamics [29]. These works give the sufficient conditions for the conjugate pairing rule. On the other hand, it was suggested numerically that it can be violated in the presence of a magnetic field [30] and in inhomogeneously thermostated systems such as a system under temperature gradient [31] or a system in which the peculiar momenta are thermostated [32]. Another numerical work also suggested that it is not exact in the iso-energetic thermostat with a finite number of particles [33], although the iso-energetic thermostat should be equivalent to the iso-kinetic thermostat in the thermodynamic limit [34,35]. A special interest is the iso-kinetic thermostated system with a shear field, which is described by the Sllod equation for the planar Couette flow [36]. The Sllod equation, so named because of its close relationship to the Dolls tensor algorithm has an explicit parameter expressing the shear rate to realize a shear flow, and is different from the dynamics in which a shear flow is realized only by a boundary condition such as the Lees-Edwards periodic boundary condition [36]. Early investigations supported the conjugate pairing rule for the Sllod dynamics [19,20,37]. References [32,38] suggested a small deviation from the conjugate pairing rule. An analytical consideration showed that the deviation from the conjugate pairing rule should be at most fourth order in the shear rate in the case of a small shear rate in the thermodynamic limit [39]. However, a recent numerical calculation with a more careful numbering of the Lyapunov exponents and with numerical error bars showed that within the numerical precision the conjugate pairing rule was satisfied [40]. After all these trials, a justification of the conjugate pairing rule for the iso-kinetic thermostated system with a shear field still remains as an open problem.

This paper has two main purposes. First we generalize the master equation approach to the Lyapunov spectrum to non-equilibrium thermostated systems. Such a generalization of this approach to nonequilibrium systems is not known. As the second purpose of this paper we discuss the conjugate pairing rule of the Lyapunov spectrum for the iso-kinetic thermostated system with a shear field by using this generalized master equation approach. In this paper we concentrate on the case where the particles interact with a Gaussian white randomness. We also restrict our consideration in the thermodynamic limit, in which the fluctuations of the friction coefficient can be neglected [37]. In this case the friction coefficient in the iso-kinetic thermostated system is simply replaced by a constant. This is actually the case considered in Ref. [39], but the proof of the conjugate pairing rule for the Sllod dynamics has not known even in this simplified case. One of difficult problems in the proof of the conjugate pairing rule for the Sllod dynamics is that this dynamics does not have the  $\mu$ -symplectic structure, which is a generalized symplectic structure and have been essential in the past trials to prove the conjugate pairing rule for the thermostated systems. On the other hand, as will be shown in this paper, in order to discuss the conjugate pairing rule using the master equation approach a structure like the  $\mu$ -symplectic structure is not necessary, and this is the reason why the master equation approach allows us to access to the problem of the conjugate pairing rule for the Sllod dynamics, for which deterministic approaches have not been successful. However a problem in the master equation approach is that the time-forward master equation for the tangent space dynamics can give the only positive branch of the Lyapunov spectrum (at least in the equilibrium case), although we need the negative branch of the Lyapunov spectrum to discuss the conjugate pairing rule for thermostated systems. To overcome this problem in this paper we introduce another master equation to describe the time-reversed tangent vector dynamics, and propose a method to calculate the negative branch of the Lyapunov spectrum using this time-reversed master equation. Under the assumptions of the Gaussian white random interactions and the constant friction coefficient we show that the conjugate pairing rule for the thermostated system with a shear field given by the Sllod equation is satisfied. As a special case we also discuss briefly an explicit form to connect the Lyapunov exponents with the time-correlation of the interaction matrix in a thermostated system without a shear field.

## II. ISOKINETIC THERMOSTATED SYSTEM WITH A SHEAR FIELD AND ITS TANGENT VECTOR DYNAMICS

We consider nonequilibrium systems with an iso-kinetic thermostat. Our consideration includes the case where a shear flow is sustained by an external restriction, and for simplicity we consider a two-dimensional system consisting of  $N$  particles with the same mass  $m$ . We introduce  $\mathbf{q}^{(j)}(t) \equiv (q_x^{(j)}(t), q_y^{(j)}(t))^T$  and  $\mathbf{p}^{(j)}(t) \equiv (p_x^{(j)}(t), p_y^{(j)}(t))^T$  as the spatial coordinate vector and the momentum vector of the  $j$ th particle, respectively, at time  $t$  with the transpose operation  $T$ . (Note that all vectors in this paper are introduced as col-

umn vectors.) Equations for  $\mathbf{q}^{(j)}(t)$  and  $\mathbf{p}^{(j)}(t)$  are expressed as [36]

$$\frac{d\mathbf{q}^{(j)}(t)}{dt} = \frac{1}{m}\mathbf{p}^{(j)}(t) + \gamma\Xi_{2k}\mathbf{q}^{(j)}(t) \quad (1)$$

$$\frac{d\mathbf{p}^{(j)}(t)}{dt} = -\frac{\partial U(t)}{\partial \mathbf{q}^{(j)}(t)} - [\gamma\Xi_{2k} + \alpha(t)I_{2k}]\mathbf{p}^{(j)}(t), \quad (2)$$

where  $U(t)$  is the potential energy as a function of  $\mathbf{q}^{(j)}(t), j=1, 2, \dots, N$  and  $t$  only, and we introduce  $\Xi_{2k}$  is the  $2k \times 2k$  matrix defined by

$$\Xi_{2k} \equiv \begin{pmatrix} 0_k & I_k \\ 0_k & 0_k \end{pmatrix} \quad (3)$$

with the  $k \times k$  identical matrix  $I_k$  and the  $k \times k$  null matrix  $0_k$ . Here  $\gamma$  is the shear rate as an external parameter, namely, a constant gradient of the  $x$  component of the local velocity in the  $y$  direction, and  $\alpha(t)$  is defined by

$$\alpha(t) \equiv -\frac{\sum_{j=1}^N \mathbf{p}^{(j)}(t)^T \left( \frac{\partial U(t)}{\partial \mathbf{q}^{(j)}(t)} + \gamma\Xi_{2k}\mathbf{p}^{(j)}(t) \right)}{\sum_{j=1}^N |\mathbf{p}^{(j)}(t)|^2} \quad (4)$$

so that the total kinetic energy is constant in time:  $d[\sum_{j=1}^N |\mathbf{p}^{(j)}(t)|^2 / (2m)] / dt = 0$ . Eqs. (1) and (2) are called the Sllod equation for the planar Couette flow with the isokinetic thermostat, and gives the model for the system driven by external fields and (or) a shear rate with an attached heat reservoir which removes the energy generated inside the system and maintains the temperature of the system constantly in time. As an example described by Eqs. (1) and (2), other than the system with a shear field, we may mention the color field system in which the system consists of many particles with charges of different signs and is driven by an external electric field [22,41].

In general, the quantity  $\alpha(t)$ , which is interpreted as the friction coefficient, depends on the coordinates and the momenta of the particles, so is variable in time. However, it is known that the fluctuation of the quantity  $\alpha(t)$  is small in a system consisting of many particles [37]. (For a justification of this point by the kinetic approach see Ref. [42], which shows that the quantity  $\alpha(t)$  fluctuates with the order of  $1/\sqrt{N}$  around a fixed value.) Based on this fact, in this paper we consider only the system which consists of enough particles so that the friction coefficient  $\alpha(t)$  in Eq. (2) can be replaced by a fixed constant  $\bar{\alpha}$ .

For a convenience we represent the  $4N$ -dimensional phase space vector  $\Gamma(t)$  as a vector  $(q_x^{(1)}(t), q_x^{(2)}(t), \dots, q_x^{(N)}(t), q_y^{(1)}(t), q_y^{(2)}(t), \dots, q_y^{(N)}(t), p_x^{(1)}(t), p_x^{(2)}(t), \dots, p_x^{(N)}(t), p_y^{(1)}(t), p_y^{(2)}(t), \dots, p_y^{(N)}(t))^T$ . Using this notation and the assumption explained in the previous paragraph we obtain the equation

$$\frac{d\delta\Gamma(t)}{dt} = \mathcal{L}(t)\delta\Gamma(t) \quad (5)$$

for the tangent vector  $\delta\Gamma(t)$ . Here the matrix  $\mathcal{L}(t)$  is given by

$$\mathcal{L}(t) \equiv \begin{pmatrix} \Phi & I_{2N}/m \\ R(t) & \Psi \end{pmatrix} \quad (6)$$

with  $2N \times 2N$  matrices  $\Phi$ ,  $\Psi$ , and  $R$  defined by

$$\Phi \equiv \gamma\Xi_{2N}, \quad (7)$$

$$\Psi \equiv -\gamma\Xi_{2N} - \bar{\alpha}I_{2N}, \quad (8)$$

$$R(t) \equiv -\frac{\partial^2 U(t)}{\partial \mathbf{q}(t) \partial \mathbf{q}(t)}, \quad (9)$$

where we introduced  $\mathbf{q}(t)$  as a vector  $(q_x^{(1)}(t), q_x^{(2)}(t), \dots, q_x^{(N)}(t), q_y^{(1)}(t), q_y^{(2)}(t), \dots, q_y^{(N)}(t))^T$ .

### III. RANDOM INTERACTIONS AND MASTER EQUATIONS FOR THE TANGENT VECTOR DYNAMICS

In this section we introduce a random interaction between the particles, and obtain the two kinds of master equations corresponding to the time-forward tangent vector dynamics and the time-reversed tangent vector dynamics by using the Kramers-Moyal expansion technique.

#### A. Fokker-Planck equation for the forward dynamics of the tangent vector

We consider the case that each particle interacts with the other particles randomly enough so that the matrix  $R(t) \equiv (R_{jk}(t))$  can be regarded as a Gaussian white random matrix satisfying the conditions

$$\langle R_{\mu_1 \nu_1}(t_1) R_{\mu_2 \nu_2}(t_2) \cdots R_{\mu_{2n-1} \nu_{2n-1}}(t_{2n-1}) \rangle = 0, \quad (10)$$

$$\begin{aligned} & \langle R_{\mu_1 \nu_1}(t_1) R_{\mu_2 \nu_2}(t_2) \cdots R_{\mu_{2n} \nu_{2n}}(t_{2n}) \rangle \\ &= \sum_{P_d} D_{\mu_{j_1} \nu_{j_1} \mu_{j_2} \nu_{j_2}} D_{\mu_{j_3} \nu_{j_3} \mu_{j_4} \nu_{j_4}} \cdots D_{\mu_{j_{2n-1}} \nu_{j_{2n-1}} \mu_{j_{2n}} \nu_{j_{2n}}} \\ & \quad \times \delta(t_{j_1} - t_{j_2}) \delta(t_{j_3} - t_{j_4}) \cdots \delta(t_{j_{2n-1}} - t_{j_{2n}}) \end{aligned} \quad (11)$$

for any integer  $n$  and a 4th rank constant tensor  $D_{jklm}$ , where we take the sum over only the independent permutation  $P_d: (1, 2, \dots, 2n) \rightarrow (j_1, j_2, \dots, j_{2n})$ , and the bracket  $\langle \cdots \rangle$  means the ensemble average over random processes. The tensor  $D_{jklm}$  satisfies the conditions

$$D_{lnjk} = D_{jklm}, \quad (12)$$

$$D_{jknl} = D_{kjlm} = D_{jklm}, \quad (13)$$

which are derived from the relation  $D_{jklm} \delta(s-t) = \langle R_{jk}(s) R_{lm}(t) \rangle$  and the symmetry property of the matrix  $R(t)$ .

Under the randomness conditions (10) and (11) the time-evolutional equation (5) is regarded as a stochastic equation of the Langevin type, and its corresponding master equation for the the probability density  $\rho^{(+)}(\delta\Gamma, t)$  for the tangent vector  $\delta\Gamma$  at time  $t$  is given by

$$\begin{aligned} \frac{\partial}{\partial t} \rho^{(+)}(\delta\Gamma, t) = & - \sum_{\mu=1}^{2N} \sum_{\nu=1}^{2N} \frac{\partial}{\partial \delta q_{\mu}} \\ & \times \left( \Phi_{\mu\nu} \delta q_{\nu} + \frac{\delta_{\mu\nu}}{m} \delta p_{\nu} \right) \rho^{(+)}(\delta\Gamma, t) \\ & - \sum_{\mu=1}^{2N} \sum_{\nu=1}^{2N} \frac{\partial}{\partial \delta p_{\mu}} \Psi_{\mu\nu} \delta p_{\nu} \rho^{(+)}(\delta\Gamma, t) \\ & + \sum_{\mu=1}^{2N} \sum_{\nu=1}^{2N} \sum_{\mu'=1}^{2N} \sum_{\nu'=1}^{2N} \frac{1}{2} D_{\mu'\mu\nu'\nu} \delta q_{\mu} \delta q_{\nu} \\ & \times \frac{\partial^2}{\partial \delta p_{\mu'} \partial \delta p_{\nu'}} \rho^{(+)}(\delta\Gamma, t) \end{aligned} \quad (14)$$

applying the Kramers-Moyal expansion technique to the dynamics (5). Here  $\delta q_j$  and  $\delta p_j$  are the  $j$ th components of the coordinate part  $\delta\mathbf{q}$  and the momentum part  $\delta\mathbf{p}$  in the tangent vector  $\delta\Gamma = (\delta\mathbf{q}, \delta\mathbf{p})^T$ , respectively, and  $\Phi_{\mu\nu}$  and  $\Psi_{\mu\nu}$  are the matrix elements of the matrix  $\Phi$  and  $\Psi$  defined by Eqs. (7) and (8), respectively. The derivation of Eq. (14) is given in Appendix A. Equation (14) in the special case of  $\Phi = 0_{2N}$  and  $\Psi = 0_{2N}$  have already been used to discuss the stepwise structure of the Lyapunov spectrum for a many-particle Hamiltonian system [10].

### B. Anti-Fokker-Planck equation for the time-reversed dynamics of the tangent vector

As shown in Ref. [10], in the case of  $\gamma=0$  and  $\bar{\alpha}=0$  the Fokker-Planck equation (14) provides the positive branch of Lyapunov exponents as the time-averaged exponential rate of the randomness average by the probability density  $\rho^{(+)}(\Gamma, t)$  in the time evolution of infinitesimal perturbations of the dynamical variables. However, this method does not provide directly the negative branch of Lyapunov exponents, because in the stochastic system *the randomness average of the distance between the infinitesimal nearby trajectories should not shrink in the infinite time limit*. This was not a problem in the Hamiltonian system discussed in Ref. [10], because in the Hamiltonian system the absolute values of the negative Lyapunov exponents are the same with the positive Lyapunov exponents [17]. However, in the thermostated system discussed in this paper such a simple relation of the negative and the positive Lyapunov exponents cannot be expected any more. In order to overcome this problem and to provide the negative branch of Lyapunov exponents using the master equation approach directly, we use the fact that *the negative Lyapunov exponents can be regarded as the positive Lyapunov exponents for the time-reversed motion*. This fact has been used in some works to calculate the negative Lyapunov exponents for chaotic systems [26,43,44].

In the iso-kinetic thermostated system with a shear field the time-reversed motion is expressed by the ‘‘time-reversed mapping’’ [36]:  $\mathbf{q} \rightarrow \mathbf{q}$ ,  $\mathbf{p} \rightarrow -\mathbf{p}$  and  $\gamma \rightarrow -\gamma$ . The transformation  $\gamma \rightarrow -\gamma$  is justified by the fact that the direction of the shear flow changes to the opposite direction in the time-reversed motion. This justifies the time-reversal transformation  $\bar{\alpha} \rightarrow -\bar{\alpha}$  for the friction coefficient by Eq. (4). The time-reversed mapping leads to the time-reversed operation  $\hat{T}$  defined by

$$\delta\mathbf{q} \rightarrow \delta\mathbf{q}, \quad (15)$$

$$\delta\mathbf{p} \rightarrow -\delta\mathbf{p}, \quad (16)$$

$$\Phi \rightarrow -\Phi, \quad (17)$$

$$\Psi \rightarrow -\Psi, \quad (18)$$

for the tangent vector dynamics, noting the relations (7) and (8) to connect the matrices  $\Phi$  and  $\Psi$  with the shear rate  $\gamma$  and the friction coefficient  $\bar{\alpha}$ . It is important to note that the tensor  $D_{jklm}$  itself is invariant under the time-reversed mapping.

Now we introduce the Fokker-Planck equation for the probability density  $\rho^{(-)}(\delta\Gamma, t)$  for the time-reversed tangent vector at time  $t$  as the transformed equation of the Fokker-Planck equation (14) by the time-reversed operation  $\hat{T}$  and the transformation  $t \rightarrow -t$ , namely

$$\begin{aligned} \frac{\partial}{\partial t} \rho^{(-)}(\delta\Gamma, t) = & - \sum_{\mu=1}^{2N} \sum_{\nu=1}^{2N} \frac{\partial}{\partial \delta q_{\mu}} \\ & \times \left( \Phi_{\mu\nu} \delta q_{\nu} + \frac{\delta_{\mu\nu}}{m} \delta p_{\nu} \right) \rho^{(-)}(\delta\Gamma, t) \\ & - \sum_{\mu=1}^{2N} \sum_{\nu=1}^{2N} \frac{\partial}{\partial \delta p_{\mu}} \Psi_{\mu\nu} \delta p_{\nu} \rho^{(-)}(\delta\Gamma, t) \\ & - \sum_{\mu=1}^{2N} \sum_{\nu=1}^{2N} \sum_{\mu'=1}^{2N} \sum_{\nu'=1}^{2N} \frac{1}{2} D_{\mu'\mu\nu'\nu} \delta q_{\mu} \delta q_{\nu} \\ & \times \frac{\partial^2}{\partial \delta p_{\mu'} \partial \delta p_{\nu'}} \rho^{(-)}(\delta\Gamma, t). \end{aligned} \quad (19)$$

In other words, if the dynamical evolution operator of the probability density  $\rho^{(+)}(\delta\Gamma, t)$  is expressed by the operator  $\exp(\hat{\Pi}t)$  (so that  $\rho^{(+)}(\delta\Gamma, t) = \exp(\hat{\Pi}t)\rho^{(+)}(\delta\Gamma, 0)$ ) with a time-independent operator  $\hat{\Pi}$  then the dynamical evolution operator of the probability density  $\rho^{(-)}(\delta\Gamma, t)$  is given by the operator  $\exp(-\hat{T}\hat{\Pi}\hat{T}t)$ . Equation (19) is simply the equation with the opposite sign of the diffusion term to the forward Fokker-Planck equation (14), and is interpreted as the master equation to describe the time evolution of the tangent vector whose initial condition is the time-reversed initial condition to the Fokker-Planck equation (14). We call this equation for the probability density  $\rho^{(-)}(\delta\Gamma, t)$  the ‘‘anti-Fokker-Planck equation’’ in this paper, and calculate the negative Lyapunov

exponents as the exponential rate of the randomness average by the probability density  $\rho^{(-)}(\delta\Gamma, t)$  in the time evolution of infinitesimal perturbations of the dynamical variables in the minus infinite time.

It is important to note the difference between the anti-Fokker-Planck equation (19) and the so called ‘‘backward Fokker-Planck equation’’ [46]. The backward Fokker-Planck equation describes the dynamics before an initial time in which the initial condition is the same as that in the forward Fokker-Planck equation that describes the dynamics after the initial time. However, in order to calculate the negative Lyapunov exponents from the time-reversed motion, we must use the different initial condition which has the opposite sign of the momentum to the initial condition in the forward Fokker-Planck equation. In the equilibrium case expressed by  $\gamma=0$  and  $\bar{\alpha}=0$  the backward Fokker-Planck equation coincides with the anti-Fokker-Planck equation, but otherwise it cannot be used to calculate the negative Lyapunov exponents.

The anti-Fokker-Planck equation is analogous to the anti-Lorentz-Boltzmann equation which was introduced to calculate the negative Lyapunov exponents using the kinetic approach [26,44,45]. In this approach the anti-Lorentz-Boltzmann equation is given as the Lorentz-Boltzmann equation where the collision operator has the opposite sign to the ordinary Lorentz-Boltzmann equation in an equilibrium or a nonequilibrium stationary state.

At least, in the equilibrium case expressed by  $\gamma=0$  and  $\bar{\alpha}=0$  the anti-Fokker-Planck equation must provide the negative Lyapunov exponents as the opposites of the positive Lyapunov exponents calculated by using the Fokker-Planck equation (14). In the following section we show that it is actually a special case of more general results.

#### IV. CONJUGATE PAIRING RULE FOR THERMOSTATED SYSTEMS WITH A SHEAR

We have to know the time evolution of the amplitude of the tangent vector in order to calculate the Lyapunov exponents. Such a time evolution for the forward movement (the time-reversed movement) is expressed as the dynamics of the diagonal elements of the matrix  $\mathbf{Y}^{(+)}(t)$  (the matrix  $\mathbf{Y}^{(-)}(t)$ ) given by

$$\mathbf{Y}^{(\pm)}(t) \equiv \langle \delta\mathbf{q} \delta\mathbf{q}^T \rangle_t^{(\pm)}. \quad (20)$$

Here the bracket  $\langle \dots \rangle_t^{(\pm)}$  means to take the average by the probability density  $\rho^{(\pm)}(\delta\Gamma, t)$ , namely,

$$\langle X(\delta\Gamma) \rangle_t^{(\pm)} \equiv \int d\delta\Gamma X(\delta\Gamma) \rho^{(\pm)}(\delta\Gamma, t) \quad (21)$$

for any function  $X(\delta\Gamma)$  of  $\delta\Gamma$ . In Ref. [10] the positive Lyapunov exponents were calculated by the time-averaged exponential rate of the diagonal elements of an orthogonal-transformed matrix of  $\mathbf{Y}^{(+)}(t)$ . We get the negative Lyapunov exponents from the matrix  $\mathbf{Y}^{(-)}(t)$  by a similar procedure. The introduction of Lyapunov exponents by the

spatial coordinate part only (or the momentum part only) of the tangent vector has been used previously by Refs. [44,47].

We introduce the matrix  $\tilde{\mathbf{Y}}^{(\pm)}(t)$  defined by

$$\tilde{\mathbf{Y}}^{(\pm)}(t) \equiv \mathbf{Y}^{(\pm)}(\pm t) e^{\pm \bar{\alpha} t}. \quad (22)$$

As shown in Appendix B, the matrix  $\tilde{\mathbf{Y}}^{(\pm)}(t)$  satisfies the differential equation

$$\begin{aligned} \frac{d^4 \tilde{\mathbf{Y}}^{(\pm)}(t)}{dt^4} - \frac{1}{2} \left[ \Omega^2 \frac{d^2 \tilde{\mathbf{Y}}^{(\pm)}(t)}{dt^2} + \frac{d^2 \tilde{\mathbf{Y}}^{(\pm)}(t)}{dt^2} (\Omega^2)^T \right] \\ + \frac{1}{16} [\Omega^4 \tilde{\mathbf{Y}}^{(\pm)}(t) - 2\Omega^2 \tilde{\mathbf{Y}}^{(\pm)}(t) (\Omega^2)^T + \tilde{\mathbf{Y}}^{(\pm)}(t) \\ \times (\Omega^4)^T] - \frac{2}{m^2} \hat{\mathcal{D}} \left\{ \frac{d \tilde{\mathbf{Y}}^{(\pm)}(t)}{dt} \right\} = 0, \end{aligned} \quad (23)$$

where we assumed the probability density  $\rho^{(\pm)}(\delta\Gamma, t)$  to be zero at the boundary of the tangent space. Here  $\Omega$  is the  $(2N) \times (2N)$  matrix defined by

$$\Omega \equiv \Phi - \Psi. \quad (24)$$

and  $\hat{\mathcal{D}}$  is the linear operator to map any  $(2N) \times (2N)$  matrix  $X \equiv (X_{jk})$  to the  $(2N) \times (2N)$  matrix  $\hat{\mathcal{D}}\{X\} \equiv ((\hat{\mathcal{D}}\{X\})_{jk})$  defined by

$$(\hat{\mathcal{D}}\{X\})_{jk} \equiv \sum_{\mu=1}^N \sum_{\nu=1}^N D_{j\mu k\nu} X_{\mu\nu}. \quad (25)$$

It may be noted that Eq. (23) for the matrix  $\tilde{\mathbf{Y}}^{(\pm)}(t)$  is invariant under the transformation  $\Omega \rightarrow -\Omega$ .

We can choose the initial probability density  $\rho^{(+)}(\delta\Gamma, 0)$  arbitrarily to calculate the positive Lyapunov exponents. On the other hand in order to derive the corresponding negative Lyapunov exponents we assume the initial probability density  $\rho^{(-)}(\delta\Gamma, 0)$  for the time-reversed tangent vector to satisfy the condition  $d^k \tilde{\mathbf{Y}}^{(-)}(t)/dt^k|_{t=0} = d^k \tilde{\mathbf{Y}}^{(+)}(t)/dt^k|_{t=0}$ ,  $k = 0, 1, 2, 3$  at the initial time  $t=0$ . Under this assumption it follows from Eq. (23) that

$$\mathbf{Y}^{(-)}(-t) e^{-\bar{\alpha} t} = \mathbf{Y}^{(+)}(t) e^{\bar{\alpha} t}, \quad (26)$$

because the quantities  $\tilde{\mathbf{Y}}^{(+)}(t)$  and  $\tilde{\mathbf{Y}}^{(-)}(t)$  defined by Eq. (22) satisfy the same differential equation (23) and have the same initial condition. Therefore, the diagonal element  $\tilde{Y}_{jj}^{(\pm)}(t)$  of any orthogonal-transformed matrix of  $\mathbf{Y}^{(\pm)}(t)$  must satisfy the relation

$$\tilde{Y}_{jj}^{(-)}(-t) = \tilde{Y}_{jj}^{(+)}(t) e^{2\bar{\alpha} t}. \quad (27)$$

This equation connects the time-forward evolution and the time-reversed evolution in the amplitudes of the spatial part of the tangent vector in the thermostated system.

The  $j$ th positive (or zero) Lyapunov exponent  $\lambda_j^{(+)}$  and its conjugate negative (or zero) exponent  $\lambda_j^{(-)}$  are given by

$$\lambda_j^{(\pm)} = \lim_{t \rightarrow \pm\infty} \frac{1}{2t} \ln \frac{\dot{Y}_{jj}^{(\pm)}(t)}{\dot{Y}_{jj}^{(\pm)}(0)}. \quad (28)$$

The quantity  $\dot{Y}_{jj}^{(\pm)}(t)$  satisfies the condition  $\dot{Y}_{jj}^{(+)}(0) = \dot{Y}_{jj}^{(-)}(0)$  at the initial time, and using Eqs. (27) and (28) we obtain

$$\lambda_j^{(+)} + \lambda_j^{(-)} = -\bar{\alpha}. \quad (29)$$

This is the conjugate pairing rule of the Lyapunov spectrum for the iso-kinetic thermostated system with a shear field. It is clear that it is attributed to the pairing rule of the Hamiltonian system in the case of  $\bar{\alpha} = 0$ .

### V. CONJUGATE PAIRING RULE FOR A COLOR FIELD

For an actual calculation of the Lyapunov spectrum for an iso-kinetic thermostated system by the master equation approach we have to know the value of tensor  $D_{jklm}$  and to solve the differential equation (23) for the matrix  $\tilde{Y}^{(\pm)}(t)$ . Let us discuss these points briefly by using a case without a shear field such as a color field system [22,41], namely

$$\gamma = 0. \quad (30)$$

For simplicity in this section we also assume that the tensor  $D_{jklm}$  is expressed as the multiplication of the matrix elements of a symmetric  $(2N) \times (2N)$  matrix  $W \equiv (W_{jk})$ :

$$D_{jklm} = W_{jk} W_{ln}. \quad (31)$$

Under this assumption the conditions (12) and (13) are automatically satisfied. This assumption was also used in Ref. [10] to discuss the stepwise structure of Lyapunov spectra.

As shown in Appendix C, under the assumptions (30) and (31) the equation of the matrix  $\tilde{Y}^{(\pm)}(t)$  is simplified to

$$\frac{d^3 \tilde{Y}^{(\pm)}(t)}{dt^3} - \bar{\alpha}^2 \frac{d \tilde{Y}^{(\pm)}(t)}{dt} - \frac{2}{m^2} W \tilde{Y}^{(\pm)}(t) W = 0. \quad (32)$$

It is shown that Eq. (23) is given by taking the time differential in both the sides of Eq. (32). Using the orthogonal matrix  $V$  diagonalizing the matrix  $W$ , namely

$$(V^T W V)_{jk} = \omega_j \delta_{jk} \quad (33)$$

with a real eigenvalue  $\omega_j$ , the quantity  $\dot{Y}_{jj}^{(\pm)}(t)$  is expressed as the diagonal element of the matrix  $\dot{Y}^{(\pm)}(t) \equiv (\dot{Y}_{jk}^{(\pm)}(t))$  defined by

$$\dot{Y}^{(\pm)}(t) = V^T \dot{Y}^{(\pm)}(t) V. \quad (34)$$

Using Eq. (34) we can solve the equation for the quantity  $\dot{Y}_{jj}^{(\pm)}(t)$  derived from Eq. (32), and by using Eqs. (22), (28), and (34) the Lyapunov exponents are given by

$$\lambda_j^{(\pm)} = -\frac{\bar{\alpha}}{2} \pm \frac{1}{2} \left( \Lambda_j + \frac{\bar{\alpha}^2}{3\Lambda_j} \right), \quad (35)$$

where  $\Lambda_j$  is defined by

$$\Lambda_j \equiv \left[ \left( \frac{\omega_j}{m} \right)^2 + \sqrt{\left( \frac{\omega_j}{m} \right)^4 - \left( \frac{\bar{\alpha}^2}{3} \right)^3} \right]^{1/3}. \quad (36)$$

[See Appendix C about a derivation of Eq. (35).] It is clear that the Lyapunov exponents given by Eq. (35) satisfy the conjugate pairing rule (29).

Concerning the expression (35) for the Lyapunov exponent it is important to note that the tensor  $D_{jklm}$  can depend on external force fields. This implies that the eigenvalue  $\omega_j$  of the matrix  $W$  can depend on the friction coefficient  $\bar{\alpha}$ . If we were to assume the quantity  $\omega_j$  to be independent of the friction coefficient  $\bar{\alpha}$ , then we obtain the expression of the Lyapunov exponents as  $\lambda_j^{(\pm)} = \pm |\omega_j / (2m)|^{2/3} - \bar{\alpha}/2 + O(\bar{\alpha}^2)$  from Eq. (35) in the case of  $|\bar{\alpha}| \leq \sqrt{3} |\omega_j / m|^{2/3}$ . However, this is not consistent with the numerical results in a deterministic many-hard-disk system with a color field in which the negative Lyapunov exponents rather increase as the value of the friction coefficient increases [22]. This consideration suggests that we should not neglect the external force field dependence of the correlation amplitude  $D_{jklm}$  at least in the color field case. The dependence of the tensor  $D_{jklm}$  on the shear rate and the external force fields should be a subject for a separated paper, although the conjugate pairing rule of the Lyapunov spectrum is correct regardless of their dependence as shown in this paper.

### VI. CONCLUSION AND REMARKS

In this paper, we have applied the master equation approach to Lyapunov spectra to nonequilibrium iso-kinetic thermostated systems in order to discuss a conjugate pairing rule. We considered two-dimensional many-particle system with Gaussian white random interactions between the particles. In this system the positive Lyapunov exponents are calculated by a (forward) Fokker-Planck equation for the tangent vector dynamics. We proposed a method to calculate the negative Lyapunov exponents by a time-reversed master equation, especially the anti-Fokker-Planck equation where the diffusion term has the opposite sign to the forward Fokker-Planck equation. Using the Lyapunov exponents calculated by these two Fokker-Planck equations we showed the conjugate pairing rule of the Lyapunov spectrum for iso-kinetic thermostated systems with a shear field given by the Sllod equation in the thermodynamic limit. We also gave a concrete form to connect the Lyapunov exponents with the time-correlation of the interaction matrix in a thermostated system without a shear field.

We discussed the conjugate pairing rule based on the iso-kinetic thermostat in the thermodynamic limit. However, it is known that the iso-kinetic thermostat is formally equivalent to other thermostats such as the iso-energetic thermostat in the thermodynamic limit [35]. In this sense our result should be correct in systems with such other thermostats, more explicitly as far as the friction coefficient can be regarded as a constant even in a finite number of particle systems.

In order to get the anti-Fokker-Planck equation we used

the fact that the shear rate  $\gamma$  changes its sign in the time reversed motion. However, this time-reversed change of the sign of the shear rate to get the anti-Fokker-Planck equation may not be essential to obtain the negative Lyapunov exponents, if the Lyapunov exponents are even functions of the shear rate. We have not proved the invariance of the Lyapunov exponents under the transformation  $\gamma \rightarrow -\gamma$  in this paper, but the invariance of Eq. (23) under the transformation  $\Omega \rightarrow -\Omega$  implies that the Lyapunov exponents are invariant under this transformation.

We can show that all the Lyapunov exponents  $\lambda_j^{(+)}$  ( $\lambda_j^{(-)}$ ) are non-negative (nonpositive) in the case of  $\gamma=0$  (See Appendix C). This implies that in this case the number of the positive Lyapunov exponents should be equal to the number of the negative Lyapunov exponents, possibly except for a few Lyapunov exponents making pairs with zero Lyapunov exponents. However, we have not proved that it is also correct in the presence of a shear field:  $\gamma \neq 0$ . Concerning this point we should notice that a numerical calculation of the Lyapunov spectrum for the Sllod equations (1) and (2) showed that in the case of a high shear rate the number of positive Lyapunov exponents can be less than the number of negative Lyapunov exponents [40]. Therefore, it should be interesting to check whether the master equation approach to the Lyapunov spectrum can describe such a situation or not.

It should be noted that the discussion of this paper does not conclude that the conjugate pairing rule of the Lyapunov spectrum for the thermostated system with a shear field must be satisfied rigorously in deterministic chaotic systems. To show the conjugate pairing rule in this paper we assumed the Gaussian white randomness (10) and (11) for the particle interactions, and there is no guarantee that we can justify the conjugate pairing rule by the master equation approach under a more general random interaction of particles, for example under the non-Gaussian randomness of the particle interaction matrix which leads to a more general master equation for the tangent vector rather than a simple Fokker-Planck equation (14). A generalization of the conjugate pairing rule by the master equation approach to a more general random interaction remains as one of the important future problems.

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#### APPENDIX A: MASTER EQUATION FOR THE TANGENT VECTOR

In this appendix we derive the Fokker-Planck equation (14) for the tangent vector dynamics. Using the Kramers-Moyal expansion the dynamics of the probability density  $\rho^{(+)}(\delta\Gamma, t)$  is given by [46]

$$\frac{\partial \rho^{(+)}(\delta\Gamma, t)}{\partial t} = \sum_{n=1}^{\infty} \sum_{j_1=1}^{2N} \sum_{j_2=1}^{2N} \cdots \sum_{j_n=1}^{2N} (-1)^n \times \frac{\partial^n \Xi_{j_1 j_2 \cdots j_n}^{(n)}(\delta\Gamma, t) \rho^{(+)}(\delta\Gamma, t)}{\partial \delta\Gamma_{j_1} \partial \delta\Gamma_{j_2} \cdots \partial \delta\Gamma_{j_n}}, \quad (\text{A1})$$

where  $\Xi_{j_1 j_2 \cdots j_n}^{(n)}(\delta\Gamma, t)$  is defined by

$$\begin{aligned} \Xi_{j_1 j_2 \cdots j_n}^{(n)}(\delta\Gamma, t) &\equiv \frac{1}{n!} \lim_{s \rightarrow 0} \frac{1}{s} \langle [\delta\Gamma_{j_1}(t+s) - \delta\Gamma_{j_1}(t)] \\ &\quad \times [\delta\Gamma_{j_2}(t+s) - \delta\Gamma_{j_2}(t)] \cdots \\ &\quad \times [\delta\Gamma_{j_n}(t+s) - \delta\Gamma_{j_n}(t)] \rangle_{\delta\Gamma(t)=\delta\Gamma} \quad (\text{A2}) \end{aligned}$$

and  $\delta\Gamma_{j_i}(t)$  is the  $j$ th component of the tangent vector  $\delta\Gamma(t)$ . Using Eq. (5) we obtain

$$\begin{aligned} \delta\Gamma(t+s) - \delta\Gamma(t) &= \left\{ T \exp \left[ \int_t^{t+s} d\tau \mathcal{L}(\tau) \right] - 1 \right\} \delta\Gamma(t) \\ &= \sum_{n=1}^{\infty} \int_t^{t+s} d\tau_n \int_t^{\tau_n} d\tau_{n-1} \cdots \int_t^{\tau_2} d\tau_1 \\ &\quad \times \mathcal{L}(\tau_n) \mathcal{L}(\tau_{n-1}) \cdots \mathcal{L}(\tau_1) \delta\Gamma(t). \quad (\text{A3}) \end{aligned}$$

It follows from Eqs. (6), (10), (11), (A2), and (A3) that

$$\begin{aligned} \Xi^{(1)}(\delta\Gamma, t) &\equiv (\Xi_1^{(1)}(\delta\Gamma, t), \Xi_2^{(1)}(\delta\Gamma, t), \dots, \Xi_{2N}^{(1)}(\delta\Gamma, t))^T \\ &= \lim_{s \rightarrow 0} \frac{1}{s} \langle [\delta\Gamma(t+s) - \delta\Gamma(t)] \rangle_{\delta\Gamma(t)=\delta\Gamma} \\ &= \lim_{s \rightarrow 0} \frac{1}{s} \int_t^{t+s} d\tau \langle \mathcal{L}(\tau) \rangle \delta\Gamma = \begin{pmatrix} \Phi \delta\mathbf{q} + \delta\mathbf{p}/m \\ \Psi \delta\mathbf{p}/m \end{pmatrix} \quad (\text{A4}) \end{aligned}$$

and

$$\begin{aligned} \Xi^{(2)}(\delta\Gamma, t) &\equiv (\Xi_{jk}^{(2)}(\delta\Gamma, t)) = \lim_{s \rightarrow 0} \frac{1}{2s} \langle [\delta\Gamma(t+s) - \delta\Gamma(t)] \\ &\quad \times [\delta\Gamma(t+s) - \delta\Gamma(t)]^T \rangle_{\delta\Gamma(t)=\delta\Gamma} \\ &= \lim_{s \rightarrow 0} \frac{1}{2s} \int_t^{t+s} d\kappa \int_t^{\kappa} d\tau \langle \mathcal{L}(\kappa) \delta\Gamma \delta\Gamma^T \mathcal{L}(\tau)^T \rangle \\ &= \begin{pmatrix} 0_{2N} & 0_{2N} \\ 0_{2N} & \eta(\delta\mathbf{q}) \end{pmatrix}, \quad (\text{A5}) \end{aligned}$$

where  $\eta(\delta\mathbf{q}) \equiv (\eta_{jk}(\delta\mathbf{q}))$  is defined by

$$\eta_{jk}(\delta\mathbf{q}) \equiv \frac{1}{2} \sum_{\mu=1}^N \sum_{\nu=1}^N D_{j\mu k\nu} \delta q_{\mu} \delta q_{\nu}. \quad (\text{A6})$$

Here the only nonzero contributions come from the  $n=1$  term of Eq. (A3). For general  $n$ , the number of  $\delta$  functions from Eq. (11) must be only one less than the number of time integrals, to give a nonzero contribution. It is straightforward to show that this never happens for  $n > 1$ . Concerning the terms including  $\Xi_{j_1 j_2 \cdots j_n}^{(n)}(\delta\Gamma, t)$ ,  $n=3, 4$ , etc., in the right-hand side of Eq. (A1) we obtain

$$\Xi_{j_1 j_2 \dots j_n}^{(n)}(\delta\Gamma, t) = 0, \quad n=3,4, \dots, \quad (\text{A7})$$

because of the Gaussian white properties (10) and (11) of the random matrix  $R(t)$ . Using Eqs. (A1), (A4), (A5), and (A7) we obtain the Fokker-Planck equation (14).

### APPENDIX B: EQUATION FOR THE MATRIX $\tilde{Y}^{(\pm)}$

In this appendix we give details of the derivation of Eq. (23) from Eqs. (14), (19), and (20). We start this derivation by introducing the  $(2N) \times (2N)$  matrices  $\mathcal{F}^{(\pm)}(t)$  and  $\mathcal{G}^{(\pm)}(t)$  defined by

$$\mathcal{F}^{(\pm)}(t) \equiv \langle \delta\mathbf{q} \delta\mathbf{p}^T \rangle_t^{(\pm)}, \quad (\text{B1})$$

$$\mathcal{G}^{(\pm)}(t) \equiv \langle \delta\mathbf{p} \delta\mathbf{p}^T \rangle_t^{(\pm)}. \quad (\text{B2})$$

Equations (14) and (19) lead to

$$\begin{aligned} \frac{dY^{(\pm)}(t)}{dt} &= \Phi Y^{(\pm)}(t) + Y^{(\pm)}(t) \Phi^T + \frac{1}{m} [\mathcal{F}^{(\pm)}(t) \\ &\quad + \mathcal{F}^{(\pm)}(t)^T], \end{aligned} \quad (\text{B3})$$

$$\frac{d\mathcal{F}^{(\pm)}(t)}{dt} = \Phi \mathcal{F}^{(\pm)}(t) + \mathcal{F}^{(\pm)}(t) \Psi^T + \frac{1}{m} \mathcal{G}^{(\pm)}(t), \quad (\text{B4})$$

$$\begin{aligned} \frac{d\mathcal{G}^{(\pm)}(t)}{dt} &= \Psi \mathcal{G}^{(\pm)}(t) + \mathcal{G}^{(\pm)}(t) \Psi^T \pm \hat{D}\{Y^{(\pm)}(t)\} \\ &\quad (\text{B5}) \end{aligned}$$

for the matrices  $Y^{(\pm)}(t)$ ,  $\mathcal{F}^{(\pm)}(t)$ , and  $\mathcal{G}^{(\pm)}(t)$  with the operator  $\hat{D}$  defined by Eq. (25). Here, to derive Eq. (B5) we used the relation (12).

Equations (B3), (B4), and (B5) are equivalent to

$$\frac{d\check{Y}^{(\pm)}(t)}{dt} = \check{\mathcal{F}}^{(\pm)}(t) P(t)^T + P(t) \check{\mathcal{F}}^{(\pm)}(t)^T, \quad (\text{B6})$$

$$\frac{d\check{\mathcal{F}}^{(\pm)}(t)}{dt} = P(t) \check{\mathcal{G}}^{(\pm)}(t), \quad (\text{B7})$$

$$\frac{d\check{\mathcal{G}}^{(\pm)}(t)}{dt} = \pm \hat{D}_t \{\check{Y}^{(\pm)}(t)\}, \quad (\text{B8})$$

where  $\check{Y}^{(\pm)}(t)$ ,  $\check{\mathcal{F}}^{(\pm)}(t)$ , and  $\check{\mathcal{G}}^{(\pm)}(t)$  are defined by

$$\check{Y}^{(\pm)}(t) \equiv e^{-\Phi t} Y^{(\pm)}(t) e^{-\Phi^T t}, \quad (\text{B9})$$

$$\check{\mathcal{F}}^{(\pm)}(t) \equiv e^{-\Phi t} \mathcal{F}^{(\pm)}(t) e^{-\Psi^T t}, \quad (\text{B10})$$

$$\check{\mathcal{G}}^{(\pm)}(t) \equiv e^{-\Psi t} \mathcal{G}^{(\pm)}(t) e^{-\Psi^T t}, \quad (\text{B11})$$

and  $P(t)$  is the  $(2N) \times (2N)$  matrix defined by

$$P(t) \equiv \frac{1}{m} e^{-\Omega t} \quad (\text{B12})$$

with the matrix  $\Omega$  defined by Eq. (24), and  $\hat{D}_t\{\dots\}$  is defined by

$$\hat{D}_t\{X\} \equiv e^{-\Psi t} \hat{D}\{e^{\Phi t} X e^{\Phi^T t}\} e^{-\Psi^T t} \quad (\text{B13})$$

for any  $(2N) \times (2N)$  matrix  $X$ . Here we used the relation

$$\Phi \Psi = \Psi \Phi, \quad (\text{B14})$$

so that we have the equation  $\exp\{-\Phi t\} \exp\{\Psi t\} = \exp\{-(\Phi - \Psi)t\}$ .

Noting that the matrix  $\check{\mathcal{G}}^{(\pm)}(t)$  is symmetric and the inverse matrix of the matrix  $P(t)$  is given by  $P(t)^{-1} = m \exp\{\Omega t\}$ , we obtain

$$\begin{aligned} 2\check{\mathcal{G}}^{(\pm)}(t) &= P(t)^{-1} \frac{d\check{\mathcal{F}}^{(\pm)}(t)}{dt} + \frac{d\check{\mathcal{F}}^{(\pm)}(t)^T}{dt} [P(t)^{-1}]^T \\ &= P(t)^{-1} \frac{d^2\check{Y}^{(\pm)}(t)}{dt^2} [P(t)^{-1}]^T + P(t)^{-1} \check{\mathcal{F}}^{(\pm)}(t) \Omega^T \\ &\quad + \Omega \check{\mathcal{F}}^{(\pm)}(t)^T [P(t)^{-1}]^T \end{aligned} \quad (\text{B15})$$

by using Eqs. (B6), (B7), and (B12). Besides, using Eqs. (B6), (B7), and (B12) we obtain

$$\begin{aligned} \frac{d}{dt} \{P(t)^{-1} \check{\mathcal{F}}^{(\pm)}(t) \Omega^T + \Omega \check{\mathcal{F}}^{(\pm)}(t)^T [P(t)^{-1}]^T\} \\ = \Omega P(t)^{-1} \frac{d\check{Y}^{(\pm)}(t)}{dt} [P(t)^{-1}]^T \Omega^T + \check{\mathcal{G}}^{(\pm)}(t) \Omega^T \\ + \Omega \check{\mathcal{G}}^{(\pm)}(t), \end{aligned} \quad (\text{B16})$$

where we again used the relation  $\check{\mathcal{G}}^{(\pm)}(t)^T = \check{\mathcal{G}}^{(\pm)}(t)$ . It follows from Eqs. (B6), (B7), and (B8) that

$$\begin{aligned} \pm 2 \hat{D}_t \{\check{Y}^{(\pm)}(t)\} &= \frac{d}{dt} P(t)^{-1} \frac{d^2\check{Y}^{(\pm)}(t)}{dt^2} [P(t)^{-1}]^T \\ &\quad + \Omega P(t)^{-1} \frac{d\check{Y}^{(\pm)}(t)}{dt} [P(t)^{-1}]^T \Omega^T \\ &\quad + \check{\mathcal{G}}^{(\pm)}(t) \Omega^T + \Omega \check{\mathcal{G}}^{(\pm)}(t). \end{aligned} \quad (\text{B17})$$

Taking the time differential of both the sides of Eq. (B17), and using Eq. (B8) we obtain

$$\begin{aligned} \frac{d^2}{dt^2} P(t)^{-1} \frac{d^2\check{Y}^{(\pm)}(t)}{dt^2} [P(t)^{-1}]^T \\ + \Omega \frac{d}{dt} P(t)^{-1} \frac{d\check{Y}^{(\pm)}(t)}{dt} [P(t)^{-1}]^T \Omega^T \\ \mp 2 \frac{d}{dt} \hat{D}_t \{\check{Y}^{(\pm)}(t)\} \pm \hat{D}_t \{\check{Y}^{(\pm)}(t)\} \Omega^T \\ \pm \Omega \hat{D}_t \{\check{Y}^{(\pm)}(t)\} = 0. \end{aligned} \quad (\text{B18})$$

This is the equation for the quantity  $\check{Y}^{(\pm)}(t)$  only.

Now we derive the equation for  $\check{Y}^{(\pm)}(t)$  defined by Eq. (22) from Eq. (B18) for  $\check{Y}^{(\pm)}(t)$  defined by Eq. (B9). We note

$$\Omega = 2\Phi + \bar{\alpha}I_{2N} \quad (\text{B19})$$

$$= -2\Psi - \bar{\alpha}I_{2N} \quad (\text{B20})$$

which is derived from Eqs. (7), (8), and (24). Using Eqs. (22), (B9), and (B19) the matrices  $\check{Y}^{(\pm)}(t)$  are connected with the matrix  $\check{Y}^{(\pm)}(t)$  by

$$\check{Y}^{(\pm)}(t) = e^{-\Omega t/2} \check{Y}^{(\pm)}(\pm t) e^{-\Omega^T t/2}. \quad (\text{B21})$$

We introduce the multiplication  $X \otimes Y$  of  $X$  and  $Y$  which is defined by

$$X \otimes Y \equiv \frac{1}{2} [XY + (XY)^T] \quad (\text{B22})$$

for any square matrices  $X$  and  $Y$  of the same size. This multiplication is used in the relation

$$\frac{d}{dt} e^{\pm \Omega t/2} Z(t) e^{\pm \Omega^T t/2} = e^{\pm \Omega t/2} \left[ \frac{dZ(t)}{dt} \pm \Omega \otimes Z(t) \right] e^{\pm \Omega^T t/2} \quad (\text{B23})$$

satisfied by any  $(2N) \times (2N)$  symmetric matrix  $Z(t)$  as a function of  $t$ . Noting Eqs. (B22) and (B23), Eq. (B21) leads to

$$P(t)^{-1} \frac{d\check{Y}^{(\pm)}(t)}{dt} [P(t)^{-1}]^T = m^2 e^{\Omega t/2} \left[ \frac{d\check{Y}^{(\pm)}(\pm t)}{dt} - \Omega \otimes \check{Y}^{(\pm)}(\pm t) \right] e^{\Omega^T t/2}, \quad (\text{B24})$$

$$P(t)^{-1} \frac{d^2\check{Y}^{(\pm)}(t)}{dt^2} [P(t)^{-1}]^T = m^2 e^{\Omega t/2} \left\{ \frac{d^2\check{Y}^{(\pm)}(\pm t)}{dt^2} - 2\Omega \otimes \frac{d\check{Y}^{(\pm)}(\pm t)}{dt} + \Omega \otimes [\Omega \otimes \check{Y}^{(\pm)}(\pm t)] \right\} e^{\Omega^T t/2}, \quad (\text{B25})$$

where we used the relation  $\check{Y}^{(\pm)}(t)^T = \check{Y}^{(\pm)}(t)$ . Moreover  $\hat{\mathcal{D}}_t$  operated on the matrix  $\check{Y}^{(\pm)}(t)$  is connected with  $\hat{\mathcal{D}}$  operated on the matrix  $\check{Y}^{(\pm)}(\pm t)$  as

$$\hat{\mathcal{D}}_t \{ \check{Y}^{(\pm)}(t) \} = e^{\Omega t/2} \hat{\mathcal{D}} \{ \check{Y}^{(\pm)}(\pm t) \} e^{\Omega^T t/2}, \quad (\text{B26})$$

where we used Eqs. (22), (B9), (B13), and (B20). Inserting Eqs. (B24), (B25), and (B26) into Eq. (B18) and using Eq. (B23) we obtain

$$\begin{aligned} & \frac{d^4\check{Y}^{(\pm)}(\pm t)}{dt^4} - 2\Omega \otimes \left[ \Omega \otimes \frac{d^2\check{Y}^{(\pm)}(\pm t)}{dt^2} \right] \\ & + \Omega \frac{d^2\check{Y}^{(\pm)}(\pm t)}{dt^2} \Omega^T + \Omega \otimes [\Omega \otimes [\Omega \otimes [\Omega \otimes \check{Y}^{(\pm)}(\pm t)]]] - \Omega [\Omega \otimes [\Omega \otimes \check{Y}^{(\pm)}(\pm t)]] \Omega^T \\ & \mp \frac{2}{m^2} \hat{\mathcal{D}} \left\{ \frac{d\check{Y}^{(\pm)}(\pm t)}{dt} \right\} = 0. \end{aligned} \quad (\text{B27})$$

Equation (B27) is equivalent to

$$\begin{aligned} & \frac{d^4\check{Y}^{(\pm)}(\pm t)}{dt^4} - \frac{1}{2} \left[ \Omega^2 \frac{d^2\check{Y}^{(\pm)}(\pm t)}{dt^2} + \frac{d^2\check{Y}^{(\pm)}(\pm t)}{dt^2} (\Omega^2)^T \right] \\ & + \frac{1}{16} [\Omega^4 \check{Y}^{(\pm)}(\pm t) - 2\Omega^2 \check{Y}^{(\pm)}(\pm t) (\Omega^2)^T + \check{Y}^{(\pm)}(\pm t) \times (\Omega^4)^T] \mp \frac{2}{m^2} \hat{\mathcal{D}} \left\{ \frac{d\check{Y}^{(\pm)}(\pm t)}{dt} \right\} = 0. \end{aligned} \quad (\text{B28})$$

By exchanging  $t$  with  $\pm t$  in Eq. (B28) we obtain Eq. (23).

### APPENDIX C: LYAPUNOV EXPONENTS IN THE COLOR FIELD CASE

In this appendix we consider the case with no shear field using the condition (30), and derive Eq. (32) under the assumption (31). We also give a derivation of Eq. (35) briefly.

Under the condition (30), the matrix  $\Omega$  defined by Eq. (24) is simply an identical matrix multiplied by a constant and is given by

$$\Omega = \bar{\alpha}I_{2N}, \quad (\text{C1})$$

and the matrix  $P(t)$  defined by Eq. (B12) and the operator  $\hat{\mathcal{D}}_t \{ \dots \}$  defined by Eq. (B13) are given by

$$P(t) = \frac{1}{m} e^{-\bar{\alpha}t} I_{2N}, \quad (\text{C2})$$

$$\hat{\mathcal{D}}_t \{ X \} = e^{2\bar{\alpha}t} \hat{\mathcal{D}} \{ X \} \quad (\text{C3})$$

for any  $(2N) \times (2N)$  matrix  $X$ . Noting Eqs. (C2) and (C3) and the relation  $\check{Y}^{(\pm)}(t) = Y^{(\pm)}(t)$ , Eqs. (B6), (B7), and (B8) are simply attributed into

$$\frac{dY^{(\pm)}(t)}{dt} = \frac{1}{m} e^{-\bar{\alpha}t} [\check{Y}^{(\pm)}(t) + \check{Y}^{(\pm)}(t)^T], \quad (\text{C4})$$

$$\frac{d\check{Y}^{(\pm)}(t)}{dt} = \frac{1}{m} e^{-\bar{\alpha}t} \check{Y}^{(\pm)}(t), \quad (\text{C5})$$

$$\frac{d\check{Y}^{(\pm)}(t)}{dt} = \pm e^{2\bar{\alpha}t} \hat{\mathcal{D}} \{ Y^{(\pm)}(t) \}. \quad (\text{C6})$$

Noting that the matrix  $\check{C}^{(\pm)}(t)$  is symmetric, Eqs. (C4), (C5), and (C6) lead to the differential equation

$$\frac{d}{dt}e^{\bar{\alpha}t}\frac{d}{dt}e^{-\bar{\alpha}t}\frac{d}{dt}Y^{(\pm)}(t)=\pm\frac{2}{m^2}e^{2\bar{\alpha}t}\hat{D}\{Y^{(\pm)}(t)\} \quad (C7)$$

for the matrix  $Y^{(\pm)}(t)$  only.

Now we consider the derivation of the equation for the matrix  $\check{Y}^{(\pm)}(t)$  [defined by Eq. (22)] from Eq. (C7) for the matrix  $Y^{(\pm)}(t)$ . It follows from Eqs. (22) and (C7) that

$$\frac{d^3\check{Y}^{(\pm)}(\pm t)}{dt^3}-\bar{\alpha}^2\frac{d\check{Y}^{(\pm)}(\pm t)}{dt}\mp\frac{2}{m^2}\hat{D}\{\check{Y}^{(\pm)}(\pm t)\}=0. \quad (C8)$$

By exchanging  $t$  with  $\pm t$  in Eq. (C8) and using Eqs. (25) and (31) we obtain Eq. (32).

Using Eqs. (32) and (34) the real function  $\xi_j^{(\pm)}(t)$  of  $t$  defined by

$$\xi_j^{(\pm)}(t)\equiv(V^T\check{Y}_{jj}^{(\pm)}(t)V)_{jj}=\check{Y}_{jj}^{(\pm)}(\pm t)e^{\pm\bar{\alpha}t} \quad (C9)$$

satisfies the equation

$$\frac{d^3\xi_j^{(\pm)}(t)}{dt^3}-\bar{\alpha}^2\frac{d\xi_j^{(\pm)}(t)}{dt}-\frac{2\omega_j^2}{m^2}\xi_j^{(\pm)}(t)=0. \quad (C10)$$

The real solution of the linear differential equation (C10) is expressed as

$$\xi_j^{(\pm)}(t)=\sum_{k=1}^3\text{Re}\{v_j^{(k)}e^{\xi_j^{(k)}t}\}, \quad (C11)$$

where  $v_j^{(k)}$ ,  $j=1,2,3$  are constants determined by the initial condition, and  $\xi_j^{(k)}$ ,  $j=1,2,3$  are the three solutions of the equation

$$\zeta^3-\bar{\alpha}^2\zeta-\frac{2\omega_j^2}{m^2}=0 \quad (C12)$$

for  $\zeta$ . Here  $\text{Re}\{X\}$  means to take the real part of any imaginary number  $X$ . We sort the quantities  $\zeta_j$ ,  $j=1,2,3$  as  $\text{Re}\{\zeta_j^{(1)}\}\geq\text{Re}\{\zeta_j^{(2)}\}\geq\text{Re}\{\zeta_j^{(3)}\}$ , so that using Eqs. (28), (34), and (C9) the Lyapunov exponent  $\lambda_j^{(\pm)}$  is expressed as

$$\lambda_j^{(\pm)}=\pm\lim_{t\rightarrow+\infty}\frac{1}{2t}\ln\frac{\xi_j^{(\pm)}(t)e^{\mp\bar{\alpha}t}}{\xi_j^{(\pm)}(0)}=-\frac{\bar{\alpha}}{2}\pm\frac{1}{2}\text{Re}\{\zeta_j^{(1)}\}. \quad (C13)$$

It follows from Eq. (C12) that  $\zeta=\zeta_j^{(1)}$  is a real solution of Eq. (C12) and satisfies the conditions  $\zeta_j^{(1)}\geq|\bar{\alpha}|\lim_{\omega_j\rightarrow 0}\zeta_j^{(1)}=|\bar{\alpha}|$ , noting that the point  $\zeta=\zeta_j^{(1)}$  is the maximum intersecting point of the graphs  $y=\zeta^3-\bar{\alpha}^2\zeta$  and  $y=2\omega_j^2/m^2$  in the  $\zeta$ - $y$  plain. This means that the Lyapunov exponents  $\lambda_j^{(+)}$  ( $\lambda_j^{(-)}$ ) must be non-negative (nonpositive). More concretely the quantity  $\zeta_j^{(1)}$  is given by

$$\zeta_j^{(1)}=\Lambda_j+\frac{\bar{\alpha}^2}{3\Lambda_j} \quad (C14)$$

with the quantity  $\Lambda_j$  defined by Eq. (36). We can check that in the case of  $|\bar{\alpha}|\leq\sqrt{3}|\omega_j/m|^{2/3}$  the quantities  $\Lambda_j$  and  $\zeta_j^{(1)}$  are both real numbers, and in the case of  $|\bar{\alpha}|>\sqrt{3}|\omega_j/m|^{2/3}$  the quantity  $\Lambda_j$  can be an imaginary number but the quantity  $\zeta_j^{(1)}$  given by Eq. (C14) is still a real number and satisfies the condition  $\lim_{\omega_j\rightarrow 0}\zeta_j^{(1)}=|\bar{\alpha}|$ . Using Eqs. (C13) and (C14) we obtain Eq. (35).

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