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Nonequilibrium mode-coupling theory for uniformly sheared systems

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We develop a nonequilibrium mode-coupling theory for uniformly sheared systems starting from microscopic, thermostatted Sllod equations of motion. Our theory aims at describing stationary-state properties including rheological ones of sheared systems, and this is accomplished via two steps. First, a set of self-consistent equations is formulated based on the projection-operator formalism and on the mode-coupling approach for the transient density correlators which measure the correlations between the density fluctuations in the initial equilibrium state and the ones at later times after the shearing force is turned on. The transient time-correlation function formalism is then used which, combined with the mode-coupling approximation, expresses stationary-state properties in terms of the transient density correlators. A detailed comparison of our theory is also presented with the related mode-coupling theory which is based on the Smoluchowski equation for Brownian particles under stationary shearing.

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I. INTRODUCTION

Nonlinear rheological behavior of glassy materials under stationary shearing has attracted considerable attention in recent years since it provides additional insight into the physics of glass transition [1–8]. For such systems driven far from equilibrium, the shear rate should be regarded as a relevant control parameter rather than as a small perturbation [9]. In this paper, we develop a nonequilibrium statistical mechanical theory for glass-forming systems in which the shear rate as well as temperature and density can be handled as external control parameters. This will be done by extending the projection-operator formalism [10] and the mode-coupling theory (MCT) [11] to nonequilibrium systems.

MCT has been known as the most successful microscopic theory for the glass transition. Indeed, extensive tests of the theoretical predictions carried out so far against experimental data and computer-simulation results suggest that the theory deals properly with some essential features of glass-forming systems [12,13]. It is therefore natural that extensions of MCT have been attempted to stationary sheared systems.

At present there exist two different approaches in such nonequilibrium extensions of MCT: one based on steady-state fluctuations [14,15] and the other based on the transient time-correlation function (TTCF) formalism [16,17]. In the former approach, basic objects are the steady-state density correlators defined with fluctuations around the stationary state. Rheological properties such as the shear stress are then expressed within the mode-coupling approximation in terms of these steady-state correlators. With the same spirit as MCT for quiescent systems [11], the structure factor $S_{\mathbf{q}}^{\mathrm{SS}}$ of the stationary state, which now depends on the shear rate as well as on the wave "vector" $\mathbf{q}$, enters as input into the equations describing the dynamics. At first sight, such an approach looks quite reasonable, but in fact it possesses a conceptual problem. For example, the following exact relation holds between the interaction part of the steady-state shear stress $\sigma_{\mathrm{SS}}^{\mathrm{int}}$ and the steady-state pair-correlation function $g_{\mathrm{SS}}(\mathbf{r})$

$$\sigma_{\mathrm{SS}}^{\mathrm{int}} = \frac{\rho^2}{2} \int d\mathbf{r}\, g_{\mathrm{SS}}(\mathbf{r}) \frac{xy}{r} \frac{du(r)}{dr} \tag{1}$$

for a uniform shear with velocity along the x axis and its gradient along the y axis [18]. Here ρ denotes the average number density and $u(r)$ the pair-interaction potential. Since $S_{\mathbf{q}}^{\mathrm{SS}}$ is related to the Fourier transform of $g_{\mathrm{SS}}(\mathbf{r})$, Eq. (1) states that $S_{\mathbf{q}}^{\mathrm{SS}}$ and $\sigma_{\mathrm{SS}}^{\mathrm{int}}$ should be handled on an equal footing, but this aspect is missing in the steady-state fluctuations approach of Refs. [14,15], where $S_{\mathbf{q}}^{\mathrm{SS}}$ is treated as the input while $\sigma_{\mathrm{SS}}^{\mathrm{int}}$ is the output. In addition, it is assumed in Ref. [14] that the fluctuation-dissipation theorem (FDT) holds also in the nonequilibrium stationary state. The use of such an assumption is unjustified since the violations of the FDT have been reported in the computer-simulation study of sheared systems [4].

On the other hand, no such problems arise in the theory developed by Fuchs and Cates (FC) [16,17] which is based on the TTCF formalism [19]. Starting from the Smoluchowski equation for interacting Brownian particles under stationary shearing, the FC theory aims at describing steady-state properties via two steps: first, the MCT equations for the transient density correlators—the correlators between the density fluctuations in the equilibrium starting state and the ones at later times after the shearing force is turned on—are formulated, and then the TTCF formalism is used which, combined with the mode-coupling approximation, expresses stationary-state properties in terms of these transient correlators. In this approach, only equilibrium static structure factor is required as input, whereas the steady-state structure factor $S_{\mathbf{q}}^{\mathrm{SS}}$ as well as the shear stress $\sigma_{\mathrm{SS}}^{\mathrm{int}}$ are the output of the theory. Thus, the aforementioned conceptual problem in Refs. [14,15] does not apply here. Furthermore, it is in principle possible using the FC theory to investigate the violations of the FDT, although this issue has not yet been addressed.

It is expected on physical grounds that the microscopic dynamics does not matter as far as the long-time glassy dynamics is concerned. Indeed, it was argued that the equilibrium MCT leads to the same glass transition scenario for both Newtonian and Brownian microscopic dynamics [11,12,20], and this was confirmed by computer-simulation studies [21,22]. However, it is not *a priori* obvious whether such an equivalent long-time dynamics holds true also for nonequilibrium sheared systems.

In this paper, we develop a nonequilibrium MCT starting from the Sllod equations [19]—Newtonian equations of motion under stationary shearing—which have been widely adopted in simulation studies of homogeneously sheared systems (see, e.g., Refs. [4,23]). Our theory follows the FC formulation in that the MCT equations for the transient density correlators are derived first, and then the TTCF formalism is used for describing stationary-state properties. However, we found that, although it is not difficult to adapt the FC formulation in Refs. [16,17] to the Sllod equations at the formal level, the resulting equations are too cumbersome to be useful in practice. We therefore developed an alternative formulation to be presented in the following. It is found that a new memory kernel enters into our nonequilibrium MCT equations reflecting the non-Hermitian nature of the relevant Liouville operator, which is absent in the FC theory formulated with the Brownian microscopic dynamics. In what circumstances this additional memory kernel from our theory matters is an open question. We shall elaborate on this at the end of the paper.

The paper is organized as follows. In Sec. II, we derive exact microscopic equations and relations for systems subjected to stationary shearing. These exact results serve a basis for the development of our nonequilibrium MCT. We will then derive a set of self-consistent equations for the transient density correlators based on the projection-operator formalism (Sec. III) and on the mode-coupling approach (Sec. IV). It is then described in Sec. V how the steady-state properties can be evaluated within the mode-coupling approximation based on the knowledge of the transient density correlators. The paper is summarized in Sec. VI, where a detailed comparison of our theory is also presented with the FC theory. Appendix A is devoted to a summary of miscellaneous materials which are necessary in the main text, and to various technical manipulations in the derivations of some equations. Appendix B describes details of the isotropic approximation which is useful in practical applications of our theory to systems where anisotropy in the density fluctuations is small.

II. MICROSCOPIC STARTING POINTS

In this section, we derive exact microscopic equations and relations subjected to stationary shearing along with thermostat. These exact results serve a basis for developing a nonequilibrium MCT for sheared systems to be presented in later sections.

A. Sllod equations of motion

We shall consider a system of N atoms of mass m in a volume V subjected to stationary shearing characterized by the shear-rate tensor $\boldsymbol{\kappa}$. For a simple uniform shear with velocity along the x axis and its gradient along the y axis, which we consider throughout this paper, the shear-rate tensor is $\kappa_{\lambda\mu}=\dot{\gamma}\delta_{\lambda x}\delta_{\mu y}$ with $\dot{\gamma}$ denoting the strain rate. It is postulated that the applied shear induces a homogeneous streaming-velocity profile $\mathbf{u}(\mathbf{r})=\boldsymbol{\kappa}\cdot\mathbf{r}$ at position $\mathbf{r}$, assuming that no spontaneous symmetry breaking takes place. Newtonian equations of motion describing such a homogeneously sheared system are the thermostatted Sllod equations [19]

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m} + \boldsymbol{\kappa}\cdot\mathbf{r}_i, \tag{2a}$$

$$\dot{\mathbf{p}}_i = \mathbf{F}_i - \boldsymbol{\kappa}\cdot\mathbf{p}_i - \alpha\mathbf{p}_i. \tag{2b}$$

Here $\mathbf{r}_i$ and $\mathbf{p}_i$ refer to the position and momentum of the ith particle, $\mathbf{F}_i=-\partial U/\partial\mathbf{r}_i$ with the total interaction potential U is the conservative force exerted on the ith particle by other particles, and $\alpha\mathbf{p}_i$ is the thermostatting term which prevents the system from heating up due to the work done on it by the shearing force. The momenta $\{\mathbf{p}_i\}$, referred to as the Sllod momenta, are peculiar with respect to the streaming velocity $\mathbf{u}(\mathbf{r}_i)=\boldsymbol{\kappa}\cdot\mathbf{r}_i$ at the particle position $\mathbf{r}_i$, and satisfy $\Sigma_i\mathbf{p}_i=0$.

The thermostatting multiplier α controls the kinetic temperature or some other quantity such as the internal energy. There exist various types of thermostats—stochastic or deterministic and reversible or irreversible—considered in the literature. Among them, the Gaussian isokinetic thermostat has acquired a respected status and a special importance [19]. However, from a fundamental point of view, there is no privileged thermostat, and one should not attribute a fundamental role to special assumptions about such models since they simply describe various ways to take out energy from the system. Indeed, it has been conjectured that different thermostats may lead to the same steady-state properties, in the usual sense of the macroscopic equivalence of equilibrium ensembles [24]. Although no proof is yet available, it is at least reasonable to expect that steady-state properties do not significantly depend on the types of the thermostats, and this has been tacitly assumed in simulation studies where various models have been used as practical means to control the temperature.

In the present work, we shall adopt a constant-α thermostat in which the multiplier α can be regarded as a "friction" constant. As we will see later, this thermostat greatly simplifies the equations to be handled compared, e.g., to the corresponding equations under the Gaussian isokinetic thermostat whose multiplier α_G reads [19]

$$\alpha_G = \sum_i \mathbf{p}_i\cdot(\mathbf{F}_i - \boldsymbol{\kappa}\cdot\mathbf{p}_i) \Bigg/ \sum_i \mathbf{p}_i^2. \tag{3}$$

How the steady-state temperature can be controlled with the constant-α model will be discussed in Sec. II G.

B. The Liouville equation

For nonequilibrium systems described by the Sllod equations, the form of the Liouville equation commonly used for Hamiltonian systems should be properly generalized to take into account the effect of phase-space compression [19]. The Liouville equation for the nonequilibrium phase-space distribution function $f(\mathbf{\Gamma},t)$, where $\mathbf{\Gamma}=(\mathbf{r}^N,\mathbf{p}^N)$ stands for a phase-space point, is given by

$$\frac{\partial f(\mathbf{\Gamma},t)}{\partial t}=-\left[\dot{\mathbf{\Gamma}}\cdot\frac{\partial}{\partial\mathbf{\Gamma}}+\Lambda(\mathbf{\Gamma})\right]f(\mathbf{\Gamma},t)\equiv -i\mathcal{L}^{\dagger}f(\mathbf{\Gamma},t). \quad (4)$$

The operator $i\mathcal{L}^{\dagger}$ is called the f Liouvillean, and $\Lambda(\mathbf{\Gamma})$ defined by

$$\Lambda(\mathbf{\Gamma})\equiv\frac{\partial}{\partial\mathbf{\Gamma}}\cdot\dot{\mathbf{\Gamma}} \quad (5)$$

is referred to as the phase-space compression factor. For the Sllod equations (2) with constant α, one obtains

$$\Lambda(\mathbf{\Gamma})=\sum_i\left(\frac{\partial}{\partial\mathbf{r}_i}\cdot\dot{\mathbf{r}}_i+\frac{\partial}{\partial\mathbf{p}_i}\cdot\dot{\mathbf{p}}_i\right)=-3N\alpha. \quad (6)$$

The formal solution to the Liouville equation (4) reads

$$f(\mathbf{\Gamma},t)=\exp(-i\mathcal{L}^{\dagger}t)f(\mathbf{\Gamma},0), \quad (7)$$

where $\exp(-i\mathcal{L}^{\dagger}t)$ is called the f propagator.

The time evolution of phase variables, which by definition do not depend on time explicitly and whose time dependence comes solely from that of the phase $\mathbf{\Gamma}$, is determined by

$$\frac{d}{dt}A(\mathbf{\Gamma})=\dot{\mathbf{\Gamma}}\cdot\frac{\partial}{\partial\mathbf{\Gamma}}A(\mathbf{\Gamma})\equiv i\mathcal{L}A(\mathbf{\Gamma}). \quad (8)$$

The operator $i\mathcal{L}$ is referred to as the p Liouvillean. The formal solution to this equation can be written in terms of the p propagator $\exp(i\mathcal{L}t)$ as

$$A(\mathbf{\Gamma},t)=\exp(i\mathcal{L}t)A(\mathbf{\Gamma}). \quad (9)$$

Let us summarize here for later use relations between f and p Liouvilleans and corresponding propagators. It follows from Eqs. (4) and (8) that

$$i\mathcal{L}^{\dagger}(\mathbf{\Gamma})=i\mathcal{L}(\mathbf{\Gamma})+\Lambda(\mathbf{\Gamma}). \quad (10)$$

One can show that $i\mathcal{L}$ and $i\mathcal{L}^{\dagger}$ are adjoint operators, and this is why the notation $i\mathcal{L}^{\dagger}$ is used for the f Liouvillean:

$$\int d\mathbf{\Gamma}[i\mathcal{L}A(\mathbf{\Gamma})]B(\mathbf{\Gamma})=-\int d\mathbf{\Gamma}A(\mathbf{\Gamma})[i\mathcal{L}^{\dagger}B(\mathbf{\Gamma})]. \quad (11)$$

This property can be proved from the integration by parts. By a repeated use of this property, the following relation for the propagators can be derived:

$$\int d\mathbf{\Gamma}[e^{i\mathcal{L}t}A(\mathbf{\Gamma})]B(\mathbf{\Gamma})=\int d\mathbf{\Gamma}A(\mathbf{\Gamma})[e^{-i\mathcal{L}^{\dagger}t}B(\mathbf{\Gamma})]. \quad (12)$$

If the phase-space compression factor $\Lambda(\mathbf{\Gamma})$ is identically zero, then $i\mathcal{L}^{\dagger}=i\mathcal{L}$ holds, and the Liouvillean becomes self-adjoint, or Hermitian. In general, this is not the case for nonequilibrium systems.

C. Nonequilibrium distribution function

Let us consider an equilibrium system of temperature T to which a constant shear rate $\dot{\gamma}$ is applied at time $t=0$, and thereafter the system evolves according to the Sllod equations (2). The p Liouvillean is given by

$$i\mathcal{L}=\begin{cases} i\mathcal{L}_0 & (t\leq 0),\\ i\mathcal{L}_0+i\mathcal{L}_{\dot{\gamma}}+i\mathcal{L}_{\alpha} & (t>0).\end{cases} \quad (13a)$$

Here, an unperturbed adiabatic or quiescent part $(i\mathcal{L}_0)$, a shear part $(i\mathcal{L}_{\dot{\gamma}})$, and a thermostat part $(i\mathcal{L}_{\alpha})$ are, respectively, given by

$$i\mathcal{L}_0=\sum_i\left[\frac{\mathbf{p}_i}{m}\cdot\frac{\partial}{\partial\mathbf{r}_i}+\mathbf{F}_i\cdot\frac{\partial}{\partial\mathbf{p}_i}\right], \quad (13b)$$

$$i\mathcal{L}_{\dot{\gamma}}=\sum_i\left[(\boldsymbol{\kappa}\cdot\mathbf{r}_i)\cdot\frac{\partial}{\partial\mathbf{r}_i}-(\boldsymbol{\kappa}\cdot\mathbf{p}_i)\cdot\frac{\partial}{\partial\mathbf{p}_i}\right], \quad (13c)$$

$$i\mathcal{L}_{\alpha}=\sum_i(-\alpha\mathbf{p}_i)\cdot\frac{\partial}{\partial\mathbf{p}_i}. \quad (13d)$$

Since the phase-space distribution function at $t=0$ coincides with the equilibrium one, which we choose to be the canonical distribution

$$f_{\mathrm{eq}}(\mathbf{\Gamma})\equiv f(\mathbf{\Gamma},0)=\frac{1}{\mathcal{Z}}e^{-\beta H_0(\mathbf{\Gamma})},\quad \mathcal{Z}=\int d\mathbf{\Gamma}e^{-\beta H_0(\mathbf{\Gamma})}, \quad (14)$$

where $\beta\equiv 1/k_BT$ with k_B denoting Boltzmann's constant and $H_0\equiv\Sigma_i\mathbf{p}_i^2/2m+U$, a formal solution to the Liouville equation (4) for $t>0$ is given by

$$f(\mathbf{\Gamma},t)=e^{-i\mathcal{L}^{\dagger}t}f_{\mathrm{eq}}(\mathbf{\Gamma}). \quad (15)$$

With the identity

$$e^{-i\mathcal{L}^{\dagger}t}=1+\int_0^t ds e^{-i\mathcal{L}^{\dagger}s}(-i\mathcal{L}^{\dagger}), \quad (16)$$

whose validity can easily be verified by differentiation with respect to t, Eq. (15) can be expressed as

$$f(\mathbf{\Gamma},t)=f_{\mathrm{eq}}(\mathbf{\Gamma})+\int_0^t ds e^{-i\mathcal{L}^{\dagger}s}(-i\mathcal{L}^{\dagger})f_{\mathrm{eq}}(\mathbf{\Gamma}). \quad (17)$$

Since $i\mathcal{L}_0 f_{\mathrm{eq}}(\mathbf{\Gamma})=0$, we get from Eqs. (6), (10), and (13a)–(13d)

$$i\mathcal{L}^{\dagger}f_{\mathrm{eq}}(\mathbf{\Gamma})=i\mathcal{L}_{\dot{\gamma}}f_{\mathrm{eq}}(\mathbf{\Gamma})+i\mathcal{L}_{\alpha}f_{\mathrm{eq}}(\mathbf{\Gamma})-3N\alpha f_{\mathrm{eq}}(\mathbf{\Gamma}). \quad (18)$$

The first term in this expression is given by

$$i\mathcal{L}_{\dot{\gamma}}f_{\mathrm{eq}}(\mathbf{\Gamma})=\beta\sum_i\left[(\boldsymbol{\kappa}\cdot\mathbf{r}_i)\cdot\mathbf{F}_i+(\boldsymbol{\kappa}\cdot\mathbf{p}_i)\cdot\frac{\mathbf{p}_i}{m}\right]f_{\mathrm{eq}}(\mathbf{\Gamma})$$
$$=\beta\boldsymbol{\kappa}:\boldsymbol{\sigma}f_{\mathrm{eq}}(\mathbf{\Gamma})=\frac{\dot{\gamma}}{k_BT}f_{\mathrm{eq}}(\mathbf{\Gamma})\sigma_{xy}. \quad (19)$$

Here $\boldsymbol{\kappa}:\boldsymbol{\sigma}\equiv\Sigma_{\lambda,\mu}\kappa_{\lambda\mu}\sigma_{\mu\lambda}$, and $\boldsymbol{\sigma}$ denotes the stress tensor whose elements are

$$\sigma_{\lambda\mu} = \sum_i [p_i^\lambda p_i^\mu/m + r_i^\lambda F_i^\mu] \quad (\lambda,\mu = x,y,z) \tag{20}$$

and in the final equality of Eq. (19) we used the specific form $\kappa_{\lambda\mu}=\dot{\gamma}\delta_{\lambda x}\delta_{\mu y}$ for the shear-rate tensor and the symmetry $\sigma_{\lambda\mu}=\sigma_{\mu\lambda}$ of the stress tensor (see Appendix A 1). The second term in Eq. (18) is given by

$$i\mathcal{L}_\alpha f_{\text{eq}}(\mathbf{\Gamma}) = \frac{2\alpha}{k_B T} f_{\text{eq}}(\mathbf{\Gamma}) K(\mathbf{\Gamma}) \tag{21}$$

in terms of the kinetic energy $K(\mathbf{\Gamma}) \equiv \Sigma_i \mathbf{p}_i^2/2m$. We therefore obtain

$$i\mathcal{L}^\dagger f_{\text{eq}}(\mathbf{\Gamma}) = \frac{\dot{\gamma}}{k_B T} f_{\text{eq}}(\mathbf{\Gamma})\sigma_{xy}(\mathbf{\Gamma}) + \frac{2\alpha}{k_B T} f_{\text{eq}}(\mathbf{\Gamma})\delta K(\mathbf{\Gamma}), \tag{22}$$

where we have introduced the kinetic energy fluctuation $\delta K(\mathbf{\Gamma})$ defined as

$$\delta K(\mathbf{\Gamma}) \equiv K(\mathbf{\Gamma}) - \frac{3}{2} N k_B T. \tag{23}$$

Substitution of Eq. (22) into Eq. (17) then yields

$$f(\mathbf{\Gamma},t) = f_{\text{eq}}(\mathbf{\Gamma}) - \frac{\dot{\gamma}}{k_B T}\int_0^t ds e^{-i\mathcal{L}^\dagger s}[f_{\text{eq}}(\mathbf{\Gamma})\sigma_{xy}(\mathbf{\Gamma})] - \frac{2\alpha}{k_B T}\int_0^t ds e^{-i\mathcal{L}^\dagger s}[f_{\text{eq}}(\mathbf{\Gamma})\delta K(\mathbf{\Gamma})]. \tag{24}$$

This expression for the nonequilibrium phase-space distribution function plays a fundamental role in the following. Notice that the last term in this expression vanishes if the Gaussian isokinetic thermostat [see Eq. (3)] is used for constraining $\delta K(\mathbf{\Gamma})$ to zero.

D. Transient time-correlation function formalism

In contrast to equilibrium quantities, the nonequilibrium ensemble average $\langle A(t)\rangle$ of a phase variable A depends explicitly on the time t past since the start of shearing. Similarly, the time-correlation function $\langle A(t+\tau)B(t)^*\rangle$ depends not only on the time difference τ but also on t. Using the nonequilibrium phase-space distribution function $f(\mathbf{\Gamma},t)$, $\langle A(t)\rangle$, and $\langle A(t+\tau)B(t)^*\rangle$ can be expressed as

$$\langle A(t)\rangle = \int d\mathbf{\Gamma} f(\mathbf{\Gamma},0)A(t) = \int d\mathbf{\Gamma} f(\mathbf{\Gamma},t)A(0), \tag{25}$$

$$\langle A(t+\tau)B(t)^*\rangle = \int d\mathbf{\Gamma} f(\mathbf{\Gamma},0)A(t+\tau)B(t)^* = \int d\mathbf{\Gamma} f(\mathbf{\Gamma},t)A(\tau)B(0)^*. \tag{26}$$

The two representations in terms of $f(\mathbf{\Gamma},0)$ or $f(\mathbf{\Gamma},t)$ are equivalent because of the relation (12). Hereafter, we shall reserve the notation $\langle\cdots\rangle$ for representing the averaging over the initial canonical distribution function $f(\mathbf{\Gamma},0)=f_{\text{eq}}(\mathbf{\Gamma})$:

$$\langle\cdots\rangle \equiv \int d\mathbf{\Gamma} f_{\text{eq}}(\mathbf{\Gamma})\cdots . \tag{27}$$

It should be remembered, however, that the dynamics inside the brackets $\langle\cdots\rangle$ is governed by the thermostatted Sllod equations, and only averages such as $\langle A(0)\rangle$ and $\langle A(0)B(0)^*\rangle$ coincide with equilibrium quantities.

Substituting Eq. (24) into Eqs. (25) and (26) and then using Eq. (12), one obtains

$$\langle A(t)\rangle = \langle A(0)\rangle - \frac{\dot{\gamma}}{k_B T}\int_0^t ds \langle A(s)\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\int_0^t ds\langle A(s)\delta K(0)\rangle, \tag{28}$$

$$\langle A(t+\tau)B(t)^*\rangle = \langle A(\tau)B(0)^*\rangle - \frac{\dot{\gamma}}{k_B T}\int_0^t ds\langle A(s+\tau)B(s)^*\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\int_0^t ds\langle A(s+\tau)B(s)^*\delta K(0)\rangle. \tag{29}$$

The expression (28) relates the nonequilibrium value of a phase variable A at time t to the integral of transient time-correlation function (TTCF) $\langle A(s)\sigma_{xy}(0)\rangle$—the correlation between σ_{xy} in the initial equilibrium state $\sigma_{xy}(0)$ and A at time s after the shearing force is turned on—and another integral of TTCF $\langle A(s)\delta K(0)\rangle$ formed with $\delta K(0)$. Equation (29) is a generalization of this TTCF expression to the time-correlation function.

The system is said to be in a nonequilibrium steady state if the ensemble averages of all phase variables become time independent. Let us notice that the long-time limit of Eq. (28) becomes constant if the system displays mixing [25]. This feature can be shown by taking a time derivative of Eq. (28):

$$\frac{d}{dt}\langle A(t)\rangle = -\frac{\dot{\gamma}}{k_B T}\langle A(t)\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\langle A(t)\delta K(0)\rangle. \tag{30}$$

If the system displays mixing [25], then all the long-time correlations between phase variables vanish. We therefore obtain for $t\to\infty$

$$\frac{d}{dt}\langle A(t)\rangle \to -\frac{\dot{\gamma}}{k_B T}\langle A(t)\rangle\langle\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\langle A(t)\rangle\langle\delta K(0)\rangle = 0, \tag{31}$$

since the equilibrium ensemble averages $\langle\sigma_{xy}(0)\rangle$ and $\langle\delta K(0)\rangle$ are zero [see Eqs. (A7) and (23)]. This indicates that the long-time steady state average of an arbitrary phase variable becomes constant, i.e.,

$$\lim_{t\to\infty}\langle A(t)\rangle = \langle A\rangle_{\text{SS}}, \tag{32}$$

where the steady-state average, denoted by $\langle\cdots\rangle_{\text{SS}}$ hereafter, is obtained from the $t\to\infty$ limit of Eq. (28):

$$\langle A\rangle_{SS} = \langle A(0)\rangle - \frac{\dot{\gamma}}{k_B T}\int_0^\infty ds\langle A(s)\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\int_0^\infty ds\langle A(s)\delta K(0)\rangle. \quad (33)$$

Similarly, the $t\to\infty$ limit of $\langle A(t+\tau)B(t)^*\rangle$ becomes independent of t since the time derivative of Eq. (29)

$$\frac{d}{dt}\langle A(t+\tau)B(t)^*\rangle = -\frac{\dot{\gamma}}{k_B T}\langle A(t+\tau)B(t)^*\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\langle A(t+\tau)B(t)^*\delta K(0)\rangle \quad (34)$$

becomes zero for $t\to\infty$ if the system exhibits mixing. The steady-state time-correlation function defined as

$$\langle A(\tau)B^*\rangle_{SS} \equiv \lim_{t\to\infty}\langle A(t+\tau)B(t)^*\rangle \quad (35)$$

is then given by

$$\langle A(\tau)B^*\rangle_{SS} = \langle A(\tau)B(0)^*\rangle - \frac{\dot{\gamma}}{k_B T}\int_0^\infty ds\langle A(s+\tau)B(s)^*\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\int_0^\infty ds\langle A(s+\tau)B(s)^*\delta K(0)\rangle. \quad (36)$$

The TTCF expressions (33) and (36), relating the steady-state quantities to the integrals of TTCFs, can be considered as the generalized Green-Kubo relations [19].

In deriving the nonequilibrium Zwanzig-Mori–type equation of motion to be presented in Sec. III, it is necessary to know how the p-Liouvillean $i\mathcal{L}$ behaves inside the time-correlation function. To this end, we first notice from Eq. (9)

$$\frac{d}{dt}\langle A(t+\tau)B(t)^*\rangle = \langle[i\mathcal{L}A(t+\tau)]B(t)^*\rangle + \langle A(t+\tau)[i\mathcal{L}B(t)]^*\rangle. \quad (37)$$

Combined with Eq. (34), this yields the desired result

$$\langle i\mathcal{L}A(t+\tau)B(t)^*\rangle = -\langle A(t+\tau)[i\mathcal{L}B(t)]^*\rangle - \frac{\dot{\gamma}}{k_B T}\langle A(t+\tau)B(t)^*\sigma_{xy}(0)\rangle - \frac{2\alpha}{k_B T}\langle A(t+\tau)B(t)^*\delta K(0)\rangle. \quad (38)$$

For systems exhibiting mixing, there holds for $t\to\infty$

$$\langle[i\mathcal{L}A(\tau)]B^*\rangle_{SS} = -\langle A(\tau)[i\mathcal{L}B]^*\rangle_{SS}, \quad (39)$$

i.e., the p Liouvillean becomes Hermitian in the steady state. This is expected since the time-translation symmetry is recovered in the stationary state.

E. Implication of translational invariance

Since we are dealing with amorphous systems, the equilibrium distribution function $f_{eq}(\mathbf{\Gamma})$ is assumed to be translationally invariant and isotropic. In this subsection, it is shown that the nonequilibrium distribution function $f(\mathbf{\Gamma},t)$ under shear becomes anisotropic, but remains translationally invariant. We then discuss an implication of this property. Our treatment here follows the one presented in Ref. [17].

To this end, we shall consider global translation of all particle positions

$$\mathbf{\Gamma}\to\mathbf{\Gamma}', \text{ where } \mathbf{r}_i' = \mathbf{r}_i + \mathbf{a} \text{ for all } i, \quad (40)$$

which amounts to the shift $\mathbf{a}$ of the coordinate origin. Under this shift, the nonequilibrium distribution $f(\mathbf{\Gamma},t)$ given in Eq. (24) transforms to

$$f(\mathbf{\Gamma}',t) = f_{eq}(\mathbf{\Gamma}) - \frac{\dot{\gamma}}{k_B T}\int_0^t ds e^{-i\mathcal{L}^\dagger(\mathbf{\Gamma}')s}[f_{eq}(\mathbf{\Gamma})\sigma_{xy}(\mathbf{\Gamma})] - \frac{2\alpha}{k_B T}\int_0^t ds e^{-i\mathcal{L}^\dagger(\mathbf{\Gamma}')s}[f_{eq}(\mathbf{\Gamma})\delta K(\mathbf{\Gamma})]. \quad (41)$$

Here we used

$$f_{eq}(\mathbf{\Gamma}') = f_{eq}(\mathbf{\Gamma}), \quad \sigma_{xy}(\mathbf{\Gamma}') = \sigma_{xy}(\mathbf{\Gamma}), \quad \delta K(\mathbf{\Gamma}') = \delta K(\mathbf{\Gamma}). \quad (42)$$

These hold since f_{eq}, σ_{xy} [see Eq. (A6)], and δK depend on momenta and particle separations only. How the f propagator transforms under $\mathbf{\Gamma}\to\mathbf{\Gamma}'$ is discussed in Appendix A 2 with the result [see Eq. (A17)]

$$e^{-i\mathcal{L}^\dagger(\mathbf{\Gamma}')t} = e^{-i\mathcal{L}^\dagger(\mathbf{\Gamma})t}e^{-\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}t} \text{ with } \mathbf{P}\equiv\sum_i\frac{\partial}{\partial\mathbf{r}_i}. \quad (43)$$

Here $\boldsymbol{\kappa}^T$ denotes the transposed matrix of $\boldsymbol{\kappa}$. Because of Eq. (42), we have $\mathbf{P}f_{eq}(\mathbf{\Gamma})=0$, $\mathbf{P}\sigma_{xy}(\mathbf{\Gamma})=0$, and $\mathbf{P}\delta K(\mathbf{\Gamma})=0$, so that

$$e^{-i\mathcal{L}^\dagger(\mathbf{\Gamma}')s}[f_{eq}(\mathbf{\Gamma})\sigma_{xy}(\mathbf{\Gamma})] = e^{-i\mathcal{L}^\dagger(\mathbf{\Gamma})s}[f_{eq}(\mathbf{\Gamma})\sigma_{xy}(\mathbf{\Gamma})] \quad (44)$$

and a similar equation holds in which σ_{xy} is replaced by δK. Therefore, the nonequilibrium distribution function $f(\mathbf{\Gamma},t)$ remains translationally invariant:

$$f(\mathbf{\Gamma}',t) = f(\mathbf{\Gamma},t). \quad (45)$$

We next consider how the wave-vector-dependent phase variable of the form

$$A_{\mathbf{q}}(\mathbf{\Gamma},t) = e^{i\mathcal{L}(\mathbf{\Gamma})t}\sum_i X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})e^{i\mathbf{q}\cdot\mathbf{r}_i}, \quad (46)$$

transforms under the shift of the coordinate origin. It is assumed that $X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})$ is a function of momenta and particle separations only, so that $X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma}')=X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})$. For example, $X_i^{\rho_{\mathbf{q}}}=1$ for density fluctuations, $X_i^{j_{\mathbf{q}}^\lambda}=p_i^\lambda/m$ for current density fluctuations to be introduced below, and $X_i^{\sigma_{\mathbf{q}}^{\lambda\mu}}=p_i^\lambda p_i^\mu/m - (1/2)\Sigma_{j\neq i}(r_{ij}^\lambda r_{ij}^\mu/r_{ij}^2)P_{\mathbf{q}}(\mathbf{r}_{ij})$ for the wave-vector-dependent stress tensor [see Eq. (A4)]. Using the result

$$e^{i\mathcal{L}(\mathbf{\Gamma}')t} = e^{i\mathcal{L}(\mathbf{\Gamma})t}e^{\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}t} \quad (47)$$

for the p propagator which is also derived in Appendix A 2 [see Eq. (A16)], one obtains

$$A_{\mathbf{q}}(\mathbf{\Gamma}',t) = e^{i\mathcal{L}(\mathbf{\Gamma}')t}\sum_i X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma}')e^{i\mathbf{q}\cdot(\mathbf{r}_i+\mathbf{a})}$$
$$= e^{i\mathcal{L}(\mathbf{\Gamma})t}e^{\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}t}\sum_i X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})e^{i\mathbf{q}\cdot(\mathbf{r}_i+\mathbf{a})}$$
$$= e^{i(\mathbf{q}+\mathbf{q}\cdot\boldsymbol{\kappa}t)\cdot\mathbf{a}}A_{\mathbf{q}}(\mathbf{\Gamma},t), \tag{48}$$

where we used $X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma}')=X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})$, $\mathbf{P}X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})=0$, and $e^{\mathbf{a}\cdot\boldsymbol{\kappa}^{\mathrm{T}}\cdot\mathbf{P}t}e^{i\mathbf{q}\cdot(\mathbf{r}_i+\mathbf{a})}=e^{i\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\mathbf{a}t}e^{i\mathbf{q}\cdot(\mathbf{r}_i+\mathbf{a})}$.

Since the integral over the phase space must agree for either integration variables $\mathbf{\Gamma}$ or $\mathbf{\Gamma}'$, there holds

$$\langle A_{\mathbf{q}}(t)\rangle = \int d\mathbf{\Gamma} f_{\mathrm{eq}}(\mathbf{\Gamma})A_{\mathbf{q}}(\mathbf{\Gamma},t) = \int d\mathbf{\Gamma}' f_{\mathrm{eq}}(\mathbf{\Gamma}')A_{\mathbf{q}}(\mathbf{\Gamma}',t). \tag{49}$$

Using $f_{\mathrm{eq}}(\mathbf{\Gamma}')=f_{\mathrm{eq}}(\mathbf{\Gamma})$ and Eq. (48), one obtains

$$\langle A_{\mathbf{q}}(t)\rangle = e^{i(\mathbf{q}+\mathbf{q}\cdot\boldsymbol{\kappa}t)\cdot\mathbf{a}}\langle A_{\mathbf{q}}(t)\rangle. \tag{50}$$

This means that the nonequilibrium ensemble averages of phase variables, including steady-state averages, are nonvanishing for zero wave vector only:

$$\langle A_{\mathbf{q}}(t)\rangle = \delta_{\mathbf{q},0}\langle A_{\mathbf{q}=0}(t)\rangle. \tag{51}$$

Similarly, there must hold for nonequilibrium time-correlation functions

$$\langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{k}}(t)^*\rangle = \int d\mathbf{\Gamma} f(\mathbf{\Gamma},t)A_{\mathbf{q}}(\mathbf{\Gamma},\tau)B_{\mathbf{k}}(\mathbf{\Gamma},0)^*$$
$$= \int d\mathbf{\Gamma}' f(\mathbf{\Gamma}',t)A_{\mathbf{q}}(\mathbf{\Gamma}',\tau)B_{\mathbf{k}}(\mathbf{\Gamma}',0)^*. \tag{52}$$

Using Eqs. (45) and (48), one finds

$$\langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{k}}(t)^*\rangle = e^{i(\mathbf{q}+\mathbf{q}\cdot\boldsymbol{\kappa}\tau-\mathbf{k})\cdot\mathbf{a}}\langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{k}}(t)^*\rangle. \tag{53}$$

This means that $A_{\mathbf{q}}(t+\tau)$ is statistically correlated with $B_{\mathbf{k}}(t)^*$ only if $\mathbf{k}=\mathbf{q}(\tau)$ with the advected wave vector $\mathbf{q}(\tau)\equiv\mathbf{q}+\mathbf{q}\cdot\boldsymbol{\kappa}\tau$ during the time τ, i.e.,

$$\langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{k}}(t)^*\rangle = \delta_{\mathbf{k},\mathbf{q}(\tau)}\langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{q}(\tau)}(t)^*\rangle. \tag{54}$$

Thus, as in equilibrium systems, a time-correlation function characterized by a single wave vector can be defined as

$$C_{\mathbf{q}}^{AB}(t+\tau,t) \equiv \langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{q}(\tau)}(t)^*\rangle. \tag{55}$$

For the shear-rate tensor $\kappa_{\lambda\mu}=\dot{\gamma}\delta_{\lambda x}\delta_{\mu y}$, the explicit expression for the advected wave vector reads

$$\mathbf{q}(\tau) = \mathbf{q}+\mathbf{q}\cdot\boldsymbol{\kappa}\tau = (q_x, q_y+\dot{\gamma}\tau q_x, q_z). \tag{56}$$

Equivalently, one can introduce a time-correlation of the following form:

$$\tilde{C}_{\mathbf{q}}^{AB}(t+\tau,t) \equiv \langle A_{\mathbf{q}(-\tau)}(t+\tau)B_{\mathbf{q}}(t)^*\rangle. \tag{57}$$

This also follows from Eq. (53) by noting that

$$\mathbf{q}\cdot(\mathbf{I}+\boldsymbol{\kappa}t) = \mathbf{k} \to \mathbf{q} = \mathbf{k}\cdot(\mathbf{I}+\boldsymbol{\kappa}t)^{-1} = \mathbf{k}\cdot(\mathbf{I}-\boldsymbol{\kappa}t), \tag{58}$$

since the shear-rate tensor satisfies $\boldsymbol{\kappa}\cdot\boldsymbol{\kappa}=0$. In this paper, we shall mainly use the convention (55) for time-correlation functions, and the convention (57) will be used only for the discussion in Sec. III A. Finally, we notice for later use the following relation for time-correlation functions involving three phase variables:

$$\langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{q}(\tau)}(t)^*D_{\mathbf{k}}(t)^*\rangle = \delta_{\mathbf{k},\mathbf{0}}\langle A_{\mathbf{q}}(t+\tau)B_{\mathbf{q}(\tau)}(t)^*D_{\mathbf{k}=\mathbf{0}}(t)^*\rangle, \tag{59}$$

which can be derived in the same manner as Eq. (54).

F. Implication of spatial inversion symmetry

Let us notice that the Sllod equations (2) are also invariant under spatial inversion $\mathbf{\Gamma}\to-\mathbf{\Gamma}$, and hence, the f and p Liouvilleans have even parity, $i\mathcal{L}^\dagger(-\mathbf{\Gamma})=i\mathcal{L}^\dagger(\mathbf{\Gamma})$ and $i\mathcal{L}(-\mathbf{\Gamma})=i\mathcal{L}(\mathbf{\Gamma})$. Since $f_{\mathrm{eq}}(\mathbf{\Gamma})$, $\sigma_{xy}(\mathbf{\Gamma})$, and $\delta K(\mathbf{\Gamma})$ also have even parity, so does the the nonequilibrium distribution function according to Eq. (24)

$$f(-\mathbf{\Gamma},t) = f(\mathbf{\Gamma},t). \tag{60}$$

We next consider how the wave-vector-dependent phase variable $A_{\mathbf{q}}(\mathbf{\Gamma},t)$ of the form given in Eq. (46) transforms under spatial inversion. It is assumed that $X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})$ satisfies

$$X_i^{A_{\mathbf{q}}}(-\mathbf{\Gamma}) = p_A X_i^{A_{-\mathbf{q}}}(\mathbf{\Gamma}) = p_A X_i^{A_{\mathbf{q}}}(\mathbf{\Gamma})^*, \tag{61}$$

where p_A denotes the parity of the variable A. Three examples introduced below Eq. (46) satisfy these relations with $p_\rho=+1$, $p_{j^\lambda}=-1$, and $p_{\sigma^{\lambda\mu}}=+1$. Then, it follows from Eq. (46) and $i\mathcal{L}(-\mathbf{\Gamma})=i\mathcal{L}(\mathbf{\Gamma})$ that

$$A_{\mathbf{q}}(-\mathbf{\Gamma},t) = p_A A_{-\mathbf{q}}(\mathbf{\Gamma},t) = p_A A_{\mathbf{q}}(\mathbf{\Gamma},t)^*. \tag{62}$$

Let us consider an implication of Eqs. (60) and (62) for the time correlation function $C_{\mathbf{q}}^{AB}(t+\tau,t)$ defined in Eq. (55). Since the integral over the phase space must agree for either $\mathbf{\Gamma}$ or $-\mathbf{\Gamma}$, there holds

$$C_{\mathbf{q}}^{AB}(t+\tau,t) = \int d\mathbf{\Gamma} f(\mathbf{\Gamma},t)A_{\mathbf{q}}(\mathbf{\Gamma},\tau)B_{\mathbf{q}(\tau)}(\mathbf{\Gamma},0)^*$$
$$= \int d(-\mathbf{\Gamma}) f(-\mathbf{\Gamma},t)A_{\mathbf{q}}(-\mathbf{\Gamma},\tau)B_{\mathbf{q}(\tau)}(-\mathbf{\Gamma},0)^*. \tag{63}$$

Using Eqs. (60) and (62) and noting that $\int d\mathbf{\Gamma}\cdots=\int d(-\mathbf{\Gamma})\cdots$ [e.g., $\int_{-\infty}^{\infty}dx_i\cdots\to\int_{\infty}^{-\infty}d(-x_i)\cdots=\int_{-\infty}^{\infty}dx_i\cdots$ under $x_i\to-x_i$], one finds

$$C_{\mathbf{q}}^{AB}(t+\tau,t) = p_A p_B C_{\mathbf{q}}^{AB}(t+\tau,t)^*. \tag{64}$$

In particular, the autocorrelation function is real:

$$C_{\mathbf{q}}^{AA}(t+\tau,t) = C_{\mathbf{q}}^{AA}(t+\tau,t)^*. \tag{65}$$

G. Steady-state properties

Among various stationary-state properties, we shall specifically be interested in this paper in the steady-state shear stress, kinetic temperature, and density fluctuations. Here we summarize the TTCF expressions for these quantities.

The steady-state shear stress shall be defined via

$$\sigma_{\mathrm{SS}} \equiv -\langle \sigma_{xy} \rangle_{\mathrm{SS}}/V. \tag{66}$$

Since the equilibrium ensemble average of σ_{xy} is zero, $\langle\sigma_{xy}(0)\rangle=0$ [see Eq. (A7)], one obtains from Eq. (33) the following TTCF expression for σ_{SS}:

$$\sigma_{\mathrm{SS}} = \frac{\dot{\gamma}}{k_B T V}\int_0^\infty ds\langle \sigma_{xy}(s)\sigma_{xy}(0)\rangle + \frac{2\alpha}{k_B T V}\int_0^\infty ds\langle \sigma_{xy}(s)\delta K(0)\rangle. \tag{67}$$

The steady-state temperature shall be defined as

$$T_{\mathrm{SS}} \equiv \frac{2}{3Nk_B}\langle K\rangle_{\mathrm{SS}}, \tag{68}$$

in terms of the kinetic energy. Let us show that T_{SS} is connected to σ_{SS} via a simple relation. To this end, we notice that the rate of the change of the internal energy $H_0=K+U$ is given by

$$\dot{H}_0 = \sum_i \left[\frac{\dot{\mathbf{p}}_i\cdot\mathbf{p}_i}{m} - \dot{\mathbf{r}}_i\cdot\mathbf{F}_i\right] = -\dot{\gamma}\sigma_{xy} - 2\alpha K, \tag{69}$$

where the specific form $\kappa_{\lambda\mu}=\dot{\gamma}\delta_{\lambda x}\delta_{\mu y}$ for the shear-rate tensor and Eq. (20) for the shear stress have been used in the final equality. Since there is no internal-energy change in the steady state, i.e., $\langle\dot{H}_0\rangle_{\mathrm{SS}}=0$, one finds from Eqs. (66), (68), and (69) that

$$T_{\mathrm{SS}} = \frac{\dot{\gamma}}{3k_B\rho\alpha}\sigma_{\mathrm{SS}}, \tag{70}$$

where $\rho=N/V$ denotes the average number density. Thus, it suffices to know σ_{SS} to obtain T_{SS}. This relation can also be used to control T_{SS} by varying the thermostatting multiplier α. However, a self-consistent treatment is necessary in order to set T_{SS} to a desired value since σ_{SS} also depends on α.

In view of Eqs. (35) and (55), the steady-state correlator $F_{\mathbf{q}}^{\mathrm{SS}}(t)$ of the density fluctuations

$$\rho_{\mathbf{q}}(t) \equiv \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i(t)} - N\delta_{\mathbf{q},\mathbf{0}} \tag{71}$$

shall be defined via

$$F_{\mathbf{q}}^{\mathrm{SS}}(t) \equiv \lim_{s\to\infty}\frac{1}{N}\langle \rho_{\mathbf{q}}(s+t)\rho_{\mathbf{q}(t)}(s)^*\rangle. \tag{72}$$

One understands from Eq. (65) that $F_{\mathbf{q}}^{\mathrm{SS}}(t)$ is a real function of time. From Eq. (36), one obtains the following TTCF expression for $F_{\mathbf{q}}^{\mathrm{SS}}(t)$

$$F_{\mathbf{q}}^{\mathrm{SS}}(t) = F_{\mathbf{q}}(t) - \frac{\dot{\gamma}}{Nk_BT}\int_0^\infty ds\langle \rho_{\mathbf{q}}(s+t)\rho_{\mathbf{q}(t)}(s)^*\sigma_{xy}(0)\rangle - \frac{2\alpha}{Nk_BT}\int_0^\infty ds\langle \rho_{\mathbf{q}}(s+t)\rho_{\mathbf{q}(t)}(s)^*\delta K(0)\rangle \tag{73}$$

in terms of the transient density correlator defined by

$$F_{\mathbf{q}}(t) \equiv \frac{1}{N}\langle \rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}(0)^*\rangle, \tag{74}$$

and other transient cross correlators formed with $\sigma_{xy}(0)$ and $\delta K(0)$. As a corollary, one gets for the steady-state "static" or equal-time structure factor $S_{\mathbf{q}}^{\mathrm{SS}} \equiv F_{\mathbf{q}}^{\mathrm{SS}}(t=0)$

$$S_{\mathbf{q}}^{\mathrm{SS}} = S_q - \frac{\dot{\gamma}}{Nk_BT}\int_0^\infty ds\langle \rho_{\mathbf{q}}(s)\rho_{\mathbf{q}}(s)^*\sigma_{xy}(0)\rangle - \frac{2\alpha}{Nk_BT}\int_0^\infty ds\langle \rho_{\mathbf{q}}(s)\rho_{\mathbf{q}}(s)^*\delta K(0)\rangle, \tag{75}$$

where $S_q=F_{\mathbf{q}}(t=0)$ denotes the equilibrium static structure factor. While S_q depends only on the wave-vector modulus $q=|\mathbf{q}|$ reflecting the isotropy of the initial equilibrium state, the steady-state structure factor $S_{\mathbf{q}}^{\mathrm{SS}}$ also depends on the direction of the wave vector due to the anisotropy of the sheared stationary state. It is also clear from Eq. (75) that $S_{\mathbf{q}}^{\mathrm{SS}}$ should be considered as a dynamic object in the sense it is given by the time integrals of the transient time-correlation functions.

Finally, let us show the connection between the TTCF expressions for the steady-state shear stress σ_{SS} and the structure factor $S_{\mathbf{q}}^{\mathrm{SS}}$ given by Eqs. (67) and (75), respectively. For this purpose, we first write $\sigma_{xy}(s)$ appearing in the integrands of Eq. (67) as [see Eq. (A6)]

$$\begin{aligned}\sigma_{xy}(s) &= \sum_i \frac{p_i^x(s)p_i^y(s)}{m} - \frac{1}{2}\sum_{i\neq j}\frac{r_{ij}^x(s)r_{ij}^y(s)}{r_{ij}(s)}u'(r_{ij}(s)) \\ &= \sum_i \frac{p_i^x(s)p_i^y(s)}{m} \\ &\quad - \frac{N}{2}\int d\mathbf{r}\frac{xy}{r}u'(r)\int\frac{d\mathbf{q}}{(2\pi)^3}e^{-i\mathbf{q}\cdot\mathbf{r}}\left[\frac{1}{N}\rho_{\mathbf{q}}(s)\rho_{\mathbf{q}}(s)^* - 1\right],\end{aligned} \tag{76}$$

where we have used $f(\mathbf{r}_{ij})=\int d\mathbf{r}f(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}_{ij})$ and $\delta(\mathbf{r}-\mathbf{r}_{ij})=(1/2\pi)^3\int d\mathbf{q}e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}_{ij})}$ with $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$ in the final equality. Substituting this into the integrands of Eq. (67), one obtains

$$\sigma_{\mathrm{SS}} = -\frac{1}{V}\left\langle\sum_i\frac{p_i^xp_i^y}{m}\right\rangle_{\mathrm{SS}} + \frac{\rho}{2}\int d\mathbf{r}\frac{xy}{r}u'(r) \times \int\frac{d\mathbf{q}}{(2\pi)^3}e^{-i\mathbf{q}\cdot\mathbf{r}}(S_{\mathbf{q}}^{\mathrm{SS}} - S_q). \tag{77}$$

Here, the definition (33) for the steady-state average has been exploited for the first term, and Eq. (75) for the steady-state structure factor $S_{\mathbf{q}}^{\mathrm{SS}}$ has been used for the second term. Notice that $(S_{\mathbf{q}}^{\mathrm{SS}}-S_q)$ in the second term can be replaced, e.g., by $(S_{\mathbf{q}}^{\mathrm{SS}}-1)$, since isotropic terms do not survive after spatial integral involving the anisotropic term xy. Equation (77) simply expresses that anisotropic density fluctuations are responsible for the steady-state shear stress. Since the steady-state pair correlation function $g_{\mathrm{SS}}(\mathbf{r})$ is related to $S_{\mathbf{q}}^{\mathrm{SS}}$ via

$$\rho g_{\mathrm{SS}}(\mathbf{r}) = \int \frac{d\mathbf{q}}{(2\pi)^3} e^{-i\mathbf{q}\cdot\mathbf{r}} (S_{\mathbf{q}}^{\mathrm{SS}} - 1), \tag{78}$$

one understands that the interaction part of Eq. (77) is equivalent to Eq. (1). Such an equal handling of σ_{SS} and $S_{\mathbf{q}}^{\mathrm{SS}}$ based on the TTCF formalism is expected since no approximation has yet been introduced.

In the following sections, we will first derive a set of self-consistent equations for the transient density correlators $F_{\mathbf{q}}(t)$ using the projection-operator formalism (Sec. III) and the mode-coupling approach (Sec. IV). We will then argue that the mentioned TTCF expressions for the steady-state properties can be evaluated within the mode-coupling approximation based on the knowledge of $F_{\mathbf{q}}(t)$ (Sec. V). In this way, we construct the nonequilibrium MCT for stationary sheared systems.

III. ZWANZIG-MORI–TYPE EQUATIONS

In this section, we derive exact Zwanzig-Mori–type equations of motion for the transient density correlator $F_{\mathbf{q}}(t)$ for a system that is initially at equilibrium and subsequently subjected to stationary shearing along with thermostat. A "standard" approach [10] for a quiescent system is that a Zwanzig-Mori equation for a correlator $\langle A(t)A(0)^*\rangle$ of some phase variable A evolving with a time-independent p Liouvillean is derived based on the static projection operator onto the subspace spanned by A. As we will see below, due to the presence of the time-dependent wave-vector advection $\mathbf{q}(t)$, this standard approach should be appropriately generalized for sheared systems. We start our discussion by pointing this out.

A. Difficulties in applying previous formulations

Recently, McPhie *et al.* [26] developed a projection-operator formalism which generalizes the standard approach to nonequilibrium systems and allows one to derive a Zwanzig-Mori–type equation for a transient correlator $\langle A(t)A(0)^*\rangle$. Their formalism is also based on the time-independent p Liouvillean and on the static projection operator. Using the convention (57), one can introduce the transient density correlator of the form

$$\tilde{F}_{\mathbf{q}}(t) = \frac{1}{N}\langle \rho_{\mathbf{q}(-t)}(t)\rho_{\mathbf{q}}(0)^*\rangle. \tag{79}$$

Thus, apparently, there seems no problem to apply the formalism developed in Ref. [26] by setting $A(t)=\rho_{\mathbf{q}(-t)}(t)$. However, $\rho_{\mathbf{q}(-t)}(t)$ is not a phase variable since its time evolution is also affected by the wave-vector advection $\mathbf{q}(-t)$ and its equation of motion cannot be written solely in terms of the time-independent p Liouvillean as in Eq. (8). Their formalism, therefore, cannot be directly applied to derive the equation for $\tilde{F}_{\mathbf{q}}(t)$. Nevertheless, we mention here that our equations of motion derived below resemble those presented in Ref. [26] in that new memory kernels enter in addition to the one familiar in the equilibrium Zwanzig-Mori equations.

More recently, Fuchs and Cates [17] derived the Zwanzig-Mori–type equation for $F_{\mathbf{q}}(t)$, starting from the Smoluchowski equation for interacting Brownian particles under stationary shearing. It is not difficult, at least formally, to adapt their formulation to the Sllod equations, and we briefly summarize its consequences here.

Because of the equivalence of the particles, the transient density correlator $F_{\mathbf{q}}(t)$ defined in Eq. (74) can be written as

$$F_{\mathbf{q}}(t) = \frac{1}{N}\langle \rho_{\mathbf{q}(t)}(0)^*\rho_{\mathbf{q}}(t)\rangle = \langle \rho_{\mathbf{q}}^{s*} e^{-i\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\mathbf{r}_s t} e^{i\mathcal{L}t}\rho_{\mathbf{q}}\rangle, \tag{80}$$

where $\rho_{\mathbf{q}}^{s} \equiv e^{i\mathbf{q}\cdot\mathbf{r}_s}$ denotes the density of a single tagged particle (labeled s), which is identical to the others. Hereafter, the absence of the argument t implies that the associated quantities are evaluated at $t=0$. By this trick of singling out a particle, the motion of the collective density fluctuations $\rho_{\mathbf{q}}$ can be described by one, but time-dependent, p Liouvillean $i\mathcal{L}_s(t)$ defined via

$$\frac{\partial}{\partial t} e^{-i\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\mathbf{r}_s t} e^{i\mathcal{L}t} \equiv i\mathcal{L}_s(t) e^{-i\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\mathbf{r}_s t} e^{i\mathcal{L}t}. \tag{81}$$

Based on the p Liouvillean $i\mathcal{L}$ for the Sllod equations, the operator $i\mathcal{L}_s(t)$ can be worked out explicitly,

$$i\mathcal{L}_s(t) = i\mathcal{L} - i\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\mathbf{r}_s + i\mathbf{q}\cdot\boldsymbol{\kappa}\cdot(\mathbf{p}_s/m)t. \tag{82}$$

Integrating Eq. (81) in time, one obtains

$$F_{\mathbf{q}}(t) = \langle \rho_{\mathbf{q}}^{s*} e_+^{\int_0^t d\tau i\mathcal{L}_s(\tau)}\rho_{\mathbf{q}}\rangle. \tag{83}$$

Here e_+ denotes the time-ordered exponential, where earlier times appear on the right. This expression also explains why the formalism developed in Ref. [26], which is based on the time-independent p Liouvillean, cannot deal with $F_{\mathbf{q}}(t)$.

Equation (83) can be handled by manipulations based on the static projection operator $\mathcal{P}_s = \rho_{\mathbf{q}}\rangle(1/S_q)\langle\rho_{\mathbf{q}}^{s*}$, and one can derive the following exact Zwanzig-Mori–type equation of motion for $F_{\mathbf{q}}(t)$ in the same manner as detailed in Ref. [17]:

$$\frac{\partial}{\partial t}F_{\mathbf{q}}(t) - \frac{1}{S_q}\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}S_q\right]F_{\mathbf{q}}(t) + \int_0^t ds K_{\mathbf{q}}(t,s)F_{\mathbf{q}}(s) = 0. \tag{84a}$$

Here the memory kernel is given by

$$K_{\mathbf{q}}(t,t') = -\frac{1}{S_q}\langle \rho_{\mathbf{q}}^{s*} i\mathcal{L}_s(t)\mathcal{Q}_s e_+^{\int_{t'}^{t} d\tau \mathcal{Q}_s i\mathcal{L}_s(\tau)\mathcal{Q}_s}\mathcal{Q}_s i\mathcal{L}_s(t')\rho_{\mathbf{q}}\rangle, \tag{84b}$$

in which $\mathcal{Q}_s \equiv I - \mathcal{P}_s$ with I denoting the identity operator. Equations (84a) and (84b) serve as the starting equations for Brownian particles exhibiting overdamped dynamics, since in this case the velocity entering into $\mathcal{Q}_s i\mathcal{L}_s(t)\rho_{\mathbf{q}}$ is proportional to the force, and hence, $K(t,t')$ essentially describes the fluctuating-force correlations. Such an incorporation of the fluctuating-force correlations is essential in developing self-consistent equations for $F_{\mathbf{q}}(t)$.

On the other hand, we need an additional Zwanzig-Mori–type equation for $K(t,t')$ in constructing a self-consistent theory since the time derivative of the (peculiar) momentum is proportional to the force in the Sllod equations (2). For this purpose, one needs to introduce a time-dependent projection operator onto the subspace spanned by $\mathcal{Q}_s i\mathcal{L}_s(t)\rho_{\mathbf{q}}$. We found that the resulting equation of motion for $K(t,t')$ is too cumbersome to be adopted as our starting equation. (See, e.g., Ref. [27] for the application of the time-dependent projection-operator formalism.)

Here we shall take an alternative route. Adopting the original definition

$$F_{\mathbf{q}}(t) = \frac{1}{N}\langle \rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}(0)^*\rangle = \frac{1}{N}\langle [e^{i\mathcal{L}t}\rho_{\mathbf{q}}]\rho^*_{\mathbf{q}(t)}\rangle \tag{85}$$

of the transient density correlator, we will first derive an exact continuity equation which relates $F_{\mathbf{q}}(t)$ to the transient cross correlator

$$H^{\lambda}_{\mathbf{q}}(t) = \frac{1}{N}\langle j^{\lambda}_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}(0)^*\rangle = \frac{1}{N}\langle [e^{i\mathcal{L}t}j^{\lambda}_{\mathbf{q}}]\rho^*_{\mathbf{q}(t)}\rangle \tag{86}$$

for $\lambda = x,y,z$, formed with the current density fluctuations $j^{\lambda}_{\mathbf{q}}$ defined by

$$j^{\lambda}_{\mathbf{q}} = \sum_i \frac{p^{\lambda}_i}{m} e^{i\mathbf{q}\cdot\mathbf{r}_i}. \tag{87}$$

Here it is necessary to take into account all the λ components of $j^{\lambda}_{\mathbf{q}}$ due to the anisotropic nature of the sheared system. We will then derive a Zwanzig-Mori–type equation of motion for $H^{\lambda}_{\mathbf{q}}(t)$, which can be done via a partial use of the static projection operator as we will see below.

B. Continuity equation

We start with the time-evolution equation for the number density fluctuations. Since [see Eqs. (13a)–(13d)]

$$i\mathcal{L}\rho_{\mathbf{q}} = (i\mathcal{L}_0 + i\mathcal{L}_{\dot\gamma} + i\mathcal{L}_{\alpha})\rho_{\mathbf{q}} = i\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}} + \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\rho_{\mathbf{q}}, \tag{88}$$

one finds the following continuity equation for the sheared system relating the partial time derivative of $\rho_{\mathbf{q}}(t) = e^{i\mathcal{L}t}\rho_{\mathbf{q}}$ to $j^{\lambda}_{\mathbf{q}}(t) = e^{i\mathcal{L}t}j^{\lambda}_{\mathbf{q}}$:

$$\left[\frac{\partial}{\partial t} - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]\rho_{\mathbf{q}}(t) = i\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}}(t). \tag{89}$$

On the other hand, the density fluctuation at the advected wave vector $\rho^*_{\mathbf{q}(t)}$ obeys the equation

$$\left[\frac{\partial}{\partial t} - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]\rho^*_{\mathbf{q}(t)} = i\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\sum_i(\boldsymbol{\kappa}t)\cdot\mathbf{r}_i e^{-i\mathbf{q}(t)\cdot\mathbf{r}_i} = 0, \tag{90}$$

since the shear-rate tensor satisfies $\boldsymbol{\kappa}\cdot\boldsymbol{\kappa}=0$. One can readily obtain from the above two equations that the transient density correlator $F_{\mathbf{q}}(t) = \langle\rho_{\mathbf{q}}(t)\rho^*_{\mathbf{q}(t)}\rangle/N$ and the transient cross correlator $H^{\lambda}_{\mathbf{q}}(t) = \langle j^{\lambda}_{\mathbf{q}}(t)\rho^*_{\mathbf{q}(t)}\rangle/N$ is connected via

$$\left[\frac{\partial}{\partial t} - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]F_{\mathbf{q}}(t) = i\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t). \tag{91}$$

C. Exact equation for the transient cross correlator

We next derive an exact equation of motion for the transient cross correlator $H^{\lambda}_{\mathbf{q}}(t)$. We start from

$$\begin{aligned} i\mathcal{L}j^{\lambda}_{\mathbf{q}} &= (i\mathcal{L}_0 + i\mathcal{L}_{\dot\gamma} + i\mathcal{L}_{\alpha})j^{\lambda}_{\mathbf{q}} \\ &= i\mathcal{L}_0 j^{\lambda}_{\mathbf{q}} + \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}j^{\lambda}_{\mathbf{q}} - (\boldsymbol{\kappa}\cdot\mathbf{j}_{\mathbf{q}})^{\lambda} - \alpha j^{\lambda}_{\mathbf{q}}. \end{aligned} \tag{92}$$

One therefore gets for $j^{\lambda}_{\mathbf{q}}(t) = e^{i\mathcal{L}t}j_{\mathbf{q}}$

$$\left[\frac{\partial}{\partial t} - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]j^{\lambda}_{\mathbf{q}}(t) = e^{i\mathcal{L}t}i\mathcal{L}_0 j^{\lambda}_{\mathbf{q}} - [\boldsymbol{\kappa}\cdot\mathbf{j}_{\mathbf{q}}(t)]^{\lambda} - \alpha j^{\lambda}_{\mathbf{q}}(t). \tag{93}$$

It is straightforward to obtain from this equation and Eq. (90) for the correlator $H^{\lambda}_{\mathbf{q}}(t) = \langle j^{\lambda}_{\mathbf{q}}(t)\rho^*_{\mathbf{q}(t)}\rangle/N$

$$\begin{aligned} \left[\frac{\partial}{\partial t} - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]H^{\lambda}_{\mathbf{q}}(t) &= \frac{1}{N}\langle[e^{i\mathcal{L}t}i\mathcal{L}_0 j^{\lambda}_{\mathbf{q}}]\rho^*_{\mathbf{q}(t)}\rangle - [\boldsymbol{\kappa}\cdot\mathbf{H}_{\mathbf{q}}(t)]^{\lambda} \\ &\quad - \alpha H^{\lambda}_{\mathbf{q}}(t). \end{aligned} \tag{94}$$

It is already clear at this point that one cannot derive a closed equation for the "longitudinal" component $\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t)$ alone due to the presence of the second term on the right-hand side of Eq. (94). This reflects the anisotropic nature of the sheared system. We also notice that the thermostatting multiplier α can be taken outside of the ensemble average in the last term of Eq. (94) since we have adopted the constant-α model. If, for example, the Gaussian isokinetic multiplier α_G were used [see Eq. (3)], then one would have to consider an additional equation of motion for $(1/N)\langle[e^{i\mathcal{L}t}\alpha_G j^{\lambda}_{\mathbf{q}}]\rho^*_{\mathbf{q}(t)}\rangle$. Thus, a considerable simplification is achieved via the adoption of the constant-α model.

D. Projection-operator formalism

In the following, we shall apply a projection-operator formalism, but only to the first term on the right-hand side of Eq. (94). As will be shown below, this can be done via a static projection operator, and thereby the aforementioned difficulty connected with Eq. (84b) can be avoided. In this way, we complete the derivation of the Zwanzig-Mori–type equation of motion for $H^{\lambda}_{\mathbf{q}}(t)$, which together with the continuity equation (91) provides our starting equations for developing a nonequilibrium MCT for transient density correlators.

For this purpose, let us introduce the static projection operator $\mathcal{P}$ onto the subspace spanned by $\rho_{\mathbf{k}}$ and $j^{\mu}_{\mathbf{k}}$ ($\mu = x,y,z$). Since $\langle\rho_{\mathbf{k}}\rho^*_{\mathbf{k}'}\rangle = \delta_{\mathbf{k},\mathbf{k}'}NS_k$, $\langle j^{\lambda}_{\mathbf{k}}j^{\mu*}_{\mathbf{k}'}\rangle = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda\mu}Nv^2$ with $v = \sqrt{k_BT/m}$ denoting the thermal velocity, and $\langle\rho_{\mathbf{k}}j^{\mu*}_{\mathbf{k}'}\rangle = 0$ (remember that the averaging is over the initial canonical distribution), the projection operator $\mathcal{P}$ is given by

$$\mathcal{P}X = \sum_{\mathbf{k}}\langle X\rho^*_{\mathbf{k}}\rangle\frac{1}{NS_k}\rho_{\mathbf{k}} + \sum_{\mathbf{k}}\sum_{\mu}\langle Xj^{\mu*}_{\mathbf{k}}\rangle\frac{1}{Nv^2}j^{\mu}_{\mathbf{k}}. \tag{95}$$

The complementary projection operator is defined by $\mathcal{Q} \equiv I - \mathcal{P}$. One can easily show that $\mathcal{P}$ and $\mathcal{Q}$ are idempotent and Hermitian.

The time evolution of $i\mathcal{L}_0 j^\lambda_{\mathbf{q}}$ appearing in the first term on the right-hand side of Eq. (94) shall then be separated into parts correlated and uncorrelated with $\{\rho_{\mathbf{k}}, j^\mu_{\mathbf{k}}\}$:

$$e^{i\mathcal{L}t} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} = e^{i\mathcal{L}t}\mathcal{P} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} + e^{i\mathcal{L}t}\mathcal{Q} i\mathcal{L}_0 j^\lambda_{\mathbf{q}}. \tag{96}$$

As derived in Appendix A 3, one obtains

$$\mathcal{P} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} = i q_\lambda \frac{v^2}{S_q}\rho_{\mathbf{q}}, \tag{97}$$

and hence, the first term on the right-hand side of Eq. (96) is given by

$$e^{i\mathcal{L}t}\mathcal{P} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} = i q_\lambda \frac{v^2}{S_q} e^{i\mathcal{L}t}\rho_{\mathbf{q}}. \tag{98}$$

The second term on the right-hand side of Eq. (96) shall be handled using the identity

$$e^{i\mathcal{L}t} = e^{\mathcal{Q}i\mathcal{L}t} + \int_0^t ds e^{i\mathcal{L}(t-s)}\mathcal{P} i\mathcal{L} e^{\mathcal{Q}i\mathcal{L}s}. \tag{99}$$

Applying this to $\mathcal{Q} i\mathcal{L}_0 j^\lambda_{\mathbf{q}}$ and exploiting the relation $e^{\mathcal{Q}i\mathcal{L}t}\mathcal{Q} = e^{it}\mathcal{Q}$ which holds due to the idempotency of the operator $\mathcal{Q}$, we obtain

$$e^{i\mathcal{L}t}\mathcal{Q} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} = e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{Q} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} + \int_0^t ds e^{i\mathcal{L}(t-s)}\mathcal{P} i\mathcal{L} e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}s}\mathcal{Q} i\mathcal{L}_0 j^\lambda_{\mathbf{q}}. \tag{100}$$

Let us introduce

$$R^\lambda_{\mathbf{q}}(t) \equiv e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t} R^\lambda_{\mathbf{q}} \tag{101}$$

with

$$R^\lambda_{\mathbf{q}} \equiv \mathcal{Q} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} = i\mathcal{L}_0 j^\lambda_{\mathbf{q}} - i q_\lambda \frac{v^2}{S_q}\rho_{\mathbf{q}}, \tag{102}$$

where we have used Eq. (97). Since $\mathcal{Q}\rho^*_{\mathbf{q}(t)} = \mathcal{Q} j^{\mu *}_{\mathbf{q}(t)} = 0$, there holds

$$\langle R^\lambda_{\mathbf{q}}(t)\rho^*_{\mathbf{q}(t)}\rangle = 0 \quad \text{and} \quad \langle R^\lambda_{\mathbf{q}}(t) j^{\mu *}_{\mathbf{q}(t)}\rangle = 0. \tag{103}$$

Thus, $R^\lambda_{\mathbf{q}}(t)$ is always uncorrelated with $\{\rho_{\mathbf{k}}, j^\mu_{\mathbf{k}}\}$, and we follow the usual convention to call this phase variable the random or fluctuating force.

In terms of the fluctuating force $R^\lambda_{\mathbf{q}}(t)$, the second term in Eq. (100) can be expressed as

$$\begin{aligned}\int_0^t ds e^{i\mathcal{L}(t-s)}\mathcal{P} i\mathcal{L} R^\lambda_{\mathbf{q}}(s) &= \int_0^t ds \sum_{\mathbf{k}} \langle [i\mathcal{L} R^\lambda_{\mathbf{q}}(s)]\rho^*_{\mathbf{k}}\rangle \frac{1}{NS_k} e^{i\mathcal{L}(t-s)}\rho_{\mathbf{k}} \\ &\quad + \int_0^t ds \sum_{\mathbf{k}}\sum_\mu \langle [i\mathcal{L} R^\lambda_{\mathbf{q}}(s)] j^{\mu *}_{\mathbf{k}}\rangle \\ &\quad \times \frac{1}{Nv^2} e^{i\mathcal{L}(t-s)} j^\mu_{\mathbf{k}} \\ &= \int_0^t ds \langle [i\mathcal{L} R^\lambda_{\mathbf{q}}(s)]\rho^*_{\mathbf{q}(s)}\rangle \\ &\quad \times \frac{1}{NS_{q(s)}} e^{i\mathcal{L}(t-s)}\rho_{\mathbf{q}(s)} \\ &\quad + \sum_\mu \int_0^t ds \langle [i\mathcal{L} R^\lambda_{\mathbf{q}}(s)] j^{\mu *}_{\mathbf{q}(s)}\rangle \\ &\quad \times \frac{1}{Nv^2} e^{i\mathcal{L}(t-s)} j^\mu_{\mathbf{q}(s)},\end{aligned} \tag{104}$$

where the last equality holds since $\langle R^\lambda_{\mathbf{q}}(s) f^*_{\mathbf{k}}\rangle$ is nonzero only for $\mathbf{k} = \mathbf{q}(s)$ [see Eq. (54)]. We also noticed that the ensemble averaged terms are independent of the phase and are unaffected by the propagator. The evaluation of the ensemble averaged terms in the integrands of Eq. (104) is presented in Appendix A 4, and the results are given by

$$\begin{aligned}\langle [i\mathcal{L} R^\lambda_{\mathbf{q}}(s)]\rho^*_{\mathbf{q}(s)}\rangle = &- \frac{\dot\gamma}{k_B T}\langle R^\lambda_{\mathbf{q}}(s)\mathcal{Q}[\rho^*_{\mathbf{q}(s)}\sigma_{xy}]\rangle \\ &- \frac{2\alpha}{k_B T}\langle R^\lambda_{\mathbf{q}}(s)\mathcal{Q}[\rho^*_{\mathbf{q}(s)}\delta K]\rangle,\end{aligned} \tag{105}$$

$$\begin{aligned}\langle [i\mathcal{L} R^\lambda_{\mathbf{q}}(s)] j^{\mu *}_{\mathbf{q}(s)}\rangle = &- \langle R^\lambda_{\mathbf{q}}(s) R^{\mu *}_{\mathbf{q}(s)}\rangle - \frac{\dot\gamma}{k_B T}\langle R^\lambda_{\mathbf{q}}(s)\mathcal{Q}[j^{\mu *}_{\mathbf{q}(s)}\sigma_{xy}]\rangle \\ &- \frac{2\alpha}{k_B T}\langle R^\lambda_{\mathbf{q}}(s)\mathcal{Q}[j^{\mu *}_{\mathbf{q}(s)}\delta K]\rangle.\end{aligned} \tag{106}$$

Let us notice that Eq. (106) has been simplified due to the adoption of the constant-α model for the thermostat [see the comment below Eq. (A32)]: otherwise, e.g., when the Gaussian isokinetic thermostat is used, one has to add a term $\langle R^\lambda_{\mathbf{q}}(s)\mathcal{Q}[\alpha_G j^{\mu *}_{\mathbf{q}(s)}]\rangle$ to the right-hand side of Eq. (106).

With Eqs. (100)–(102) and (104)–(106), we now obtain

$$\begin{aligned}e^{i\mathcal{L}t}\mathcal{Q} i\mathcal{L}_0 j^\lambda_{\mathbf{q}} = R^\lambda_{\mathbf{q}}(t) &- \sum_\mu \int_0^t ds M^{\lambda\mu}_{\mathbf{q}}(s) e^{i\mathcal{L}(t-s)} j^\mu_{\mathbf{q}(s)} \\ &+ \dot\gamma \int_0^t ds i L^\lambda_{\mathbf{q}}(s) e^{i\mathcal{L}(t-s)}\rho_{\mathbf{q}(s)} \\ &- \dot\gamma \sum_\mu \int_0^t ds L'^{\lambda\mu}_{\mathbf{q}}(s) e^{i\mathcal{L}(t-s)} j^\mu_{\mathbf{q}(s)} \\ &+ \alpha \int_0^t ds i N^\lambda_{\mathbf{q}}(s) e^{i\mathcal{L}(t-s)}\rho_{\mathbf{q}(s)} \\ &- \alpha \sum_\mu \int_0^t ds N'^{\lambda\mu}_{\mathbf{q}}(s) e^{i\mathcal{L}(t-s)} j^\mu_{\mathbf{q}(s)}.\end{aligned} \tag{107}$$

Here we have introduced the following memory kernels:

$$M^{\lambda\mu}_{\mathbf{q}}(t) \equiv \frac{1}{Nv^2}\langle R^\lambda_{\mathbf{q}}(t) R^{\mu *}_{\mathbf{q}(t)}\rangle, \tag{108}$$

$$L^\lambda_{\mathbf{q}}(t) \equiv i\frac{1}{Nk_B T S_{q(t)}}\langle R^\lambda_{\mathbf{q}}(t)\mathcal{Q}[\rho^*_{\mathbf{q}(t)}\sigma_{xy}]\rangle, \tag{109}$$

$$L'^{\lambda\mu}_{\mathbf{q}}(t) \equiv \frac{m}{N(k_B T)^2}\langle R^\lambda_{\mathbf{q}}(t)\mathcal{Q}[j^{\mu *}_{\mathbf{q}(t)}\sigma_{xy}]\rangle, \tag{110}$$

$$N_{\mathbf{q}}^{\lambda}(t) \equiv i \frac{2}{N k_B T S_{q(t)}} \langle R_{\mathbf{q}}^{\lambda}(t) \mathcal{Q}[\rho_{\mathbf{q}(t)}^{*} \delta K] \rangle, \tag{111}$$

$$N_{\mathbf{q}}^{\prime \lambda \mu}(t) \equiv \frac{2m}{N(k_B T)^2} \langle R_{\mathbf{q}}^{\lambda}(t) \mathcal{Q}[j_{\mathbf{q}(t)}^{\mu *} \delta K] \rangle. \tag{112}$$

Substituting Eqs. (96), (98), and (107) along with Eq. (103) into the first term on the right-hand side of Eq. (94), we finally obtain the following Zwanzig-Mori–type equation for $H_{\mathbf{q}}^{\lambda}(t)$:

$$\begin{aligned}\left[\frac{\partial}{\partial t} - \mathbf{q} \cdot \boldsymbol{\kappa} \cdot \frac{\partial}{\partial \mathbf{q}}\right] H_{\mathbf{q}}^{\lambda}(t) = {} & i q_{\lambda} \frac{v^2}{S_q} F_{\mathbf{q}}(t) - [\boldsymbol{\kappa} \cdot \mathbf{H}_{\mathbf{q}}(t)]^{\lambda} - \alpha H_{\mathbf{q}}^{\lambda}(t) \\ & - \sum_{\mu} \int_0^t ds M_{\mathbf{q}}^{\lambda \mu}(s) H_{\mathbf{q}(s)}^{\mu}(t-s) \\ & + \dot{\gamma} \int_0^t ds i L_{\mathbf{q}}^{\lambda}(s) F_{\mathbf{q}(s)}(t-s) \\ & - \dot{\gamma} \sum_{\mu} \int_0^t ds L_{\mathbf{q}}^{\prime \lambda \mu}(s) H_{\mathbf{q}(s)}^{\mu}(t-s) \\ & + \alpha \int_0^t ds i N_{\mathbf{q}}^{\lambda}(s) F_{\mathbf{q}(s)}(t-s) \\ & - \alpha \sum_{\mu} \int_0^t ds N_{\mathbf{q}}^{\prime \lambda \mu}(s) H_{\mathbf{q}(s)}^{\mu}(t-s). \end{aligned} \tag{113}$$

Here, we have noticed $(1/N)\langle [e^{i\mathcal{L}(t-s)} \rho_{\mathbf{q}(s)}] \rho_{\mathbf{q}(t)}^{*} \rangle = F_{\mathbf{q}(s)}(t-s)$ and $(1/N)\langle [e^{i\mathcal{L}(t-s)} j_{\mathbf{q}(s)}^{\mu}] \rho_{\mathbf{q}(t)}^{*} \rangle = H_{\mathbf{q}(s)}^{\mu}(t-s)$. One can easily confirm that these are consistent with the definitions (85) and (86).

The memory kernel $M_{\mathbf{q}}^{\lambda\mu}(t)$ describing the fluctuating force correlations is already familiar from the equilibrium Zwanzig-Mori equation of motion for the density correlator [11]. The additional memory kernels $L_{\mathbf{q}}^{\lambda}(t)$ and $L_{\mathbf{q}}^{\prime\lambda\mu}(t)$ are due to couplings between the fluctuating force and the shear stress and $N_{\mathbf{q}}^{\lambda}(t)$ and $N_{\mathbf{q}}^{\prime\lambda\mu}(t)$ are associated with couplings between the fluctuating force and temperature fluctuations. In the following section, we introduce mode-coupling approximations for these memory kernels to obtain a set of self-consistent equations of motion for the transient density correlators.

IV. MODE-COUPLING APPROXIMATION

We have encountered five memory kernels in the Zwanzig-Mori–type exact equations of motion for the transient correlators. We need to invoke approximations for these memory kernels in order to obtain closed equations for $F_{\mathbf{q}}(t)$. In this section, we apply the mode-coupling approximations [11] to these memory kernels.

The basic idea behind MCT is that the fluctuation of a given dynamical variable decays, at intermediate and long times, predominantly into pairs of hydrodynamic modes associated with quasiconserved dynamical variables. It is therefore reasonable to expect that the decay of the memory kernels at intermediate and long times is dominated by those mode correlations which have the longest relaxation times. The sluggishness of the structural relaxation processes in glass-forming systems suggests that the slow decay of the memory kernels is basically due to couplings to pair-density modes. The simplest way to extract such a slowly decaying part is to introduce another projection operator $\mathcal{P}_2$ which projects any variable onto the subspace spanned by $\rho_{\mathbf{k}}\rho_{\mathbf{p}}$, i.e.,

$$\mathcal{P}_2 X = \sum_{\mathbf{k} > \mathbf{p}} \langle X \rho_{\mathbf{k}}^{*} \rho_{\mathbf{p}}^{*} \rangle \frac{1}{N^2 S_k S_p} \rho_{\mathbf{k}} \rho_{\mathbf{p}}. \tag{114}$$

Here we already used the static version of the factorization approximation introduced below [see Eq. (120)]. It is readily verified that $\mathcal{P}_2$ is idempotent and Hermitian.

The first approximation in the mode-coupling approach thus corresponds to replacing the propagator $e^{i\mathcal{QLQ}t}$ governing the time-evolution of the memory kernels by its projection on the subspace spanned by the pair-density modes $e^{i\mathcal{QLQ}t} \approx \mathcal{P}_2 e^{i\mathcal{QLQ}t} \mathcal{P}_2$. Under this approximation, the memory kernel $M_{\mathbf{q}}^{\lambda\mu}(t)$ defined in Eq. (108) is given by

$$\begin{aligned} M_{\mathbf{q}}^{\lambda\mu}(t) &\approx \frac{1}{N v^2} \langle [\mathcal{P}_2 e^{i\mathcal{QLQ}t} \mathcal{P}_2 R_{\mathbf{q}}^{\lambda}] R_{\mathbf{q}(t)}^{\mu *} \rangle \\ &= \frac{1}{N v^2} \langle [e^{i\mathcal{QLQ}t} \mathcal{P}_2 R_{\mathbf{q}}^{\lambda}] \mathcal{P}_2 R_{\mathbf{q}(t)}^{\mu *} \rangle. \end{aligned} \tag{115}$$

The expression for the projected random force $\mathcal{P}_2 R_{\mathbf{q}}^{\lambda}$ is derived in Appendix A 5 within the convolution approximation for triple correlations

$$\langle \rho_{\mathbf{q}} \rho_{\mathbf{k}}^{*} \rho_{\mathbf{p}}^{*} \rangle \approx \delta_{\mathbf{q},\mathbf{k}+\mathbf{p}} N S_q S_k S_p \tag{116}$$

and is given by

$$\mathcal{P}_2 R_{\mathbf{q}}^{\lambda} = - i \frac{\rho v^2}{N} \sum_{\mathbf{k} > \mathbf{p}} \delta_{\mathbf{q},\mathbf{k}+\mathbf{p}} [k_{\lambda} c_k + p_{\lambda} c_p] \rho_{\mathbf{k}} \rho_{\mathbf{p}}. \tag{117}$$

Here c_q is the direct correlation function defined via

$$\rho c_q = 1 - \frac{1}{S_q}. \tag{118}$$

Substituting Eq. (117) into Eq. (115), we obtain

$$\begin{aligned} M_{\mathbf{q}}^{\lambda\mu}(t) = {} & \frac{\rho^2 v^2}{N^3} \sum_{\mathbf{k} > \mathbf{p}} \sum_{\mathbf{k}' > \mathbf{p}'} \delta_{\mathbf{q},\mathbf{k}+\mathbf{p}} \delta_{\mathbf{q}(t),\mathbf{k}'+\mathbf{p}'} [k_{\lambda} c_k + p_{\lambda} c_p] \\ & \times [k'_{\mu} c_{k'} + p'_{\mu} c_{p'}] \langle [e^{i\mathcal{QLQ}t} \rho_{\mathbf{k}} \rho_{\mathbf{p}}] \rho_{\mathbf{k}'}^{*} \rho_{\mathbf{p}'}^{*} \rangle. \end{aligned} \tag{119}$$

The final approximation in the mode-coupling approach is to factorize averages of products, evolving in time with the propagator $e^{i\mathcal{QLQ}t}$, into products of averages formed with the variables evolving with $e^{i\mathcal{L}t}$ (factorization approximation):

$$\begin{aligned} \langle [e^{i\mathcal{QLQ}t} \rho_{\mathbf{k}} \rho_{\mathbf{p}}] \rho_{\mathbf{k}'}^{*} \rho_{\mathbf{p}'}^{*} \rangle &\approx \langle [e^{i\mathcal{L}t} \rho_{\mathbf{k}}] \rho_{\mathbf{k}'}^{*} \rangle \langle [e^{i\mathcal{L}t} \rho_{\mathbf{p}}] \rho_{\mathbf{p}'}^{*} \rangle \\ &= \delta_{\mathbf{k}',\mathbf{k}(t)} \delta_{\mathbf{p}',\mathbf{p}(t)} N^2 F_{\mathbf{k}}(t) F_{\mathbf{p}}(t). \end{aligned} \tag{120}$$

Here the translational invariance of the sheared system is taken into account [see Eq. (54)]. Applying this approximation to Eq. (119), we obtain

$$M_{\mathbf{q}}^{\lambda\mu}(t) = \frac{\rho v^2}{2(2\pi)^3} \int d\mathbf{k} [k_\lambda c_k + p_\lambda c_p] \times [k_\mu(t) c_{k(t)} + p_\mu(t) c_{p(t)}] F_{\mathbf{k}}(t) F_{\mathbf{p}}(t), \quad (121)$$

where the wave vector $\mathbf{p}$ in this and the following expressions for the memory kernels abbreviates $\mathbf{p} \equiv \mathbf{q} - \mathbf{k}$, and should not be confused with the momentum variable.

In the absence of shear, the MCT expression (121) reduces to the one familiar from the equilibrium MCT [11] describing nonlinear interactions of density fluctuations, called the cage effect, relevant for structural slowing down. The matrix structure as well as the wave-vector dependence in $M_{\mathbf{q}}^{\lambda\mu}(t)$ can be simplified, i.e., it can be decomposed into longitudinal and transversal components which depend on the modulus $q = |\mathbf{q}|$ only, and this is possible because of the isotropic nature of the quiescent equilibrium system. In the presence of shear, on the other hand, the "dephasing" of the vertex function in Eq. (121) occurs, which reduces the nonlinear interactions, and hence, enhances the structural relaxation. In addition, the structure of $M_{\mathbf{q}}^{\lambda\mu}(t)$ cannot be simplified in a mentioned way due to the wave-vector dependence of the vertex function and of the transient density correlators, which are associated with the anisotropic nature of the sheared system.

The memory kernel $L_{\mathbf{q}}^{\lambda}(t)$ defined in Eq. (109) can be handled in a similar manner under the mode-coupling approximation, and its detailed derivation is presented in Appendix A 6 with the result

$$L_{\mathbf{q}}^{\lambda}(t) = -\frac{v^2}{2(2\pi)^3} \int d\mathbf{k} [k_\lambda c_k + p_\lambda c_p] \times \left[\frac{k_x k_y(t)}{k(t)} \frac{S'_{k(t)}}{S_{k(t)}} + \frac{p_x p_y(t)}{p(t)} \frac{S'_{p(t)}}{S_{p(t)}} \right] F_{\mathbf{k}}(t) F_{\mathbf{p}}(t). \quad (122)$$

Here $S'_q \equiv \partial S_q / \partial q$. It is anticipated that this memory kernel becomes relevant only if significant anisotropy is developed in the density fluctuations. This is because the shear stress σ_{xy} entering into its defining equation (109), which is reflected in the quantities in the second square brackets in Eq. (122), is intrinsically an anisotropic quantity. For example, one finds from Eq. (122) that $L_{\mathbf{q}}^{\lambda}(0) = 0$ reflecting the isotropy of the initial equilibrium state.

The other memory kernels defined in Eqs. (110)–(112) are found to vanish under the mode-coupling approximation as demonstrated in Appendixes A 7 and A 8:

$$L_{\mathbf{q}}^{\prime\lambda\mu}(t) = 0. \quad (123)$$

$$N_{\mathbf{q}}^{\lambda}(t) = 0, \quad N_{\mathbf{q}}^{\prime\lambda\mu}(t) = 0. \quad (124)$$

Thus, only the memory kernels $M_{\mathbf{q}}^{\lambda\mu}(t)$ and $L_{\mathbf{q}}^{\lambda}(t)$ survive under the mode-coupling approximation formulated with the projection operator $\mathcal{P}_2$.

V. STEADY-STATE PROPERTIES

In this section, we provide the TTCF expressions for the steady-state properties (see Sec. II G) under the mode-coupling approximation. This enables one to obtain the stationary-state properties based on the knowledge of the transient density correlators $F_{\mathbf{q}}(t)$.

A. Remarks on TTCF expressions

Let us first notice that the transient time-correlation functions appearing in the TTCF expressions in Sec. II G can be abbreviated as

$$G_X(t) \equiv \langle [e^{i\mathcal{L}t} X] \sigma_{xy} \rangle, \quad H_X(t) \equiv \langle [e^{i\mathcal{L}t} X] \delta K \rangle. \quad (125)$$

For example, the TTCF formed with $\sigma_{xy}(0)$ in Eq. (67) is given by $\langle [e^{i\mathcal{L}s} \sigma_{xy}] \sigma_{xy} \rangle$, and the one in Eq. (73) by $\langle [e^{i\mathcal{L}s} \{\rho_{\mathbf{q}}(t) \rho^*_{\mathbf{q}(t)}\}] \sigma_{xy} \rangle$.

As discussed in Appendix A 9, the functions $G_X(t)$ and $H_X(t)$ evolve in time within the subspace orthogonal to $\{\rho_{\mathbf{k}}, j_{\mathbf{k}}^{\mu}\}$, i.e., there hold

$$G_X(t) = \langle [e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t} \mathcal{Q}X] \mathcal{Q}\sigma_{xy} \rangle, \quad (126a)$$

$$H_X(t) = \langle [e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t} \mathcal{Q}X] \mathcal{Q}\delta K \rangle, \quad (126b)$$

in terms of the projection operator $\mathcal{Q}$ complementary to $\mathcal{P}$ defined in Eq. (95). This feature is exactly the one sheared with the memory kernels [see Eqs. (101), (103), and (108)–(112)]. Thus, no additional approximation than those introduced in Sec. IV is necessary to deal with $G_X(t)$ and $H_X(t)$. The only difference here is that, since both σ_{xy} and δK are "zero wave-vector" quantities, the second projection operator $\mathcal{P}_2$ given in Eq. (114) has to be replaced by $\mathcal{P}_2^0$ defined via

$$\mathcal{P}_2^0 X \equiv \sum_{\mathbf{k}>0} \langle X \rho_{\mathbf{k}} \rho^*_{\mathbf{k}} \rangle \frac{1}{N^2 S_k^2} \rho_{\mathbf{k}} \rho^*_{\mathbf{k}}. \quad (127)$$

We thus obtain under the first mode-coupling approximation, in which the propagator $e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}$ is approximated by the projected one $\mathcal{P}_2^0 e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t} \mathcal{P}_2^0$,

$$G_X(t) = \langle [e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t} \mathcal{P}_2^0 \mathcal{Q}X] \mathcal{P}_2^0 \sigma_{xy} \rangle, \quad (128a)$$

$$H_X(t) = \langle [e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t} \mathcal{P}_2^0 \mathcal{Q}X] \mathcal{P}_2^0 \delta K \rangle. \quad (128b)$$

Here we have noticed $\mathcal{Q}\sigma_{xy} = \sigma_{xy}$ and $\mathcal{Q}\delta K = \delta K$ [see Eq. (A73)].

The evaluation of $\mathcal{P}_2^0 \sigma_{xy}$ is presented in Appendix A 10 with the result

$$\mathcal{P}_2^0 \sigma_{xy} = -\frac{k_B T}{N} \sum_{\mathbf{k}>0} \frac{k_x k_y}{k} \frac{S'_k}{S_k^2} \rho_{\mathbf{k}} \rho^*_{\mathbf{k}}. \quad (129)$$

In view of Eq. (23), one easily understands that $\langle \delta K \rho_{\mathbf{k}} \rho^*_{\mathbf{k}} \rangle = 0$, and hence,

$$\mathcal{P}_2^0 \delta K = 0. \quad (130)$$

Thus, under the mode-coupling approximation, only those contributions abbreviated as $G_X(t)$ survive in the TTCF expressions for the steady-state properties.

B. Steady-state shear stress

With the results in the previous subsection, the TTCF expression (67) for the steady-state shear stress under the mode-coupling approximation is given by

$$\sigma_{\rm SS} = \frac{\dot\gamma}{k_BTV}\int_0^\infty ds\langle[e^{i\mathcal{QLQ}s}\mathcal{P}_2^0\sigma_{xy}]\mathcal{P}_2^0\sigma_{xy}\rangle. \quad (131)$$

Substituting Eq. (129) into this expression yields

$$\sigma_{\rm SS} = \frac{k_BT\dot\gamma}{VN^2}\int_0^\infty ds\sum_{\mathbf{k}>0}\sum_{\mathbf{k}'>0}\frac{k_xk_y}{k}\frac{S_k'}{S_k^2}\frac{k_x'k_y'}{k'}\frac{S_{k'}'}{S_{k'}^2} \times\langle[e^{i\mathcal{QLQ}s}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*]\rho_{\mathbf{k}'}\rho_{\mathbf{k}'}^*\rangle. \quad (132)$$

Applying the factorization approximation (120), one gets

$$\langle[e^{i\mathcal{QLQ}s}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*]\rho_{\mathbf{k}'}\rho_{\mathbf{k}'}^*\rangle \approx \langle[e^{i\mathcal{L}s}\rho_{\mathbf{k}}]\rho_{\mathbf{k}'}^*\rangle\langle[e^{i\mathcal{L}s}\rho_{\mathbf{k}}^*]\rho_{\mathbf{k}'}\rangle = \delta_{\mathbf{k}',\mathbf{k}(s)}N^2F_{\mathbf{k}}(s)^2, \quad (133)$$

where in the final equality we have noticed that $F_{\mathbf{k}}(s)$ is a real function of time [see Eq. (65)]. This leads to the following MCT expression for the steady-state shear stress $\sigma_{\rm SS}$ in terms of the transient density correlators

$$\sigma_{\rm SS} = \frac{k_BT\dot\gamma}{2(2\pi)^3}\int_0^\infty ds\int d\mathbf{k}\frac{k_x^2k_yk_y(s)}{kk(s)}\frac{S_k'S_{k(s)}'}{S_k^2S_{k(s)}^2}F_{\mathbf{k}}(s)^2. \quad (134)$$

The steady-state kinetic temperature $T_{\rm SS}$ can then be obtained via Eq. (70).

C. Steady-state density fluctuations

With the remarks in Sec. V A, the TTCF expression (73) for the steady-state density correlator $F_{\mathbf{q}}^{\rm SS}(t)$ under the mode-coupling approximation is given by

$$F_{\mathbf{q}}^{\rm SS}(t) = F_{\mathbf{q}}(t) - \frac{\dot\gamma}{Nk_BT}\int_0^\infty ds\langle[e^{i\mathcal{QLQ}s}\mathcal{Q}\{\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*\}]\mathcal{P}_2^0\sigma_{xy}\rangle. \quad (135)$$

Here we do not apply $\mathcal{P}_2^0$ to $\mathcal{Q}\{\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*\}$ since it already has the form of the density product. Let us notice that, since $\rho_{\mathbf{k}=0}=0$ [see Eq. (71)] and $j_{\mathbf{k}=0}^\mu=(1/m)\Sigma_ip_i^\mu=0$ [see the comment below Eq. (2b)], it follows from Eq. (59) that $\langle\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*\rho_{\mathbf{k}}^*\rangle=\delta_{\mathbf{k},0}\langle\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*\rho_{\mathbf{k}=0}^*\rangle=0$ and $\langle\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*j_{\mathbf{k}}^{\mu*}\rangle=\delta_{\mathbf{k},0}\langle\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*j_{\mathbf{k}=0}^{\mu*}\rangle=0$. One therefore obtains $\mathcal{P}\{\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*\}=0$ [see Eq. (95)], and hence, $\mathcal{Q}\{\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*\}=\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*$. Thus, we have for the integrand of Eq. (135)

$$\langle[e^{i\mathcal{QLQ}s}\mathcal{Q}\{\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*\}]\mathcal{P}_2^0\sigma_{xy}\rangle = -\frac{k_BT}{N}\sum_{\mathbf{k}>0}\frac{k_xk_y}{k}\frac{S_k'}{S_k^2}\langle[e^{i\mathcal{QLQ}s}\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*]\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\rangle, \quad (136)$$

where we have used Eq. (129). Here we apply the factorization approximation [see Eq. (120)]

$$\langle[e^{i\mathcal{QLQ}s}\rho_{\mathbf{q}}(t)\rho_{\mathbf{q}(t)}^*]\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\rangle \approx \langle[e^{i\mathcal{L}s}\rho_{\mathbf{q}}(t)]\rho_{\mathbf{k}}^*\rangle\langle[e^{i\mathcal{L}s}\rho_{\mathbf{q}(t)}^*]\rho_{\mathbf{k}}\rangle = \delta_{\mathbf{k},\mathbf{q}(t+s)}N^2F_{\mathbf{q}}(t+s)F_{\mathbf{q}(t)}(s), \quad (137)$$

where in the final equality we have noticed that $F_{\mathbf{q}(t)}(s)$ is a real function of time [see Eq. (65)]. This yields the following MCT expression for the steady-state density correlator $F_{\mathbf{q}}^{\rm SS}(t)$ in terms of the transient density correlators:

$$F_{\mathbf{q}}^{\rm SS}(t) = F_{\mathbf{q}}(t) + \dot\gamma\int_0^\infty ds\frac{q_xq_y(t+s)}{q(t+s)}\frac{S_{q(t+s)}'}{S_{q(t+s)}^2}F_{\mathbf{q}}(t+s)F_{\mathbf{q}(t)}(s). \quad (138)$$

As a corollary, we obtain for the steady-state structure factor $S_{\mathbf{q}}^{\rm SS}=F_{\mathbf{q}}^{\rm SS}(t=0)$

$$S_{\mathbf{q}}^{\rm SS} = S_q + \dot\gamma\int_0^\infty ds\frac{q_xq_y(s)}{q(s)}\frac{S_{q(s)}'}{S_{q(s)}^2}F_{\mathbf{q}}(s)^2. \quad (139)$$

Let us see the connection between $\sigma_{\rm SS}$ and $S_{\mathbf{q}}^{\rm SS}$ under the mode-coupling approximation. By comparing Eqs. (134) and (139), one finds

$$\sigma_{\rm SS} = \frac{k_BT}{2(2\pi)^3}\int d\mathbf{k}\frac{k_xk_y}{k}\frac{S_k'}{S_k^2}S_{\mathbf{k}}^{\rm SS}, \quad (140)$$

where we have noticed that the isotropic term in $S_{\mathbf{k}}^{\rm SS}$ does not contribute to the integral. Thus, $\sigma_{\rm SS}$ and $S_{\mathbf{q}}^{\rm SS}$ are handled on an equal footing naturally under the mode-coupling approximation. Compared to Eq. (77), the kinetic part is missing here since only the interaction part is dealt with under the mode-coupling approach. In addition, since $S_k'/S_k^2=\rho c_k'$ [see Eq. (118)], the bare potential in Eq. (77) is replaced by the "renormalized" [10] direct correlation function in Eq. (140). Finally, we notice that Eq. (140) can directly be derived from Eq. (129) by approximating $\sigma_{\rm SS}\approx-\langle\mathcal{P}_2^0\sigma_{xy}\rangle_{\rm SS}/V$ and using the definition $S_{\mathbf{k}}^{\rm SS}=(1/N)\langle\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\rangle_{\rm SS}$.

VI. SUMMARY AND DISCUSSION

In this paper, we developed a nonequilibrium MCT for uniformly sheared systems starting from microscopic, thermostatted Sllod equations of motion. Our theory aims at describing stationary-state properties including rheological ones, and this is accomplished via two steps. First, a set of self-consistent equations of motion is formulated for the transient density correlators $F_{\mathbf{q}}(t)$ based on the projection-operator formalism and on the mode-coupling approach, which enables the calculation of $F_{\mathbf{q}}(t)$ provided the static structure factor S_q of the initial equilibrium state is given as input. The transient time-correlation function formalism is then used which, combined with the mode-coupling approximation, expresses stationary-state properties in terms of $F_{\mathbf{q}}(t)$. Thereby, steady-state quantities such as the shear stress $\sigma_{\rm SS}$, temperature $T_{\rm SS}$, density correlators $F_{\mathbf{q}}^{\rm SS}(t)$, and the structure factor $S_{\mathbf{q}}^{\rm SS}$ can all be calculated in terms of S_q. We also addressed how the steady-state temperature $T_{\rm SS}$ can be controlled using the constant-α model for the thermostat:

this can be done via a self-consistent treatment of the thermostatting multiplier α based on Eq. (70). Our theory is able to treat σ_{SS} and $S_{\mathbf{q}}^{\mathrm{SS}}$ on an equal footing, which is missing in the steady-state-fluctuations approach of Refs. [14,15]. In addition, we need not assume the validity of the fluctuation-dissipation theorem in sheared states, which was necessary in Ref. [14].

The transient density correlators $F_{\mathbf{q}}(t)$ thus play a distinguished role in our approach. Let us collect here all the relevant MCT equations for $F_{\mathbf{q}}(t)$ derived in Secs. III and IV to highlight new features of our theory compared to the equilibrium MCT [11] and to the nonequilibrium MCT developed by Fuchs and Cates (FC) for sheared Brownian systems [16,17]. The exact Zwanzig-Mori–type equations consist of the continuity equation

$$\left[\frac{\partial}{\partial t} - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial \mathbf{q}}\right]F_{\mathbf{q}}(t) = i\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t), \tag{141a}$$

and the time-evolution equation for the transient density-current cross correlator $H_{\mathbf{q}}^{\lambda}(t)$

$$\left[\frac{\partial}{\partial t} - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial \mathbf{q}}\right]H_{\mathbf{q}}^{\lambda}(t) = iq_{\lambda}\frac{v^2}{S_q}F_{\mathbf{q}}(t) - [\boldsymbol{\kappa}\cdot\mathbf{H}_{\mathbf{q}}(t)]^{\lambda} - \alpha H_{\mathbf{q}}^{\lambda}(t) - \sum_{\mu}\int_0^t ds M_{\mathbf{q}}^{\lambda\mu}(s)H_{\mathbf{q}(s)}^{\mu}(t-s) + \dot{\gamma}\int_0^t ds\, iL_{\mathbf{q}}^{\lambda}(s)F_{\mathbf{q}(s)}(t-s). \tag{141b}$$

In this equation, we already omitted those memory kernels which vanish under the mode-coupling approximation (see Sec. IV). The MCT expressions for the memory kernels $M_{\mathbf{q}}^{\lambda\mu}(t)$ and $L_{\mathbf{q}}^{\lambda}(t)$ are given by

$$M_{\mathbf{q}}^{\lambda\mu}(t) = \frac{\rho v^2}{2(2\pi)^3}\int d\mathbf{k}[k_{\lambda}c_k + p_{\lambda}c_p] \times [k_{\mu}(t)c_{k(t)} + p_{\mu}(t)c_{p(t)}]F_{\mathbf{k}}(t)F_{\mathbf{p}}(t), \tag{142a}$$

$$L_{\mathbf{q}}^{\lambda}(t) = -\frac{v^2}{2(2\pi)^3}\int d\mathbf{k}[k_{\lambda}c_k + p_{\lambda}c_p] \times \left[\frac{k_x k_y(t)}{k(t)}\frac{S'_{k(t)}}{S_{k(t)}} + \frac{p_x p_y(t)}{p(t)}\frac{S'_{p(t)}}{S_{p(t)}}\right]F_{\mathbf{k}}(t)F_{\mathbf{p}}(t). \tag{142b}$$

Here $\mathbf{p}\equiv\mathbf{q}-\mathbf{k}$. Compared to the equilibrium MCT [11], new features entering here are (i) the replacement of $\partial/\partial t$ by $[\partial/\partial t - \mathbf{q}\cdot\boldsymbol{\kappa}\cdot(\partial/\partial\mathbf{q})]$, (ii) the presence of the second (shear) and the third (thermostat) terms on the right-hand side of Eq. (141b), (iii) the matrix structure of the memory kernel $M_{\mathbf{q}}^{\lambda\mu}(t)$ describing the fluctuating-force correlations which cannot be decomposed into the longitudinal and transversal parts, and (iv) the presence of the additional memory kernel $L_{\mathbf{q}}^{\lambda}(t)$. Furthermore, when compared with the FC theory [16,17], we see in addition to those rather trivial differences reflecting the Newtonian and Brownian short-time microscopic dynamics (v) the memory kernel in the FC theory describing the fluctuating-force correlations, to be denoted as $M_{\mathbf{q}}^{\mathrm{FC}}(t,t')$, has a different mathematical structure in that it depends on two times t and t' after the shearing force is turned on, while only one time enters into our $M_{\mathbf{q}}^{\lambda\mu}(t)$, and (vi) the memory kernel corresponding to $L_{\mathbf{q}}^{\lambda}(t)$ is absent also in the FC theory.

The first and second features just mentioned arise from the shear part ($i\mathcal{L}_{\dot{\gamma}}$) and the thermostat part ($i\mathcal{L}_{\alpha}$) in the p Liouvillean for the Sllod equations [see Eqs. (13a)–(13d)], which are absent in the p Liouvillean for quiescent systems. The third feature reflects the anisotropic nature of the sheared system: in the presence of shear, the longitudinal and transversal current density fluctuations cannot be separately handled as in isotropic systems since their cross correlators do not vanish. In this connection, we notice that the second term on the right-hand side of Eq. (141b), which cannot be expressed in terms of the λ component $H_{\mathbf{q}}^{\lambda}(t)$ alone, also reflects the anisotropy of the sheared system. Therefore, without introducing any further approximation (see below), Eqs. (141a) and (141b) cannot be combined to yield a single second-order integrodifferential equation for $F_{\mathbf{q}}(t)$ as in the equilibrium MCT [11]. The fourth feature originates from the non-Hermitian nature of the p Liouvillean describing nonequilibrium dynamics [see Eq. (38)], i.e., the presence of the additional memory kernel $L_{\mathbf{q}}^{\lambda}(t)$ is expected on general grounds.

The fifth feature, when compared with the FC theory, is due to different strategies employed in deriving the Zwanzig-Mori–type equations for $F_{\mathbf{q}}(t)$: the two-time structure in $M_{\mathbf{q}}^{\mathrm{FC}}(t,t')$ is an exact consequence of the Zwanzig-Mori–type equations (84a) and (84b) for $F_{\mathbf{q}}(t)$ upon which the FC theory is based (see Ref. [17]), while the one-time structure in our $M_{\mathbf{q}}^{\lambda\mu}(t)$ follows from another exact equation (94) to which the projection-operator formalism is applied (see Sec. III D). One therefore cannot judge which of the memory kernels is superior at the formal level: we can only state that ours has a simpler mathematical structure. Furthermore, both the memory kernels $M_{\mathbf{q}}^{\lambda\mu}(t)$ and $M_{\mathbf{q}}^{\mathrm{FC}}(t,t')$ under the mode-coupling approximation describe essentially the same physics concerning the competition between the cage effect and the shear advection of density fluctuations (see also below).

Thus, the sixth feature mentioned above, i.e., the presence or absence of the memory kernel $L_{\mathbf{q}}^{\lambda}(t)$ is the major difference between our and the FC theory. It is unlikely that this difference originates from the different microscopic dynamics—Newtonian or Brownian—adopted in these theories since, as we stated above, the presence of such a memory kernel is expected on general grounds.

It is anticipated that the memory kernel $L_{\mathbf{q}}^{\lambda}(t)$ becomes relevant only if significant anisotropy is developed in the density fluctuations. This is because the shear stress σ_{xy} entering into the defining equation (109) of $L_{\mathbf{q}}^{\lambda}(t)$ is intrinsically an anisotropic quantity. We indeed confirmed from our preliminary numerical calculations based on the MCT expression (142b) that the contribution from $L_{\mathbf{q}}^{\lambda}(t)$ is quite small under the isotropic approximation for the density fluctuations to be discussed below. It will be interesting to pursue in what circumstances this additional memory kernel becomes important whose presence is naturally expected for nonequilibrium sheared systems.

To further facilitate the comparison of our theory with the equilibrium MCT and with the FC theory, the MCT equations (141a), (141b), and (142) shall be simplified using the isotropic approximation introduced in Appendix B 1. Such a simplifying approximation is also useful in practical applications of our theory to systems where anisotropy in the density fluctuations is small.

The MCT equations (B13), (B19), and (B23) derived in Appendix B 1 under the isotropic approximation shall be rewritten in the following form for the normalized transient density correlators $\phi_q(t) \equiv F_q(t)/S_q$:

$$\ddot{\phi}_q(t) + \Omega_q^2 \phi_q(t) + \alpha \dot{\phi}_q(t) + \Omega_q^2 \int_0^t ds m_q^{\rm iso}(s) \dot{\phi}_{\bar{q}(s)}(t-s) + \dot{\gamma}\Omega_q^2 \int_0^t ds l_q^{\rm iso}(s) \phi_{\bar{q}(s)}(t-s) = 0. \tag{143}$$

Here all the functions depend on the wave-vector modulus only; the dot denotes the partial time derivative; $\Omega_q^2 \equiv q^2 v^2/S_q$ the square of the characteristic frequency relevant for the short-time dynamics; and $\bar{q}(s) \equiv q[1+(\dot{\gamma}s)^2/3]^{1/2}$ the modulus of the advected wave vector under the isotropic approximation. The memory kernels, from which Ω_q^2 is factored out following the convention in the equilibrium MCT [11], are given by

$$m_q^{\rm iso}(t) = \int d\mathbf{k} V_{\mathbf{q},\mathbf{k},\mathbf{p}}^{(\dot{\gamma})}(t) \phi_k(t) \phi_p(t), \tag{144a}$$

$$l_q^{\rm iso}(t) = \int d\mathbf{k} V_{\mathbf{q},\mathbf{k},\mathbf{p}}^{(\dot{\gamma})\prime}(t) \phi_k(t) \phi_p(t), \tag{144b}$$

with the time-dependent vertex functions

$$V_{\mathbf{q},\mathbf{k},\mathbf{p}}^{(\dot{\gamma})}(t) = \frac{\rho S_q S_k S_p}{2(2\pi)^3 q^4} [\mathbf{q}\cdot\mathbf{k} c_k + \mathbf{q}\cdot\mathbf{p} c_p] \times [\mathbf{q}\cdot\mathbf{k} c_{\bar{k}(t)} + \mathbf{q}\cdot\mathbf{p} c_{\bar{p}(t)}], \tag{144c}$$

$$V_{\mathbf{q},\mathbf{k},\mathbf{p}}^{(\dot{\gamma})\prime}(t) = -\frac{\dot{\gamma}t}{3\sqrt{1+(\dot{\gamma}t)^2/3}} \frac{S_q S_k S_p}{2(2\pi)^3 q^2} [\mathbf{q}\cdot\mathbf{k} c_k + \mathbf{q}\cdot\mathbf{p} c_p] \times \left[k\frac{S'_{\bar{k}(t)}}{S_{\bar{k}(t)}} + \frac{S'_{\bar{p}(t)}}{S_{\bar{p}(t)}} \right]. \tag{144d}$$

The resemblance of these equations to those in the equilibrium MCT [11] is apparent: the major differences are the dephasing in the vertex function $V_{qkp}^{(\dot{\gamma})}(t)$ for $m_q^{\rm iso}(t)$, which enhances the relaxation of the density fluctuations, and the presence of the additional memory kernel $l_q^{\rm iso}(t)$.

Now, let us "derive" the MCT equations for sheared Brownian systems, starting from Eq. (143) with the procedure adopted in Ref. [28] for converting the microscopic dynamics from Newtonian to Brownian. Assuming that the "friction" constant α is large, the inertia term in Eq. (143) shall be neglected. As a result, the generalized oscillator equation (143) is specialized to generalized relaxator equation

$$\dot{\phi}_q(t) + \Gamma_q \phi_q(t) + \Gamma_q \int_0^t ds m_q^{\rm iso}(s) \dot{\phi}_{\bar{q}(s)}(t-s) + \dot{\gamma}\Gamma_q \int_0^t ds l_q^{\rm iso}(s) \phi_{\bar{q}(s)}(t-s) = 0, \tag{145}$$

where we have defined $\Gamma_q \equiv \Omega_q^2/\alpha$. This equation, combined with Eqs. (144a) and (144c) and neglecting $l_q^{\rm iso}(t)$ which is found to be small from our preliminary calculations, is formally identical to the corresponding equation in the FC theory. [See Eqs. (4)–(6) of the second article cited in Ref. [16]. There is a minor difference that $\dot{\phi}_{\bar{q}(s)}(t-s)$ at the advected wave number $\bar{q}(s)$ enters into the third term in Eq. (145), while $\dot{\phi}_q(t-s)$ at the wave number q appears in the corresponding FC equation. Again, this reflects the difference of the starting Zwanzig-Mori–type equations.] In this sense, our and the FC theory are equivalent. But, it should be remembered that this holds only under the isotropic approximation: when anisotropy in the density fluctuations is significant, one has to go back to Eqs. (141a), (141b), and (142), and the presence or absence of the memory kernel $L_{\mathbf{q}}^{\lambda}(t)$ may have significant consequences.

Finally, we notice that our exact formulation in Secs. II and III based on the Liouville equation can find wider applications for nonequilibrium sheared systems than the one presented in this work. For example, it has been recognized that long-range spatial correlations emerge in sheared systems via anisotropic couplings between density and current-density fluctuations [29,30]. So far, most of the studies on long-range correlations have been based on a naive extension of fluctuating hydrodynamics to nonequilibrium states, and we expect that our formulation in Secs. II and III, into which anisotropic couplings between density and current-density fluctuations naturally enter, provides a microscopic foundation also for the research in this direction.

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APPENDIX A: MISCELLANEOUS MATERIALS AND DETAILS OF SOME DERIVATIONS

This appendix is devoted to a summary of miscellaneous materials which are necessary in the main text, and to various technical manipulations in the derivations of some equations. In these derivations, we repeatedly use the relation

$$\langle (i\mathcal{L}_0 A) B^* \rangle = -\langle A (i\mathcal{L}_0 B)^* \rangle, \tag{A1}$$

which holds for the unperturbed or quiescent p Liouvillean $i\mathcal{L}_0$ given in Eq. (13b), and

$$\langle A F_i^{\lambda} \rangle = -\left\langle A \frac{\partial U}{\partial r_i^{\lambda}} \right\rangle = -k_B T \left\langle \frac{\partial A}{\partial r_i^{\lambda}} \right\rangle, \tag{A2}$$

where $F_i^{\lambda} = -\partial U/\partial r_i^{\lambda}$ denotes the λ component of the conservative force acting on the ith particle. These relations, well known from equilibrium statistical mechanics [10], hold here since the averaging $\langle\cdots\rangle$ in this paper is defined with the canonical distribution function [see Eq. (27)]. Also, terms involving odd number of momentum variables vanish under such canonical averaging.

1. Microscopic expression for stress tensor

Here we summarize the microscopic expression for the stress tensor. For simplicity, we deal with quiescent equilibrium system for which the p Liouvillean is given by $i\mathcal{L}=i\mathcal{L}_0$ [see Eq. (13b)]. In handling sheared systems, momenta appearing in the following expressions should be understood as peculiar or Sllod momenta [19].

The wave-vector-dependent stress tensor $\sigma_{\mathbf{q}}^{\lambda\mu}$ is introduced via the continuity equation for the current density fluctuation $j_{\mathbf{q}}^{\lambda}=\Sigma_i(p_i^{\lambda}/m)\exp(i\mathbf{q}\cdot\mathbf{r}_i)$

$$i\mathcal{L}_0 j_{\mathbf{q}}^{\lambda}=\sum_{\mu}\frac{iq_{\mu}}{m}\sigma_{\mathbf{q}}^{\lambda\mu}, \tag{A3}$$

and is given by [10]

$$\sigma_{\mathbf{q}}^{\lambda\mu}=\sum_i\left[p_i^{\lambda}p_i^{\mu}/m-\frac{1}{2}\sum_{j\neq i}\frac{r_{ij}^{\lambda}r_{ij}^{\mu}}{r_{ij}^2}P_{\mathbf{q}}(\mathbf{r}_{ij})\right]\exp(i\mathbf{q}\cdot\mathbf{r}_i). \tag{A4}$$

Here $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$, $r_{ij}=|\mathbf{r}_{ij}|$, $r_{ij}^{\lambda}=r_i^{\lambda}-r_j^{\lambda}$, and

$$P_{\mathbf{q}}(\mathbf{r})=ru'(r)\frac{1-\exp(-i\mathbf{q}\cdot\mathbf{r})}{i\mathbf{q}\cdot\mathbf{r}}, \tag{A5}$$

in which $u(r)$ denotes the pair-interaction potential; the total interaction potential of the system is thus given by $U=(1/2)\Sigma_i\Sigma_{j\neq i}u(r_{ij})$. Obviously, $\sigma_{\mathbf{q}}^{\lambda\mu}$ is a symmetric tensor.

The "stress tensor" referred to in the main text is the zero-wave-vector limit of $\sigma_{\mathbf{q}}^{\lambda\mu}$:

$$\sigma_{\lambda\mu}\equiv\sigma_{\mathbf{q}=0}^{\lambda\mu}=\sum_i\left[p_i^{\lambda}p_i^{\mu}/m-\frac{1}{2}\sum_{j\neq i}\frac{r_{ij}^{\lambda}r_{ij}^{\mu}}{r_{ij}}u'(r_{ij})\right]. \tag{A6}$$

Exploiting the isotropy of the quiescent equilibrium system, one can show that [10]

$$\langle\sigma_{\lambda\mu}\rangle=0\ (\lambda\neq\mu). \tag{A7}$$

The equivalence of expression (A6) and Eq. (20) in the main text can be demonstrated as follows. Since $\mathbf{F}_i=\Sigma_{j\neq i}\mathbf{F}_{ij}$, where $\mathbf{F}_{ij}$ denotes the force acting on the ith particle from the jth particle and $\mathbf{F}_{ji}=-\mathbf{F}_{ij}$ due to Newton's third law, there holds

$$\sum_i\mathbf{r}_i\mathbf{F}_i=\frac{1}{2}\left[\sum_i\mathbf{r}_i\sum_{j\neq i}\mathbf{F}_{ij}+\sum_j\mathbf{r}_j\sum_{i\neq j}\mathbf{F}_{ji}\right]=\frac{1}{2}\sum_i\sum_{j\neq i}\mathbf{r}_{ij}\mathbf{F}_{ij}. \tag{A8}$$

Expressing the force $\mathbf{F}_{ij}$ in terms of the pair-interaction potential as

$$\mathbf{F}_{ij}=-\frac{\partial}{\partial\mathbf{r}_i}u(r_{ij})=-\frac{\mathbf{r}_{ij}}{r_{ij}}u'(r_{ij}), \tag{A9}$$

one obtains

$$\sum_i r_i^{\lambda}F_i^{\mu}=-\frac{1}{2}\sum_i\sum_{j\neq i}\frac{r_{ij}^{\lambda}r_{ij}^{\mu}}{r_{ij}}u'(r_{ij}) \tag{A10}$$

indicating the equivalence of Eqs. (A6) and (20).

2. Propagators under the global translation

Here we discuss how the f and p propagators transform under the global translation $\mathbf{\Gamma}\to\mathbf{\Gamma}'$ defined by Eq. (40). The p Liouvillean corresponding to the Sllod equations is given by [see Eqs. (13a)–(13d)]

$$i\mathcal{L}(\mathbf{\Gamma})=\sum_i\left[(\mathbf{p}_i/m+\boldsymbol{\kappa}\cdot\mathbf{r}_i)\cdot\frac{\partial}{\partial\mathbf{r}_i}+(\mathbf{F}_i-\boldsymbol{\kappa}\cdot\mathbf{p}_i-\alpha\mathbf{p}_i)\cdot\frac{\partial}{\partial\mathbf{p}_i}\right] \tag{A11}$$

and it transforms under $\mathbf{\Gamma}\to\mathbf{\Gamma}'$ to

$$i\mathcal{L}(\mathbf{\Gamma}')=i\mathcal{L}(\mathbf{\Gamma})+\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}\ \text{with}\ \mathbf{P}\equiv\sum_i\frac{\partial}{\partial\mathbf{r}_i}, \tag{A12}$$

since $\mathbf{p}_i$ and $\mathbf{F}_i=\Sigma_{j\neq i}\mathbf{F}_{ij}$ (where $\mathbf{F}_{ij}$ denotes the force acting on the ith particle by the jth particle and is a function of $\mathbf{r}_{ij}$ only) are not affected by $\mathbf{\Gamma}\to\mathbf{\Gamma}'$. Here $\boldsymbol{\kappa}^T$ denotes the transpose of $\boldsymbol{\kappa}$.

Let us notice that, when $\mathbf{P}(\mathbf{\Gamma})$ acts on a phase variable $X(\mathbf{\Gamma})$ that depends on momenta $\{\mathbf{p}_i\}$ and particle separations $\{\mathbf{r}_{ij}\}$ only, there holds $\mathbf{P}X(\mathbf{\Gamma})=0$. Therefore, the only term in $i\mathcal{L}(\mathbf{\Gamma})$ that does not commute with $\mathbf{P}$ is the second term in Eq. (A11), for which we have

$$P_{\nu}\sum_i\left[(\boldsymbol{\kappa}\cdot\mathbf{r}_i)\cdot\frac{\partial}{\partial\mathbf{r}_i}\right]=\sum_i[P_{\nu}(\boldsymbol{\kappa}\cdot\mathbf{r}_i)]\cdot\frac{\partial}{\partial\mathbf{r}_i}+\sum_i\left[(\boldsymbol{\kappa}\cdot\mathbf{r}_i)\cdot\frac{\partial}{\partial\mathbf{r}_i}\right]P_{\nu}. \tag{A13}$$

We therefore obtain

$$\begin{aligned}P_{\nu}i\mathcal{L}(\mathbf{\Gamma})-i\mathcal{L}(\mathbf{\Gamma})P_{\nu}&=\sum_i[P_{\nu}(\boldsymbol{\kappa}\cdot\mathbf{r}_i)]\cdot\frac{\partial}{\partial\mathbf{r}_i}\\&=\sum_{i,j}\left[\frac{\partial}{\partial r_j^{\nu}}\left(\sum_{\lambda,\mu}\kappa_{\lambda\mu}r_i^{\mu}\right)\right]\frac{\partial}{\partial r_i^{\lambda}}\\&=\sum_i\sum_{\lambda}\kappa_{\lambda\nu}\frac{\partial}{\partial r_i^{\lambda}},\end{aligned} \tag{A14}$$

and hence, there holds

$$\begin{aligned}&(\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P})i\mathcal{L}(\mathbf{\Gamma})-i\mathcal{L}(\mathbf{\Gamma})(\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P})\\&\quad=\sum_{\lambda,\mu}a_{\lambda}\kappa_{\lambda\mu}^T[P_{\mu}i\mathcal{L}(\mathbf{\Gamma})-i\mathcal{L}(\mathbf{\Gamma})P_{\mu}]\\&\quad=\sum_{\lambda,\mu}a_{\lambda}\kappa_{\mu\lambda}\sum_i\sum_{\lambda'}\kappa_{\lambda'\mu}\frac{\partial}{\partial r_i^{\lambda'}}=\sum_{\lambda,\lambda'}a_{\lambda}(\boldsymbol{\kappa}\cdot\boldsymbol{\kappa})_{\lambda'\lambda}P_{\lambda'}=0,\end{aligned} \tag{A15}$$

since the shear-rate tensor satisfies $\boldsymbol{\kappa}\cdot\boldsymbol{\kappa}=0$. Thus, $i\mathcal{L}(\mathbf{\Gamma})$ and $\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}$ commute. This means that f Liouvillean $i\mathcal{L}^{\dagger}(\mathbf{\Gamma})$ and

$\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}$ also commute since the difference between f and p Liouvilleans for the Sllod equations with the constant-α model for the thermostat is simply a constant [see Eqs. (6) and (10)].

Using the Campbell-Baker-Hausdorff theorem which states that $e^{\mathcal{A}+\mathcal{B}}=e^{\mathcal{A}}e^{\mathcal{B}}$ for commuting operators $\mathcal{A}$ and $\mathcal{B}$, one obtains from Eqs. (A12) and (A15)

$$e^{i\mathcal{L}(\Gamma')t} = e^{i\mathcal{L}(\Gamma)t+\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}t} = e^{i\mathcal{L}(\Gamma)t}e^{\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}t}. \tag{A16}$$

Similarly, there holds for the f propagator

$$e^{-i\mathcal{L}^\dagger(\Gamma')t} = e^{-i\mathcal{L}^\dagger(\Gamma)t}e^{-\mathbf{a}\cdot\boldsymbol{\kappa}^T\cdot\mathbf{P}t}. \tag{A17}$$

3. Derivation of Eq. (97)

Here we derive an expression for $\mathcal{P}i\mathcal{L}_0 j_{\mathbf{q}}^\lambda$. To this end, one needs to evaluate the ensemble averages $\langle[i\mathcal{L}_0 j_{\mathbf{q}}^\lambda]\rho_{\mathbf{k}}^*\rangle$ and $\langle[i\mathcal{L}_0 j_{\mathbf{q}}^\lambda]j_{\mathbf{k}}^{\mu *}\rangle$ [see Eq. (95)]. Using Eq. (A1) and the relation $i\mathcal{L}_0\rho_{\mathbf{q}}=i\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}}$, the former is given by

$$\begin{aligned}\langle[i\mathcal{L}_0 j_{\mathbf{q}}^\lambda]\rho_{\mathbf{k}}^*\rangle &= -\delta_{\mathbf{q},\mathbf{k}}\langle j_{\mathbf{q}}^\lambda[i\mathcal{L}_0\rho_{\mathbf{q}}]^*\rangle = \delta_{\mathbf{q},\mathbf{k}}\langle j_{\mathbf{q}}^\lambda(i\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}}^*)\rangle\\ &= \delta_{\mathbf{q},\mathbf{k}} i q_\lambda N v^2.\end{aligned} \tag{A18}$$

For the latter, we use Eq. (A3) to obtain

$$\langle[i\mathcal{L}_0 j_{\mathbf{q}}^\lambda]j_{\mathbf{k}}^{\mu *}\rangle = \delta_{\mathbf{q},\mathbf{k}}\sum_\nu \frac{iq_\nu}{m}\langle\sigma_{\mathbf{q}}^{\lambda\nu}j_{\mathbf{q}}^{\mu *}\rangle = 0, \tag{A19}$$

since only odd number of momentum variables are involved. It thus follows from these results and Eq. (95)

$$\mathcal{P}i\mathcal{L}_0 j_{\mathbf{q}}^\lambda = \sum_{\mathbf{k}}\langle[i\mathcal{L}_0 j_{\mathbf{q}}^\lambda]\rho_{\mathbf{k}}^*\rangle\frac{1}{NS_k}\rho_{\mathbf{k}} = iq_\lambda\frac{v^2}{S_q}\rho_{\mathbf{q}}. \tag{A20}$$

4. Derivation of Eqs. (105) and (106)

Using Eq. (38), the ensemble averages in the integrands of Eq. (104) are given by

$$\begin{aligned}\langle[i\mathcal{L}R_{\mathbf{q}}^\lambda(s)]\rho_{\mathbf{q}(s)}^*\rangle = &-\langle R_{\mathbf{q}}^\lambda(s)[i\mathcal{L}\rho_{\mathbf{q}(s)}]^*\rangle - \frac{\dot\gamma}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)\rho_{\mathbf{q}(s)}^*\sigma_{xy}\rangle\\ &-\frac{2\alpha}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)\rho_{\mathbf{q}(s)}^*\delta K\rangle,\end{aligned} \tag{A21}$$

$$\begin{aligned}\langle[i\mathcal{L}R_{\mathbf{q}}^\lambda(s)]j_{\mathbf{q}(s)}^{\mu *}\rangle = &-\langle R_{\mathbf{q}}^\lambda(s)[i\mathcal{L}j_{\mathbf{q}(s)}^\mu]^*\rangle - \frac{\dot\gamma}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)j_{\mathbf{q}(s)}^{\mu *}\sigma_{xy}\rangle\\ &-\frac{2\alpha}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)j_{\mathbf{q}(s)}^{\mu *}\delta K\rangle.\end{aligned} \tag{A22}$$

Since $\mathcal{Q}R_{\mathbf{q}}^\lambda(s)=R_{\mathbf{q}}^\lambda(s)$ [see Eqs. (101) and (102)] and the operator $\mathcal{Q}$ is idempotent and Hermitian, the above equations can be written as

$$\begin{aligned}\langle[i\mathcal{L}R_{\mathbf{q}}^\lambda(s)]\rho_{\mathbf{q}(s)}^*\rangle = &-\langle R_{\mathbf{q}}^\lambda(s)[\mathcal{Q}i\mathcal{L}\rho_{\mathbf{q}(s)}]^*\rangle\\ &-\frac{\dot\gamma}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)\mathcal{Q}[\rho_{\mathbf{q}(s)}^*\sigma_{xy}]\rangle\\ &-\frac{2\alpha}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)\mathcal{Q}[\rho_{\mathbf{q}(s)}^*\delta K]\rangle,\end{aligned} \tag{A23}$$

$$\begin{aligned}\langle[i\mathcal{L}R_{\mathbf{q}}^\lambda(s)]j_{\mathbf{q}(s)}^{\mu *}\rangle = &-\langle R_{\mathbf{q}}^\lambda(s)[\mathcal{Q}i\mathcal{L}j_{\mathbf{q}(s)}^\mu]^*\rangle\\ &-\frac{\dot\gamma}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)\mathcal{Q}[j_{\mathbf{q}(s)}^{\mu *}\sigma_{xy}]\rangle\\ &-\frac{2\alpha}{k_BT}\langle R_{\mathbf{q}}^\lambda(s)\mathcal{Q}[j_{\mathbf{q}(s)}^{\mu *}\delta K]\rangle.\end{aligned} \tag{A24}$$

In the following, we will show that

$$\langle R_{\mathbf{q}}^\lambda(s)[\mathcal{Q}i\mathcal{L}\rho_{\mathbf{q}(s)}]^*\rangle = 0, \tag{A25}$$

$$\langle R_{\mathbf{q}}^\lambda(s)[\mathcal{Q}i\mathcal{L}j_{\mathbf{q}(s)}^\mu]^*\rangle = \langle R_{\mathbf{q}}^\lambda(s)R_{\mathbf{q}(s)}^{\mu *}\rangle. \tag{A26}$$

Substituting these results into Eqs. (A23) and (A24) yields Eqs. (105) and (106), respectively.

To derive Eq. (A25), we first notice from Eq. (88)

$$\begin{aligned}i\mathcal{L}\rho_{\mathbf{q}(s)} &= i\mathbf{q}(s)\cdot\mathbf{j}_{\mathbf{q}(s)} + \sum_j i[\mathbf{q}(s)\cdot\boldsymbol{\kappa}\cdot\mathbf{r}_j]e^{i\mathbf{q}(s)\cdot\mathbf{r}_j}\\ &= i\mathbf{q}(s)\cdot\mathbf{j}_{\mathbf{q}(s)} + \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\rho_{\mathbf{q}(s)},\end{aligned} \tag{A27}$$

since $\boldsymbol{\kappa}\cdot\boldsymbol{\kappa}=0$. We therefore obtain, since $\mathcal{Q}j_{\mathbf{q}(s)}^\lambda=0$,

$$\langle R_{\mathbf{q}}^\lambda(s)[\mathcal{Q}i\mathcal{L}\rho_{\mathbf{q}(s)}]^*\rangle = \left\langle R_{\mathbf{q}}^\lambda(s)\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\rho_{\mathbf{q}(s)}^*\right]\right\rangle. \tag{A28}$$

On the other hand, it follows by taking a partial time derivative of the first relation in Eq. (103) that

$$\begin{aligned}0 &= \frac{\partial}{\partial s}\langle R_{\mathbf{q}}^\lambda(s)\rho_{\mathbf{q}(s)}^*\rangle\\ &= \left\langle\left\{\frac{\partial}{\partial s}[e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}s}R_{\mathbf{q}}^\lambda]\right\}\rho_{\mathbf{q}(s)}^*\right\rangle + \left\langle R_{\mathbf{q}}^\lambda(s)\left[\frac{\partial}{\partial s}\rho_{\mathbf{q}(s)}^*\right]\right\rangle\\ &= \langle[\mathcal{Q}i\mathcal{L}R_{\mathbf{q}}^\lambda(s)]\rho_{\mathbf{q}(s)}^*\rangle + \left\langle R_{\mathbf{q}}^\lambda(s)\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\rho_{\mathbf{q}(s)}^*\right]\right\rangle,\end{aligned} \tag{A29}$$

where in the final equality we have used Eq. (90) for the second term. The first term in this expression is zero since $\mathcal{Q}$ is Hermitian and $\mathcal{Q}\rho_{\mathbf{q}(s)}^*=0$. We thus obtain

$$\left\langle R_{\mathbf{q}}^\lambda(s)\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\rho_{\mathbf{q}(s)}^*\right]\right\rangle = 0. \tag{A30}$$

Equation (A25) then follows from Eqs. (A28) and (A30).

We next derive Eq. (A26). To this end, we notice from Eq. (92) that, since $\boldsymbol{\kappa}\cdot\boldsymbol{\kappa}=0$,

$$i\mathcal{L}j^{\mu}_{\mathbf{q}(s)} = i\mathcal{L}_0 j^{\mu}_{\mathbf{q}(s)} + \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}j^{\mu}_{\mathbf{q}(s)} - [\boldsymbol{\kappa}\cdot\mathbf{j}_{\mathbf{q}(s)}]^{\mu} - \alpha j^{\mu}_{\mathbf{q}(s)}. \tag{A31}$$

We therefore obtain, since $\mathcal{Q}j^{\lambda}_{\mathbf{q}(s)}=0$,

$$\langle R^{\lambda}_{\mathbf{q}}(s)\mathcal{Q}[i\mathcal{L}j^{\mu}_{\mathbf{q}(s)}]^*\rangle = \langle R^{\lambda}_{\mathbf{q}}(s)\mathcal{Q}[i\mathcal{L}_0 j^{\mu}_{\mathbf{q}(s)}]^*\rangle + \left\langle R^{\lambda}_{\mathbf{q}}(s)\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}j^{\mu*}_{\mathbf{q}(s)}\right]\right\rangle. \tag{A32}$$

Notice that the thermostat term $\alpha j^{\mu}_{\mathbf{q}(s)}$ does not contribute here since we have adopted the constant-α model. If, e.g., the Gaussian isokinetic thermostat is used, the contribution $\langle R^{\lambda}_{\mathbf{q}}(s)\mathcal{Q}[\alpha_G j^{\mu*}_{\mathbf{q}(s)}]\rangle$ cannot be discarded.

The vanishing of the second term in Eq. (A32) can be demonstrated as follows. Using the equation

$$\frac{\partial}{\partial s}j^{\mu*}_{\mathbf{q}(s)} = \mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}j^{\mu*}_{\mathbf{q}(s)}, \tag{A33}$$

a partial time derivative of the second relation in Eq. (103) is given by

$$\begin{aligned}0 &= \frac{\partial}{\partial s}\langle R^{\lambda}_{\mathbf{q}}(s)j^{\mu*}_{\mathbf{q}(s)}\rangle\\ &= \left\langle\left\{\frac{\partial}{\partial s}[e^{i\mathcal{QLQ}s}R^{\lambda}_{\mathbf{q}}]\right\}j^{\mu*}_{\mathbf{q}(s)}\right\rangle + \left\langle R^{\lambda}_{\mathbf{q}}(s)\left[\frac{\partial}{\partial s}j^{\mu*}_{\mathbf{q}(s)}\right]\right\rangle\\ &= \langle[\mathcal{Q}i\mathcal{L}R^{\lambda}_{\mathbf{q}}(s)]j^{\mu*}_{\mathbf{q}(s)}\rangle + \left\langle R^{\lambda}_{\mathbf{q}}(s)\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}j^{\mu*}_{\mathbf{q}(s)}\right]\right\rangle.\end{aligned} \tag{A34}$$

The first term is zero since $\mathcal{Q}j^{\mu*}_{\mathbf{q}(s)}=0$, and this leads to

$$\left\langle R^{\lambda}_{\mathbf{q}}(s)\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}j^{\mu*}_{\mathbf{q}(s)}\right]\right\rangle = 0. \tag{A35}$$

One therefore obtains from Eqs. (A32) and (A35)

$$\langle R^{\lambda}_{\mathbf{q}}(s)\mathcal{Q}[i\mathcal{L}j^{\mu}_{\mathbf{q}(s)}]^*\rangle = \langle R^{\lambda}_{\mathbf{q}}(s)\mathcal{Q}[i\mathcal{L}_0 j^{\mu}_{\mathbf{q}(s)}]^*\rangle = \langle R^{\lambda}_{\mathbf{q}}(s)R^{\mu*}_{\mathbf{q}(s)}\rangle, \tag{A36}$$

where in the final equality we have used Eq. (102) for the definition of the fluctuating force. This completes the derivation of Eq. (A26).

5. Derivation of Eq. (117)

Here we calculate the projected random force $\mathcal{P}_2 R^{\lambda}_{\mathbf{q}}$:

$$\mathcal{P}_2 R^{\lambda}_{\mathbf{q}} = \sum_{\mathbf{k}>\mathbf{p}}\langle R^{\lambda}_{\mathbf{q}}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle\frac{1}{N^2 S_k S_p}\rho_{\mathbf{k}}\rho_{\mathbf{p}}. \tag{A37}$$

To this end, we need to evaluate [see Eq. (102)]

$$\langle R^{\lambda}_{\mathbf{q}}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle = \langle[i\mathcal{L}_0 j^{\lambda}_{\mathbf{q}}]\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle - iq_{\lambda}\frac{v^2}{S_q}\langle\rho_{\mathbf{q}}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle. \tag{A38}$$

Using Eq. (A1) and the relation $i\mathcal{L}_0\rho_{\mathbf{q}} = i\mathbf{q}\cdot\mathbf{j}_{\mathbf{q}}$, the first term is given by

$$\begin{aligned}\langle[i\mathcal{L}_0 j^{\lambda}_{\mathbf{q}}]\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle &= -\langle j^{\lambda}_{\mathbf{q}}[i\mathcal{L}_0\rho_{\mathbf{k}}]^*\rho^*_{\mathbf{p}}\rangle - \langle j^{\lambda}_{\mathbf{q}}\rho^*_{\mathbf{k}}[i\mathcal{L}_0\rho_{\mathbf{p}}]^*\rangle\\ &= \langle j^{\lambda}_{\mathbf{q}}(i\mathbf{k}\cdot\mathbf{j}^*_{\mathbf{k}})\rho^*_{\mathbf{p}}\rangle + \langle j^{\lambda}_{\mathbf{q}}\rho^*_{\mathbf{k}}(i\mathbf{p}\cdot\mathbf{j}^*_{\mathbf{p}})\rangle\\ &= \delta_{\mathbf{q},\mathbf{k}+\mathbf{p}}iNv^2[k_{\lambda}S_p + p_{\lambda}S_k].\end{aligned} \tag{A39}$$

For the second term in Eq. (A38), we use the convolution approximation (116):

$$iq_{\lambda}\frac{v^2}{S_q}\langle\rho_{\mathbf{q}}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle \approx \delta_{\mathbf{q},\mathbf{k}+\mathbf{p}}iNv^2 q_{\lambda}S_k S_p. \tag{A40}$$

One thus obtains from Eqs. (A38)–(A40)

$$\langle R^{\lambda}_{\mathbf{q}}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle = -\delta_{\mathbf{q},\mathbf{k}+\mathbf{p}}iN\rho v^2 S_k S_p[k_{\lambda}c_k + p_{\lambda}c_p], \tag{A41}$$

in terms of the direct correlation function [see Eq. (118)]. Substituting this result into Eq. (A37) finally yields

$$\mathcal{P}_2 R^{\lambda}_{\mathbf{q}} = -i\frac{\rho v^2}{N}\sum_{\mathbf{k}>\mathbf{p}}\delta_{\mathbf{q},\mathbf{k}+\mathbf{p}}[k_{\lambda}c_k + p_{\lambda}c_p]\rho_{\mathbf{k}}\rho_{\mathbf{p}}. \tag{A42}$$

6. Derivation of Eq. (122)

Here we derive the MCT expression for the memory kernel $L^{\lambda}_{\mathbf{q}}(t)$ defined in Eq. (109). Under the first mode-coupling approximation $e^{i\mathcal{QLQ}t} \approx \mathcal{P}_2 e^{i\mathcal{QLQ}t}\mathcal{P}_2$ (see Sec. IV), one obtains

$$L^{\lambda}_{\mathbf{q}}(t) \approx i\frac{1}{Nk_B TS_{q(t)}}\langle[e^{i\mathcal{QLQ}t}\mathcal{P}_2 R^{\lambda}_{\mathbf{q}}]\mathcal{P}_2\mathcal{Q}[\rho^*_{\mathbf{q}(t)}\sigma_{xy}]\rangle. \tag{A43}$$

Since $\mathcal{P}_2 R^{\lambda}_{\mathbf{q}}$ is already given in Eq. (A42), we only need to consider

$$\mathcal{P}_2\mathcal{Q}[\rho_{\mathbf{q}(t)}\sigma_{xy}] = \sum_{\mathbf{k}>\mathbf{p}}\langle\{\mathcal{Q}[\rho_{\mathbf{q}(t)}\sigma_{xy}]\}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle\frac{1}{N^2 S_k S_p}\rho_{\mathbf{k}}\rho_{\mathbf{p}}. \tag{A44}$$

Let us start from $\mathcal{Q}[\rho_{\mathbf{q}(t)}\sigma_{xy}]$, for which we need to know the averages $\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]\rho^*_{\mathbf{k}}\rangle$ and $\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]j^{\mu*}_{\mathbf{k}}\rangle$ [see Eq. (95)]. The latter is zero, $\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]j^{\mu*}_{\mathbf{k}}\rangle=0$, since this term involves odd number of momentum variables only. For the former, one obtains using Eq. (20)

$$\begin{aligned}\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]\rho^*_{\mathbf{k}}\rangle &= \delta_{\mathbf{k},\mathbf{q}(t)}\langle\rho_{\mathbf{q}(t)}\sigma_{xy}\rho^*_{\mathbf{q}(t)}\rangle\\ &= -\delta_{\mathbf{k},\mathbf{q}(t)}\left\langle\sum_{i,j,l}x_j\frac{\partial U}{\partial y_j}e^{i\mathbf{q}(t)\cdot(\mathbf{r}_i-\mathbf{r}_l)}\right\rangle,\end{aligned} \tag{A45}$$

since the kinetic-part contribution from σ_{xy} vanishes. Here we have expressed F^y_j in terms of the total interaction potential, $F^y_j = -\partial U/\partial y_j$. Applying Eq. (A2) to this equation yields

$$\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]\rho_{\mathbf{k}}^{*}\rangle = -\delta_{\mathbf{k},\mathbf{q}(t)}k_BT\left\langle \sum_{i,j,l} x_j\frac{\partial}{\partial y_j}e^{i\mathbf{q}(t)\cdot(\mathbf{r}_i-\mathbf{r}_l)}\right\rangle = -\delta_{\mathbf{k},\mathbf{q}(t)}k_BTq_y(t)\left\langle \sum_{i,l} i(x_i-x_l)e^{i\mathbf{q}(t)\cdot(\mathbf{r}_i-\mathbf{r}_l)}\right\rangle = -\delta_{\mathbf{k},\mathbf{q}(t)}Nk_BTq_y(t)\frac{\partial S_{q(t)}}{\partial q_x(t)} = -\delta_{\mathbf{k},\mathbf{q}(t)}Nk_BT\frac{q_xq_y(t)}{q}S'_{q(t)}, \tag{A46}$$

since $q_x(t)=q_x$ [see Eq. (56)] and $\partial S_{q(t)}/\partial q_x=(q_x/q)S'_{q(t)}$. We therefore obtain from Eq. (95)

$$\mathcal{P}[\rho_{\mathbf{q}(t)}\sigma_{xy}] = \sum_{\mathbf{k}}\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]\rho_{\mathbf{k}}^{*}\rangle\frac{1}{NS_k}\rho_{\mathbf{k}} = -k_BT\frac{q_xq_y(t)}{q}\frac{S'_{q(t)}}{S_{q(t)}}\rho_{\mathbf{q}(t)} \tag{A47}$$

and hence

$$\mathcal{Q}[\rho_{\mathbf{q}(t)}\sigma_{xy}] = \rho_{\mathbf{q}(t)}\sigma_{xy} + k_BT\frac{q_xq_y(t)}{q}\frac{S'_{q(t)}}{S_{q(t)}}\rho_{\mathbf{q}(t)}. \tag{A48}$$

Now let us calculate

$$\langle[\mathcal{Q}\{\rho_{\mathbf{q}(t)}\sigma_{xy}\}]\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle = \langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle + k_BT\frac{q_xq_y(t)}{q}\frac{S'_{q(t)}}{S_{q(t)}}\langle\rho_{\mathbf{q}(t)}\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle. \tag{A49}$$

Using Eq. (20), the first term is given by

$$\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle = -\delta_{\mathbf{q}(t),\mathbf{k}+\mathbf{p}} \times\left\langle \sum_i e^{i\mathbf{q}(t)\cdot\mathbf{r}_i}\sum_j x_j\frac{\partial U}{\partial y_j}\sum_l e^{-i\mathbf{k}\cdot\mathbf{r}_l}\sum_m e^{-i\mathbf{p}\cdot\mathbf{r}_m}\right\rangle = -\delta_{\mathbf{q}(t),\mathbf{k}+\mathbf{p}}k_BT \times\left\langle \sum_{i,j,l,m} x_j\frac{\partial}{\partial y_j}(e^{i\mathbf{q}(t)\cdot\mathbf{r}_i}e^{-i\mathbf{k}\cdot\mathbf{r}_l}e^{-i\mathbf{p}\cdot\mathbf{r}_m})\right\rangle, \tag{A50}$$

where we have employed Eq. (A2) in the second equality. The calculation of this term can be continued in the same manner as in Eq. (A46) with the result

$$\langle[\rho_{\mathbf{q}(t)}\sigma_{xy}]\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle = -\delta_{\mathbf{q}(t),\mathbf{k}+\mathbf{p}}k_BT\left(k_y\frac{\partial}{\partial k_x}+p_y\frac{\partial}{\partial p_x}\right)\langle\rho_{\mathbf{q}(t)}\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle. \tag{A51}$$

Substituting this into Eq. (A49) yields

$$\langle[\mathcal{Q}\{\rho_{\mathbf{q}(t)}\sigma_{xy}\}]\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle = -\delta_{\mathbf{q}(t),\mathbf{k}+\mathbf{p}}k_BT \times\left\{k_y\frac{\partial}{\partial k_x}+p_y\frac{\partial}{\partial p_x}-\frac{q_xq_y(t)}{q}\frac{S'_{q(t)}}{S_{q(t)}}\right\} \times\langle\rho_{\mathbf{q}(t)}\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle. \tag{A52}$$

This expression can further be simplified under the convolution approximation (116)

$$\langle\rho_{\mathbf{q}(t)}\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle \approx \delta_{\mathbf{q}(t),\mathbf{k}+\mathbf{p}}NS_{q(t)}S_kS_p. \tag{A53}$$

Let us notice that, when $\mathbf{q}(t)=\mathbf{k}+\mathbf{p}$, there holds

$$\frac{\partial}{\partial k_x}[S_{q(t)}S_kS_p] = \frac{q_x}{q(t)}S'_{q(t)}S_kS_p + \frac{k_x}{k}S_{q(t)}S'_kS_p. \tag{A54}$$

Similarly, we have

$$\frac{\partial}{\partial p_x}[S_{q(t)}S_kS_p] = \frac{q_x}{q(t)}S'_{q(t)}S_kS_p + \frac{p_x}{p}S_{q(t)}S_kS'_p. \tag{A55}$$

It then follows from Eqs. (A52)–(A55) that

$$\langle[\mathcal{Q}\{\rho_{\mathbf{q}(t)}\sigma_{xy}\}]\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle = -\delta_{\mathbf{q}(t),\mathbf{k}+\mathbf{p}}Nk_BTS_{q(t)}S_kS_p \times\left\{\frac{k_xk_y}{k}\frac{S'_k}{S_k}+\frac{p_xp_y}{p}\frac{S'_p}{S_p}\right\} \tag{A56}$$

and substituting this into Eq. (A44) yields

$$\mathcal{P}_2\mathcal{Q}[\rho_{\mathbf{q}(t)}\sigma_{xy}] = -\frac{k_BT}{N}S_{q(t)}\sum_{\mathbf{k}>\mathbf{p}}\delta_{\mathbf{q}(t),\mathbf{k}+\mathbf{p}} \times\left\{\frac{k_xk_y}{k}\frac{S'_k}{S_k}+\frac{p_xp_y}{p}\frac{S'_p}{S_p}\right\}\rho_{\mathbf{k}}\rho_{\mathbf{p}}. \tag{A57}$$

Substituting Eqs. (A42) and (A57) into Eq. (A43) and then using the factorization approximation (120), we finally obtain with $\mathbf{p}\equiv\mathbf{q}-\mathbf{k}$

$$L_{\mathbf{q}}^{\lambda}(t) = -\frac{v^2}{2(2\pi)^3}\int d\mathbf{k}[k_\lambda c_k+p_\lambda c_p] \times\left[\frac{k_xk_y(t)}{k(t)}\frac{S'_{k(t)}}{S_{k(t)}}+\frac{p_xp_y(t)}{p(t)}\frac{S'_{p(t)}}{S_{p(t)}}\right]F_{\mathbf{k}}(t)F_{\mathbf{p}}(t). \tag{A58}$$

7. Derivation of Eq. (123)

Here we show that the memory kernel $L_{\mathbf{q}}^{\prime\lambda\mu}(t)$ defined in Eq. (110) vanishes under the mode-coupling approximation formulated with $\mathcal{P}_2$. We start from

$$L_{\mathbf{q}}^{\prime\lambda\mu}(t) \approx \frac{m}{N(k_BT)^2}\langle[e^{i\mathcal{QLQ}t}\mathcal{P}_2R_{\mathbf{q}}^{\lambda}(t)]\mathcal{P}_2\mathcal{Q}[j_{\mathbf{q}(t)}^{\mu*}\sigma_{xy}]\rangle \tag{A59}$$

under the first mode-coupling approximation $e^{i\mathcal{QLQ}t}\approx\mathcal{P}_2e^{i\mathcal{QLQ}t}\mathcal{P}_2$ (see Sec. IV). In the following, we demonstrate $\langle\{\mathcal{Q}[j_{\mathbf{q}(t)}^{\mu}\sigma_{xy}]\}\rho_{\mathbf{k}}^{*}\rho_{\mathbf{p}}^{*}\rangle=0$, i.e., $\mathcal{P}_2\mathcal{Q}[j_{\mathbf{q}(t)}^{\mu}\sigma_{xy}]=0$, which completes the derivation of $L_{\mathbf{q}}^{\prime\lambda\mu}(t)=0$.

Let us start from $\mathcal{Q}[j_{\mathbf{q}(t)}^{\mu}\sigma_{xy}]$, for which we need to know the averages $\langle[j_{\mathbf{q}(t)}^{\mu}\sigma_{xy}]\rho_{\mathbf{k}}^{*}\rangle$ and $\langle[j_{\mathbf{q}(t)}^{\mu}\sigma_{xy}]j_{\mathbf{k}}^{\nu*}\rangle$ [see Eq. (95)]. The former is zero, $\langle[j_{\mathbf{q}(t)}^{\mu}\sigma_{xy}]\rho_{\mathbf{k}}^{*}\rangle=0$, since this term involves odd number of momentum variables only. Using Eq. (20), the latter reads

$$\langle [j^{\mu}_{\mathbf{q}(t)}\sigma_{xy}]j^{\nu *}_{\mathbf{k}}\rangle = \delta_{\mathbf{k},\mathbf{q}(t)}\langle j^{\mu}_{\mathbf{q}(t)}\sigma_{xy}j^{\nu *}_{\mathbf{q}(t)}\rangle = \delta_{\mathbf{k},\mathbf{q}(t)}\left\langle \sum_i \frac{p_i^{\mu}}{m}e^{i\mathbf{q}(t)\cdot\mathbf{r}_i} \times \sum_j \left(\frac{p_j^x p_j^y}{m} - x_j\frac{\partial U}{\partial y_j}\right)\sum_l \frac{p_l^{\nu}}{m}e^{-i\mathbf{q}(t)\cdot\mathbf{r}_l}\right\rangle. \tag{A60}$$

In this equation, the kinetic-part contribution survives only when (i) $i=j=l$, $\mu=x$, $\nu=y$, and (ii) $i=j=l$, $\mu=y$, $\nu=x$, and the potential-term contribution survives only when $i=l$, $\mu=\nu$. This leads to

$$\langle [j^{\mu}_{\mathbf{q}(t)}\sigma_{xy}]j^{\nu *}_{\mathbf{k}}\rangle = \delta_{\mathbf{k},\mathbf{q}(t)}Nmv^4(\delta_{\mu x}\delta_{\nu y} + \delta_{\mu y}\delta_{\nu x}), \tag{A61}$$

since the potential-term contribution vanishes after applying Eq. (A2). We therefore obtain from Eq. (95)

$$\mathcal{P}[j^{\mu}_{\mathbf{q}(t)}\sigma_{xy}] = \sum_{\mathbf{k}}\sum_{\nu}\langle [j^{\mu}_{\mathbf{q}(t)}\sigma_{xy}]j^{\nu *}_{\mathbf{k}}\rangle\frac{1}{Nv^2}j^{\nu}_{\mathbf{k}} = mv^2[\delta_{\mu x}j^{y}_{\mathbf{q}(t)} + \delta_{\mu y}j^{x}_{\mathbf{q}(t)}], \tag{A62}$$

and hence

$$\mathcal{Q}[j^{\mu}_{\mathbf{q}(t)}\sigma_{xy}] = j^{\mu}_{\mathbf{q}(t)}\sigma_{xy} - mv^2[\delta_{\mu x}j^{y}_{\mathbf{q}(t)} + \delta_{\mu y}j^{x}_{\mathbf{q}(t)}]. \tag{A63}$$

Since the right-hand side of this equation involves odd number of momentum variables only, there holds

$$\langle \{\mathcal{Q}[j^{\mu}_{\mathbf{q}(t)}\sigma_{xy}]\}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle = 0. \tag{A64}$$

8. Derivation of Eq. (124)

Here we show that the memory kernels $N^{\lambda}_{\mathbf{q}}(t)$ and $N'^{\lambda\mu}_{\mathbf{q}}(t)$ defined in Eqs. (111) and (112) vanish under the mode-coupling approximation formulated with $\mathcal{P}_2$. We start from the following expressions under the approximation $e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t} \approx \mathcal{P}_2 e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{P}_2$ (see Sec. IV):

$$N^{\lambda}_{\mathbf{q}}(t) \approx i\frac{2}{Nk_BTS_{q(t)}}\langle [e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{P}_2R^{\lambda}_{\mathbf{q}}]\mathcal{P}_2\mathcal{Q}[\rho^*_{\mathbf{q}(t)}\delta K]\rangle, \tag{A65}$$

$$N'^{\lambda\mu}_{\mathbf{q}}(t) \approx \frac{2m}{N(k_BT)^2}\langle [e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{P}_2R^{\lambda}_{\mathbf{q}}]\mathcal{P}_2\mathcal{Q}[j^{\mu *}_{\mathbf{q}(t)}\delta K]\rangle. \tag{A66}$$

In the following, we demonstrate $\langle\{\mathcal{Q}[\rho_{\mathbf{q}(t)}\delta K]\}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle=0$ and $\langle\{\mathcal{Q}[j^{\mu}_{\mathbf{q}(t)}\delta K]\}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle=0$. This means $\mathcal{P}_2\mathcal{Q}[\rho_{\mathbf{q}(t)}\delta K]=0$ and $\mathcal{P}_2\mathcal{Q}[j^{\mu}_{\mathbf{q}(t)}\delta K]=0$, and hence, completes the derivation of $N^{\lambda}_{\mathbf{q}}(t)=0$ and $N'^{\lambda\mu}_{\mathbf{q}}(t)=0$.

Let us start from $\mathcal{Q}[\rho_{\mathbf{q}(t)}\delta K]$, for which we need to know the averages $\langle[\rho_{\mathbf{q}(t)}\delta K]\rho^*_{\mathbf{k}}\rangle$ and $\langle[\rho_{\mathbf{q}(t)}\delta K]j^{\mu *}_{\mathbf{k}}\rangle$ [see Eq. (95)]. In view of Eq. (23), one easily obtains

$$\langle[\rho_{\mathbf{q}(t)}\delta K]\rho^*_{\mathbf{k}}\rangle = 0, \quad \langle[\rho_{\mathbf{q}(t)}\delta K]j^{\mu *}_{\mathbf{k}}\rangle = 0. \tag{A67}$$

Thus, $\mathcal{P}[\rho_{\mathbf{q}(t)}\delta K]=0$, and hence,

$$\mathcal{Q}[\rho_{\mathbf{q}(t)}\delta K] = \rho_{\mathbf{q}(t)}\delta K. \tag{A68}$$

Likewise, one obtains

$$\mathcal{Q}[j^{\mu}_{\mathbf{q}(t)}\delta K] = j^{\mu}_{\mathbf{q}(t)}\delta K. \tag{A69}$$

It is then obvious that

$$\langle\{\mathcal{Q}[\rho_{\mathbf{q}(t)}\delta K]\}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle = 0, \quad \langle\{\mathcal{Q}[j^{\mu}_{\mathbf{q}(t)}\delta K]\}\rho^*_{\mathbf{k}}\rho^*_{\mathbf{p}}\rangle = 0. \tag{A70}$$

9. Derivation of Eqs. (126)

Here we show that the functions $G_X(t)$ and $H_X(t)$ defined in Eq. (125) evolve in time within the subspace orthogonal to $\{\rho_{\mathbf{k}}, j^{\mu}_{\mathbf{k}}\}$, i.e., there hold

$$G_X(t) = \langle[e^{i\mathcal{L}t}X]\sigma_{xy}\rangle = \langle[e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{Q}X]\mathcal{Q}\sigma_{xy}\rangle, \tag{A71}$$

$$H_X(t) = \langle[e^{i\mathcal{L}t}X]\delta K\rangle = \langle[e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{Q}X]\mathcal{Q}\delta K\rangle, \tag{A72}$$

in terms of the projection operator $\mathcal{Q}$ complementary to $\mathcal{P}$ defined in Eq. (95). Before embarking on the derivation, let us notice

$$\mathcal{Q}\sigma_{xy} = \sigma_{xy} \quad \text{and} \quad \mathcal{Q}\delta K = \delta K. \tag{A73}$$

The first relation follows from $\langle\sigma_{xy}\rho_{\mathbf{k}}\rangle=\delta_{\mathbf{k},0}\langle\sigma_{xy}\rho_{\mathbf{k}=0}\rangle=0$ [see Eq. (71)] and $\langle\sigma_{xy}j^{\mu *}_{\mathbf{k}}\rangle=0$, and the second relation can be derived in a similar manner. Thus, the presence of the operator $\mathcal{Q}$ in front of σ_{xy} and δK in Eqs. (A71) and (A72) is irrelevant.

In the following, we shall deal with the function $G_X(t)$ only, since $H_X(t)$ can be handled in a similar manner. Applying the identity

$$e^{i\mathcal{L}t} = e^{i\mathcal{L}\mathcal{Q}t} + \int_0^t ds\, e^{i\mathcal{L}(t-s)}i e^{i\mathcal{L}\mathcal{Q}s} \tag{A74}$$

[notice the difference in the order of operators compared to the identity (99)], one finds

$$e^{i\mathcal{L}t}X = e^{i\mathcal{L}\mathcal{Q}t}X + \int_0^t ds\, e^{i\mathcal{L}(t-s)}i e^{i\mathcal{L}\mathcal{Q}s}X = e^{i\mathcal{L}\mathcal{Q}t}X + \sum_{\mathbf{k}}\frac{1}{NS_k}\int_0^t ds\langle[e^{i\mathcal{L}\mathcal{Q}s}X]\rho^*_{\mathbf{k}}\rangle e^{i\mathcal{L}(t-s)}i\mathcal{L}\rho_{\mathbf{k}} + \sum_{\mathbf{k}}\sum_{\mu}\frac{1}{Nv^2}\int_0^t ds\langle[e^{i\mathcal{L}\mathcal{Q}s}X]j^{\mu *}_{\mathbf{k}}\rangle e^{i\mathcal{L}(t-s)}i\mathcal{L}j^{\mu}_{\mathbf{k}}, \tag{A75}$$

where we have used the definition (95) of the operator $\mathcal{P}$ and noticed that the ensemble averaged terms are independent of the phase and are unaffected by the Liouvillean and the propagator. Let us notice here that

$$i\mathcal{L}\rho_{\mathbf{k}} \to 0 \quad \text{and} \quad i\mathcal{L}j^{\mu}_{\mathbf{k}} \to 0 \text{ for } \mathbf{k} \to 0. \tag{A76}$$

The former is obvious in view of Eq. (88), while the latter can be derived on the basis of Eq. (92) by noticing $i\mathcal{L}_0 j^{\lambda}_{\mathbf{k}}$

$=(1/m)\Sigma_\mu ik_\mu\sigma_{\mathbf{k}}^{\lambda\mu}$ [see Eq. (A3)] and $j_{\mathbf{k}=0}^{\lambda}=(1/m)\Sigma_i p_i^\lambda=0$ [see the comment below Eq. (2b)]. Equation (A76) simply expresses the fact that the density and the current density, the latter being defined for sheared systems in terms of the peculiar momenta, are conserved variables.

Now let us consider the transient correlator $\langle[e^{i\mathcal{L}t}X]\sigma_{xy}\rangle$ formed with the "zero wave-vector" quantity σ_{xy}. The translational invariance implies that

$$\langle[e^{i\mathcal{L}(t-s)}A_{\mathbf{k}}]\sigma_{xy}\rangle=\delta_{\mathbf{k},0}\langle[e^{i\mathcal{L}(t-s)}A_{\mathbf{k}=0}]\sigma_{xy}\rangle=0, \tag{A77}$$

for $A_{\mathbf{k}}=i\mathcal{L}\rho_{\mathbf{k}}$ and $i\mathcal{L}j_{\mathbf{k}}^{\mu}$ because of Eq. (A76). Thus, there is no contribution to $\langle[e^{i\mathcal{L}t}X]\sigma_{xy}\rangle$ from the second and third terms on the right-hand side of Eq. (A75), and we obtain

$$G_X(t)=\langle[e^{i\mathcal{L}t}X]\sigma_{xy}\rangle=\langle[e^{i\mathcal{L}\mathcal{Q}t}X]\sigma_{xy}\rangle. \tag{A78}$$

Since the operator $\mathcal{Q}$ is idempotent and Hermitian, one finds using Eq. (A73)

$$\begin{aligned}G_X(t)&=\langle[\mathcal{Q}e^{i\mathcal{L}\mathcal{Q}t}X]\mathcal{Q}\sigma_{xy}\rangle=\langle[\mathcal{Q}e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{Q}X]\mathcal{Q}\sigma_{xy}\rangle\\&=\langle[e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{Q}X]\mathcal{Q}\sigma_{xy}\rangle,\end{aligned} \tag{A79}$$

where in the second equality we have noticed

$$\mathcal{Q}e^{i\mathcal{L}\mathcal{Q}t}=\mathcal{Q}e^{i\mathcal{Q}\mathcal{L}\mathcal{Q}t}\mathcal{Q}. \tag{A80}$$

This completes the derivation of Eq. (A71), and Eq. (A72) can be derived in a similar manner.

10. Derivation of Eq. (129)

Here we derive the expression for $\mathcal{P}_2^0\sigma_{xy}$. For this purpose, we need to know the average $\langle\sigma_{xy}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\rangle$. Using Eq. (20), this average can be written as

$$\langle\sigma_{xy}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\rangle=-\sum_i\left\langle x_i\frac{\partial U}{\partial y_i}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\right\rangle=-k_BT\sum_i\left\langle x_i\frac{\partial}{\partial y_i}[\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*]\right\rangle, \tag{A81}$$

where we have used Eq. (A2). Since $\partial\rho_{\mathbf{k}}/\partial y_i=ik_ye^{i\mathbf{k}\cdot\mathbf{r}_i}$ and $\partial\rho_{\mathbf{k}}/\partial k_x=i\Sigma_i x_ie^{i\mathbf{k}\cdot\mathbf{r}_i}$, we obtain

$$\begin{aligned}\langle\sigma_{xy}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\rangle&=-k_BT\left\{ik_y\left\langle\left(\sum_i x_ie^{i\mathbf{k}\cdot\mathbf{r}_i}\right)\rho_{\mathbf{k}}^*\right\rangle\right.\\&\quad\left.-ik_y\left\langle\left(\sum_i x_ie^{-i\mathbf{k}\cdot\mathbf{r}_i}\right)\rho_{\mathbf{k}}\right\rangle\right\}\\&=-k_BTk_y\left\{\left\langle\left(\frac{\partial}{\partial k_x}\rho_{\mathbf{k}}\right)\rho_{\mathbf{k}}^*\right\rangle+\left\langle\rho_{\mathbf{k}}\left(\frac{\partial}{\partial k_x}\rho_{\mathbf{k}}^*\right)\right\rangle\right\}\\&=-Nk_BT\frac{k_xk_y}{k}S_k'.\end{aligned} \tag{A82}$$

It then follows from Eq. (127) that

$$\mathcal{P}_2^0\sigma_{xy}=\sum_{\mathbf{k}>0}\langle\sigma_{xy}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*\rangle\frac{1}{N^2S_k^2}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*=-\frac{k_BT}{N}\sum_{\mathbf{k}>0}\frac{k_xk_y}{k}\frac{S_k'}{S_k^2}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*. \tag{A83}$$

APPENDIX B: ISOTROPIC APPROXIMATION

In this appendix, we shall introduce the isotropic approximation which considerably simplifies the wave-vector-dependent MCT equations (141a), (141b), and (142) for the transient density correlators. Such a simplifying approximation is useful in practical applications of our theory to systems where anisotropy in the density fluctuations is small. We also argue that the anisotropic nature of steady-state quantities such as the shear stress can nevertheless be captured within such an approximation.

1. MCT equations for the transient correlators

The isotropic approximation consists of the following three assumptions. First, it is assumed that $F_{\mathbf{q}}(t)$ depends only on the modulus $q=|\mathbf{q}|$, i.e.,

$$F_{\mathbf{q}}(t)\approx F_q(t). \tag{B1}$$

Second, we introduce a corresponding approximation for the transient cross correlator $H_{\mathbf{q}}^{\lambda}(t)$ formed with current density fluctuations. Since $H_{\mathbf{q}}^{\lambda}(t)$ is a vector correlator whose orientational dependence comes also from the dependence on λ, one cannot introduce such a simple approximation such as $H_{\mathbf{q}}^{\lambda}(t)\approx H_q^{\lambda}(t)$. Instead, we assume that the following relation, valid for isotropic quiescent systems, to hold:

$$H_{\mathbf{q}}^{\lambda}(t)\approx-i\frac{q_\lambda}{q^2}\frac{\partial}{\partial t}F_q(t). \tag{B2}$$

The third assumption concerns the modulus of the advected wave vector $\mathbf{q}(t)$ [see Eq. (56)]:

$$q(t)^2=q^2+2(\dot\gamma t)q_xq_y+(\dot\gamma t)^2q_x^2. \tag{B3}$$

We assume that $q(t)^2$ can be approximated by its orientational average. This is equivalent to neglecting the anisotropic term q_xq_y and approximating q_x^2 by $q^2/3$ in Eq. (B3), leading to

$$q(t)\approx q\sqrt{1+(\dot\gamma t)^2/3}\equiv\bar q(t). \tag{B4}$$

In the following, we shall see consequences of these assumptions.

It follows from the approximation (B2)

$$\frac{\partial}{\partial t}F_q(t)=i\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t), \tag{B5}$$

implying that $\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t)$ also becomes an isotropic quantity. Equation (B5) is consistent with Eq. (141a) under the isotropic approximation. To see this, we first rewrite Eq. (141a) as

$$\frac{\partial}{\partial t}F_{\mathbf{q}}(t)=\dot\gamma q_x\frac{\partial}{\partial q_y}F_{\mathbf{q}}(t)+i\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t), \tag{B6}$$

where the specific form $\kappa_{\lambda\mu}=\dot\gamma\delta_{\lambda x}\delta_{\mu y}$ for the shear-rate tensor has been used. The application of the approximation (B1) then yields

$$\frac{\partial}{\partial t}F_q(t)=\dot\gamma\frac{q_xq_y}{q}\frac{\partial}{\partial q}F_q(t)+i\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t), \tag{B7}$$

because $\partial F_q(t)/\partial q_y=(q_y/q)\partial F_q(t)/\partial q$. Since now the left-hand side depends only on the modulus q, the orientational averaging of this expression gives Eq. (B5).

From a partial time derivative of Eq. (B5), we obtain

$$\frac{\partial^2}{\partial t^2}F_q(t) = i\mathbf{q}\cdot\frac{\partial}{\partial t}\mathbf{H}_{\mathbf{q}}(t). \tag{B8}$$

Substituting Eq. (141b) into the right-hand side yields

$$\frac{\partial^2}{\partial t^2}F_q(t) = \sum_\lambda iq_\lambda\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]H^\lambda_{\mathbf{q}}(t) - q^2\frac{v^2}{S_q}F_{\mathbf{q}}(t) - \sum_\lambda iq_\lambda[\boldsymbol{\kappa}\cdot\mathbf{H}_{\mathbf{q}}(t)]^\lambda - \alpha[i\mathbf{q}\cdot\mathbf{H}_{\mathbf{q}}(t)] - \sum_{\lambda,\mu}\int_0^t ds\, iq_\lambda M^{\lambda\mu}_{\mathbf{q}}(s)H^\mu_{\mathbf{q}(s)}(t-s) - \dot\gamma\sum_\lambda\int_0^t ds\, q_\lambda L^\lambda_{\mathbf{q}}(s)F_{\mathbf{q}(s)}(t-s). \tag{B9}$$

Applying the approximation (B1) to the second and sixth terms, Eq. (B2) to the fifth term, and Eq. (B5) to the fourth term, we obtain

$$\ddot F_q(t) = \sum_\lambda iq_\lambda\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]H^\lambda_{\mathbf{q}}(t) - q^2\frac{v^2}{S_q}F_q(t) - \sum_\lambda iq_\lambda[\boldsymbol{\kappa}\cdot\mathbf{H}_{\mathbf{q}}(t)]^\lambda - \alpha\dot F_q(t) - \int_0^t ds\left[\sum_{\lambda,\mu}q_\lambda M^{\lambda\mu}_{\mathbf{q}}(s)q_\mu(s)/q(s)^2\right]\dot F_{q(s)}(t-s) - \dot\gamma\int_0^t ds\left[\sum_\lambda q_\lambda L^\lambda_{\mathbf{q}}(s)\right]F_{q(s)}(t-s), \tag{B10}$$

where the overdot denotes the partial time derivative. The first and third terms on the right-hand side of this equation can be manipulated as

$$\sum_\lambda iq_\lambda\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right]H^\lambda_{\mathbf{q}}(t) = \sum_\lambda\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}\right][iq_\lambda H^\lambda_{\mathbf{q}}(t)] - \sum_\lambda\left[\mathbf{q}\cdot\boldsymbol{\kappa}\cdot\frac{\partial}{\partial\mathbf{q}}iq_\lambda\right]H^\lambda_{\mathbf{q}}(t) = \dot\gamma q_x\frac{\partial}{\partial q_y}[i\mathbf{q}\cdot\mathbf{H}_q(t)] - \sum_\lambda\left[\dot\gamma q_x\frac{\partial}{\partial q_y}iq_\lambda\right]H^\lambda_{\mathbf{q}}(t) = \dot\gamma q_x\frac{\partial}{\partial q_y}\dot F_q(t) - \dot\gamma[iq_xH^y_{\mathbf{q}}(t)] = \dot\gamma\frac{q_xq_y}{q}\left[\frac{\partial}{\partial q}-\frac{1}{q}\right]\dot F_q(t), \tag{B11}$$

$$\sum_\lambda iq_\lambda[\boldsymbol{\kappa}\cdot\mathbf{H}_{\mathbf{q}}(t)]^\lambda = \sum_\lambda iq_\lambda\left[\sum_\mu\dot\gamma\delta_{\lambda x}\delta_{\mu y}H^\mu_{\mathbf{q}}(t)\right] = \dot\gamma[iq_xH^y_{\mathbf{q}}(t)] = \dot\gamma\frac{q_xq_y}{q^2}\dot F_q(t), \tag{B12}$$

in deriving which we have used the approximations (B2) and (B5). Both of these terms are anisotropic, and vanish after taking the orientational average. [Remember that the left-hand side of Eq. (B10) depends only on the modulus q.] We therefore obtain

$$\ddot F_q(t) + q^2\frac{v^2}{S_q}F_q(t) + \alpha\dot F_q(t) + \int_0^t ds M^{\rm iso}_{\mathbf{q}}(s)\dot F_{\bar q(s)}(t-s) + \dot\gamma\int_0^t ds L^{\rm iso}_{\mathbf{q}}(s)F_{\bar q(s)}(t-s) = 0, \tag{B13}$$

where we have employed the approximation (B4) for the modulus of the advected wave number in the fourth and fifth terms, and introduced

$$M^{\rm iso}_{\mathbf{q}}(t) \equiv \sum_{\lambda,\mu}q_\lambda M^{\lambda\mu}_{\mathbf{q}}(t)q_\mu(t)/q(t)^2, \tag{B14}$$

$$L^{\rm iso}_{\mathbf{q}}(t) \equiv \sum_\lambda q_\lambda L^\lambda_{\mathbf{q}}(t). \tag{B15}$$

Now, we are left with the kernels $M^{\rm iso}_{\mathbf{q}}(t)$ and $L^{\rm iso}_{\mathbf{q}}(t)$ which still depend on the wave vector. From Eqs. (B14) and (142a), one gets for $M^{\rm iso}_{\mathbf{q}}(t)$ under the approximations (B1) and (B4)

$$M^{\rm iso}_{\mathbf{q}}(t) = \frac{\rho v^2}{2(2\pi)^3}\frac{1}{q^2[1+(\dot\gamma t)^2/3]}\int d\mathbf{k}[\mathbf{q}\cdot\mathbf{k}c_k + \mathbf{q}\cdot\mathbf{p}c_p] \times[\mathbf{q}(t)\cdot\mathbf{k}(t)c_{\bar k(t)} + \mathbf{q}(t)\cdot\mathbf{p}(t)c_{\bar p(t)}]F_k(t)F_p(t). \tag{B16}$$

It is clear from this expression that the wave-vector dependence of the this memory kernel stems from the terms $\mathbf{q}(t)\cdot\mathbf{k}(t)$ and $\mathbf{q}(t)\cdot\mathbf{p}(t)$. Using Eq. (56), the explicit expression for the former reads

$$\mathbf{q}(t)\cdot\mathbf{k}(t) = \mathbf{q}\cdot\mathbf{k} + (\dot\gamma t)(q_xk_y + q_yk_x) + (\dot\gamma t)^2q_xk_x, \tag{B17}$$

and a similar expression holds for $\mathbf{q}(t)\cdot\mathbf{p}(t)$. With the same spirit as in the approximation (B4), the anisotropic terms q_xk_y and q_yk_x shall be neglected, and q_xk_x approximated by $\mathbf{q}\cdot\mathbf{k}/3$, i.e.,

$$\mathbf{q}(t)\cdot\mathbf{k}(t) \approx \mathbf{q}\cdot\mathbf{k}[1+(\dot{\gamma}t)^2/3]. \quad \text{(B18)}$$

Substituting this and a similar approximation for $\mathbf{q}(t)\cdot\mathbf{p}(t)$ into Eq. (B16) yields the following expression which now depends only on the modulus q:

$$M_q^{\rm iso}(t) = \frac{\rho v^2}{2(2\pi)^3 q^2}\int d\mathbf{k}[\mathbf{q}\cdot\mathbf{k}c_k + \mathbf{q}\cdot\mathbf{p}c_p] \times[\mathbf{q}\cdot\mathbf{k}c_{\bar{k}(t)} + \mathbf{q}\cdot\mathbf{p}c_{\bar{p}(t)}]F_k(t)F_p(t). \quad \text{(B19)}$$

Concerning $L_{\mathbf{q}}^{\rm iso}(t)$, one gets from Eqs. (B15) and (142b) under the approximation (B1)

$$L_{\mathbf{q}}^{\rm iso}(t) = -\frac{v^2}{2(2\pi)^3}\int d\mathbf{k}[\mathbf{q}\cdot\mathbf{k}c_k + \mathbf{q}\cdot\mathbf{p}c_p] \times\left[\frac{k_xk_y(t)}{k(t)}\frac{S'_{k(t)}}{S_{k(t)}} + \frac{p_xp_y(t)}{p(t)}\frac{S'_{p(t)}}{S_{p(t)}}\right]F_k(t)F_p(t). \quad \text{(B20)}$$

In this expression, the wave vector dependence comes from

$$k_xk_y(t) = k_xk_y + (\dot{\gamma}t)k_x^2 \quad \text{(B21)}$$

and $p_xp_y(t)$. Here again, the anisotropic term k_xk_y shall be neglected, and k_x^2 approximated by $k^2/3$, i.e.,

$$k_xk_y(t) \approx (\dot{\gamma}t)k^2/3, \quad \text{(B22)}$$

and $p_xp_y(t)$ shall be approximated similarly. Along with the approximation (B4), one then obtains the following expression which now depends on the modulus q only:

$$L_q^{\rm iso}(t) = -\frac{v^2}{2(2\pi)^3}\frac{\dot{\gamma}t}{3\sqrt{1+(\dot{\gamma}t)^2/3}}\int d\mathbf{k}[\mathbf{q}\cdot\mathbf{k}c_k + \mathbf{q}\cdot\mathbf{p}c_p] \times\left[k\frac{S'_{\bar{k}(t)}}{S_{\bar{k}(t)}} + p\frac{S'_{\bar{p}(t)}}{S_{\bar{p}(t)}}\right]F_k(t)F_p(t). \quad \text{(B23)}$$

2. Steady-state quantities

Under the isotropic approximation (B1) for the transient density correlators and (B4) for the modulus of the advected wave vector, the MCT expressions (138) and (139) for the steady-state density correlator and structure factor are given by

$$F_{\mathbf{q}}^{\rm SS}(t) = F_q(t) + \dot{\gamma}\int_0^\infty ds\frac{[q_xq_y + \dot{\gamma}(t+s)q_x^2]}{\bar{q}(t+s)}\frac{S'_{\bar{q}(t+s)}}{S^2_{\bar{q}(t+s)}} \times F_q(t+s)F_{\bar{q}(t)}(s), \quad \text{(B24)}$$

$$S_{\mathbf{q}}^{\rm SS} = S_q + \dot{\gamma}\int_0^\infty ds\frac{(q_xq_y + \dot{\gamma}sq_x^2)}{\bar{q}(s)}\frac{S'_{\bar{q}(s)}}{S^2_{\bar{q}(s)}}F_q(s)^2. \quad \text{(B25)}$$

From a numerical point of view, it is not necessary to further simplify these expressions since these steady-state quantities are the final output of the theory rather than the ones involved in the self-consistent calculations. Of course, it is instructive to consider their averages over the orientation $\hat{\mathbf{q}} \equiv \mathbf{q}/q$

$$F_q^{\rm SS}(t) \equiv \frac{1}{4\pi}\int d\hat{\mathbf{q}}F_{\mathbf{q}}^{\rm SS}(t) = F_q(t) + \int_0^\infty ds\frac{(\dot{\gamma})^2(t+s)}{3\sqrt{1+[\dot{\gamma}(t+s)]^2/3}}\frac{qS'_{\bar{q}(t+s)}}{S^2_{\bar{q}(t+s)}}F_q(t+s)F_{\bar{q}(t)}(s), \quad \text{(B26)}$$

$$S_q^{\rm SS} \equiv \frac{1}{4\pi}\int d\hat{\mathbf{q}}S_{\mathbf{q}}^{\rm SS} = S_q + \int_0^\infty ds\frac{(\dot{\gamma})^2 s}{3\sqrt{1+(\dot{\gamma}s)^2/3}}\frac{qS'_{\bar{q}(s)}}{S^2_{\bar{q}(s)}}F_q(s)^2, \quad \text{(B27)}$$

to which only those terms in Eqs. (B24) and (B25) proportional to q_x^2 contribute. However, it is more informative to regard Eqs. (B24) and (B25) as the approximate expressions in which the anisotropic nature of the steady-state density fluctuations is retained to the lowest order: such anisotropy arises from the terms in Eqs. (B24) and (B25) proportional to q_xq_y. Indeed, such a viewpoint is necessary to correctly understand "the isotropic approximation for the steady-state shear stress," adopted in Ref. [16], which sounds contradictory since the shear stress is intrinsically an anisotropic quantity and vanishes under isotropic density fluctuations. We shall come back to this point in a moment.

Under the isotropic approximations (B1) and (B4), one obtains from the MCT expression (134) for the steady-state shear stress $\sigma_{\rm SS}$

$$\sigma_{\rm SS} = \frac{k_BT\dot{\gamma}}{2(2\pi)^3}\int_0^\infty ds\int d\mathbf{k}\frac{k_x^2k_y(k_y+\dot{\gamma}sk_x)}{k\bar{k}(s)}\frac{S'_kS'_{\bar{k}(s)}}{S_k^2S^2_{\bar{k}(s)}}F_k(s)^2. \quad \text{(B28)}$$

One easily understands that only the term proportional to $k_x^2k_y^2$ survives after the integration over the orientation $\hat{\mathbf{k}} \equiv \mathbf{k}/k$, yielding the following expression for $\sigma_{\rm SS}$ under the isotropic approximation

$$\sigma_{\rm SS} = \frac{k_BT\dot{\gamma}}{60\pi^2}\int_0^\infty ds\frac{1}{\sqrt{1+(\dot{\gamma}s)^2/3}}\int_0^\infty dk k^4\frac{S'_kS'_{\bar{k}(s)}}{S_k^2S^2_{\bar{k}(s)}}F_k(s)^2. \quad \text{(B29)}$$

This is essentially the same expression as adopted in Ref. [16].

To connect such an isotropic expression for $\sigma_{\rm SS}$ with anisotropic density fluctuations, we rewrite the term in Eq. (B28) which survives after the integration over $\hat{\mathbf{k}}$ in the following form:

$$\sigma_{\rm SS} = \frac{k_BT}{2(2\pi)^3}\int d\mathbf{k}\frac{k_xk_y}{k}\frac{S'_k}{S_k^2}\left\{\dot{\gamma}\int_0^\infty ds\frac{k_xk_y}{\bar{k}(s)}\frac{S'_{\bar{k}(s)}}{S^2_{\bar{k}(s)}}F_k(s)^2\right\}. \quad \text{(B30)}$$

The quantity in the curly brackets is exactly the aforementioned anisotropic term in Eq. (B25). Thus, the steady-state shear stress σ_{SS} can be handled within the isotropic approximation since its MCT expression takes a form of the product of two anisotropic terms, one from $k_x k_y$ and the other from the anisotropic part of the density fluctuations, which altogether behaves as an isotropic term inside the integral.

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