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Quasihydrodynamics of nanofluid mixtures

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The functional perturbation theory method developed earlier [L. A. Pozhar and K. E. Gubbins, J. Chem. Phys. **94**, 1367 (1991)] and used for derivation of the transport theory of pure dense, strongly inhomogeneous fluids [L. A. Pozhar and K. E. Gubbins, J. Chem. Phys. **99**, 8970 (1993)] is exploited to develop the transport theory for mixtures of dense, strongly inhomogeneous fluids. The generalized Enskog-like kinetic equations have been solved using the 13-moment approximation method to obtain linearized quasihydrodynamic equations of first order in gradients of continuum variables and to derive explicit, tractable expressions for the transport coefficients of such mixtures. The derived transport coefficients are expressed in terms of equilibrium structure factors (the number density and the pair and direct correlation functions) of the corresponding inhomogeneous fluid mixtures. Diffusion in such mixtures is considered in detail for several particular cases. [S1063-651X(97)00610-7]

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I. INTRODUCTION

The properties of strongly inhomogeneous fluids, such as those at interfaces and confined in narrow capillary pores of widths less than about 10 nm (called here nanofluids), show a rich variety of behavior, including enhanced or inhibited viscosity and diffusion rates, new and modified phase transitions, and highly selective adsorption. Experimental studies designed to investigate properties of such fluids experience difficulties due to the complicated structure of the confined systems and interfaces, the many variables involved, and the sensitivity of the properties to experimental conditions. In the few cases when reliable experimental data have been obtained, their analysis is complicated by a lack of a reliable theoretical description of the properties of such systems.

Over the past decade there has been significant progress in understanding equilibrium properties of inhomogeneous fluids, though some wide areas are still to be investigated. Much less progress has been achieved in the case of nonequilibrium properties of these fluids. Such knowledge is very important for both basic and applied research since many industrial processes are known to be limited by diffusion, selectivity, and/or flow considerations. In several recent papers [1–3] and a monograph [4] we have addressed the development of rigorous statistical mechanical methods for the description of nonequilibrium properties of nanofluids. These methods generalize existing rigorous approaches in nonequilibrium statistical mechanics of uniform systems (see Ref. [5] and references therein) and qualitative concepts [6] in statistical mechanics of confined fluids. They also suggest new developments in nonequilibrium statistical mechanics, in particular that of nanofluids. The major thrust of our approach is to generalize rigorous statistical mechanical approaches developed for the description of nonequilibrium processes in uniform (or bulk) fluids to include nonequilibrium phenomena in nanofluids [1,2,4] and their mixtures. Recent comparisons of theoretical predictions for the shear viscosity of nanofluids, obtained in the framework of this approach, with nonequilibrium molecular-dynamics (NEMD) simulation data [3] show that such a generalization leads to further insights into the nature of nonequilibrium processes in nanofluids. In particular, the theory [2,4] correctly predicts the increase in the shear viscosity due to confinement and the oscillating nature of the local shear viscosity of nanofluids. The theoretical results have been shown to agree within 1–5% with the NEMD data [3] on the shear viscosity of a nanofluid confined in a narrow slit pore of about five molecular diameters in width. This success of the theory has encouraged us to further develop the approach to include mixtures of nanofluids.

In this paper we present such a generalization of the above theory and describe transport processes in mixtures of dense, strongly inhomogeneous fluids composed of simple, structureless molecules. To do this we follow the methods developed and used in our previous works [2,4]. We start from the system of Enskog-like kinetic equations derived earlier [1] on the basis of functional perturbation theory (FPT), and use the 13-moment approximation (Grad) method, generalized by Sung and Dahler [5], to obtain the corresponding system of nonlocal moment equations (Sec. II) for the quasicontinuum variables, defined as expectation values of the first 13 moments of the velocity distribution functions of the components of the nanofluid mixtures. These definitions reflect those of the densities of the components, their hydrodynamic velocities, temperatures, kinetic contributions to the pressure tensor, and the energy flux specific to uniform fluid mixtures. However, the physical meaning of our quasicontinuum quantities may not coincide with that of the continuum characteristics of uniform fluid mixtures because we are concerned with fluid systems of a finite (sometimes very small) number of molecules. Rather, our quasicontinuum quantities are essentially expectation values of the corresponding velocity moments.

In Sec. III the system of equations for the quasicontinuum variables is reduced to obtain the linearized, Navier-Stokes-

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like, quasihydrodynamic equations of first order in gradients of the quasicontinuum variables. These quasihydrodynamic equations are derived in terms of deviations of the quasicontinuum variables from their equilibrium values. Though such nonequilibrium values are characterized by large spatial gradients, recent NEMD simulation data and experimental findings show that their deviations from the corresponding equilibrium values are small, provided that the system is not too far from its equilibrium state (see references in Ref. [4], Chap. 1). In deriving these equations, we also recover explicit expressions for the viscosities and thermal conductivities of the nanofluid mixtures. The derivation of explicit expressions for the diffusion coefficients for such mixtures includes usage of an appropriate expression for the equilibrium pressure of nanofluid mixtures and is discussed in Sec. IV. As for a pure nanofluid [2,4], the transport coefficients of a nanofluid mixture emerge in terms of the ''smoothed'' structure factors of the corresponding nanofluid mixture at equilibrium. The smoothing procedures enter these expressions automatically as a consequence of having intermolecular interaction potentials that are the sum of short-range repulsive and long-range attractive contributions. We place some emphasis on the diffusion coefficients here, in view of their prime importance for applications involving nanofluids in pores. Section V contains closing remarks, and the Appendixes supply details of the theory.

II. FPT KINETIC EQUATIONS, THE 13-MOMENT APPROXIMATION METHOD, AND NONLOCAL MOMENT EQUATIONS FOR MIXTURES OF NANOFLUIDS

A. FPT kinetic equations

Inhomogeneity of a fluid or a fluid mixture composed of simple, structureless molecules can be considered to result from a continuous external potential field, and in a general case this may be written as a sum of short-range repulsive and long-range attractive contributions. The short-range repulsive part describes hard-core-like interactions of the fluid molecules with molecules forming walls (if any). The long-range attractive contribution are caused by both the long-range intermolecular interactions of the fluid molecules with the molecules of the walls and an external potential field of a general nature. A similar representation of the fluid-fluid interactions can be made by means of the Weeks-Chandler-Andersen [7] or Barker-Henderson [8] methods. In what follows we consider an inhomogeneous fluid mixture composed of N components, in which molecules interact with the wall molecules and with each other by virtue of the above potentials. To simplify the expressions, the molecules forming the confinement (walls) are considered to be simple, structureless, and all of the same species. These expressions are easily generalized to cases where the walls are composed of a mixture of species by adding a summation over wall species to terms involving the fluid-wall pair correlation function g_{iw}. The repulsive contributions to all of the potentials of intermolecular interaction are assumed to be hard-core ones, with effective diameters σ_{ij} specific to interactions of the ith species molecules with those of the jth species, and with effective diameters σ_{iw} corresponding to the repulsive interactions of the ith species molecules with those of the walls. The attractive parts of the potentials are expected to behave as r^{-n}, $n>2$, at $r\rightarrow\infty$, where r is the distance between interacting molecules. Also, the potentials of intermolecular interaction are expected to be central and pairwise. The walls, which are of arbitrary geometry, are supposed to be impenetrable to fluid molecules and thermostated at temperature T; the wall molecules are fixed in their positions in the walls. Since the wall molecules are fixed, there will be a net momentum production in the system, but no kinetic-energy production. Such a momentum production should not affect local values of the kinetic coefficients of the nanofluid mixture, except those in the immediate vicinity of the walls. In addition, we assume that there is no chemical reaction in the system.

Neglecting delayed response of the system to thermal disturbances, and being close to the equilibrium state of the system, the kinetic stage of evolution of the above nanofluid mixture is described by the kinetic equations (4.36) of Ref. [1] [see also the kinetic equations (82) of Chap. 3, Ref. [4]] with respect to the $\delta F_i(\mathbf{q},\mathbf{v};t)$, which denote the deviations of the velocity distribution functions (where the index i specifies a component of the mixture) from their equilibrium values $\Phi_i(v)=(\beta m_i/2\pi)^{3/2}\exp(-\beta m_i|\mathbf{v}|^2/2)$, i.e., the corresponding Maxwell-Boltzmann velocity distribution functions. Here m_i is the mass of a molecule of the ith species; the vectors $\mathbf{q}$ and $\mathbf{v}$ denote the Cartesian three-vector of spatial coordinates and the velocity of a molecule, respectively; $|\mathbf{v}|$ means the absolute value of the vector $\mathbf{v}$; $\beta=1/k_BT$, where T is the equilibrium temperature of the nanofluid mixture and k_B is the Boltzmann constant. These kinetic equations can be transformed to the form

$$\frac{\partial}{\partial t}\,\delta F_i(\mathbf{q},\mathbf{v};t)+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{q}}\,\delta F_i(\mathbf{q},\mathbf{v};t)=\sum_{l=1}^{N}\int\int d\mathbf{q}'\,d\mathbf{v}'\,\Gamma_{il}(\mathbf{q},\mathbf{v};\mathbf{q}',\mathbf{v}')\,\delta F_l(\mathbf{q}',\mathbf{v}';t), \tag{2.1}$$

where

$$\Gamma_{il}(\mathbf{q},\mathbf{v};\mathbf{q}',\mathbf{v}')=\delta_{il}\sum_{j=1}^{N}\sigma_{ij}^2\int\int\int d\hat{\boldsymbol{\sigma}}\,d\mathbf{v}_i d\mathbf{v}_j\Phi_j(\mathbf{v}_j)|\mathbf{v}_{ji}\cdot\hat{\boldsymbol{\sigma}}|\,\theta(\mathbf{v}_{ji}\cdot\hat{\boldsymbol{\sigma}})\{\delta(\mathbf{v}-\mathbf{v}_i^*)n_j(\mathbf{q}-\sigma_{ij}\hat{\boldsymbol{\sigma}})g_{ij}(\mathbf{q},\mathbf{q}-\sigma_{ij}\hat{\boldsymbol{\sigma}})$$
$$-\delta(\mathbf{v}-\mathbf{v}_i)n_j(\mathbf{q}+\sigma_{ij}\hat{\boldsymbol{\sigma}})g_{ij}(\mathbf{q},\mathbf{q}+\sigma_{ij}\hat{\boldsymbol{\sigma}})\}\,\delta(\mathbf{v}'-\mathbf{v}_i)\,\delta(\mathbf{q}'-\mathbf{q})+\sigma_{il}^2\int\int\int d\hat{\boldsymbol{\sigma}}\,d\mathbf{v}_i d\mathbf{v}_l|\mathbf{v}_{li}\cdot\hat{\boldsymbol{\sigma}}|\,\theta(\mathbf{v}_{li}\cdot\hat{\boldsymbol{\sigma}})\Phi_i(\mathbf{v}_i)$$
$$\times\{\delta(\mathbf{v}-\mathbf{v}_i^*)n_i(\mathbf{q}'-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q}'-\sigma_{il}\hat{\boldsymbol{\sigma}},\mathbf{q}')\,\delta(\mathbf{q}-\mathbf{q}'+\sigma_{il}\hat{\boldsymbol{\sigma}})-\delta(\mathbf{v}-\mathbf{v}_i)n_i(\mathbf{q}'+\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q}'+\sigma_{il}\hat{\boldsymbol{\sigma}},\mathbf{q}')$$

$$\times\delta(\mathbf{q}-\mathbf{q}'-\sigma_{il}\hat{\boldsymbol{\sigma}})\}\delta(\mathbf{v}'-\mathbf{v}_l)+\delta_{il}\sigma_{iw}^2\int\int d\hat{\boldsymbol{\sigma}}\,d\mathbf{v}_i\left|\mathbf{v}_i\cdot\hat{\boldsymbol{\sigma}}\right|\theta(-\mathbf{v}_i\cdot\hat{\boldsymbol{\sigma}})\{\delta(\mathbf{v}-\mathbf{v}_i^*)n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})$$
$$\times g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})-\delta(\mathbf{v}-\mathbf{v}_i)n_w(\mathbf{q}+\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}+\sigma_{iw}\hat{\boldsymbol{\sigma}})\}\delta(\mathbf{v}'-\mathbf{v}_i)\delta(\mathbf{q}'-\mathbf{q})$$
$$+n_i(\mathbf{q})\Phi_i(\mathbf{v})\mathbf{v}\cdot\left\{\frac{\partial C_{il}(\mathbf{q},\mathbf{q}')}{\partial\mathbf{q}}-g_{il}(\mathbf{q},\mathbf{q}')\,\frac{\partial f^H(|\mathbf{q}-\mathbf{q}'|)}{\partial(\mathbf{q}-\mathbf{q}')}\right\}$$
$$+\frac{\partial n_i(\mathbf{q})}{\partial\mathbf{q}}\cdot\mathbf{v}\Phi_i(\mathbf{v})\left\{1+C_{il}(\mathbf{q},\mathbf{q}')-\sum_{k=1}^{N}\int d\mathbf{q}''n_k(\mathbf{q}'')C_{kl}(\mathbf{q}'',\mathbf{q}')\right\}. \tag{2.2}$$

In the above expressions $\partial/\partial t$ and $\partial/\partial\mathbf{q}$ denote the time derivative and spacial gradient, the centered dot means the inner product; $\mathbf{q}',\mathbf{q}''$ and $\mathbf{v}',\mathbf{v}'',\mathbf{v}_i,\mathbf{v}_l$ are dummy variables of integration over the domains of the molecular coordinates and velocities; $n_i(\mathbf{q})$ is the equilibrium number density of the ith species; $g_{ik}(\mathbf{q},\mathbf{q}\pm\sigma_{ik}\hat{\boldsymbol{\sigma}})$ and $g_{iw}(\mathbf{q},\mathbf{q}\pm\sigma_{iw}\hat{\boldsymbol{\sigma}})$ denote the contact values of the equilibrium pair-correlation functions specific to the ith and kth component interactions, and the ith component and wall molecules interactions, respectively; $C_{ik}(\mathbf{q},\mathbf{q}')$ is the equilibrium direct correlation function specific to the ith and kth species; δ_{il} stands for Kronecker's delta; σ_{ik} and σ_{iw} are the effective diameters of the hard-core interactions specific to ith and kth species, and the ith species and the wall molecules, respectively; $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ are the unit vectors of the x, y, and z directions, respectively; $\hat{\boldsymbol{\sigma}}=\sigma_x\mathbf{i}+\sigma_y\mathbf{j}+\sigma_z\mathbf{k}$; $|\sigma|^2=1$ is the unit vector; $\delta(\mathbf{q}-\mathbf{q}')$, $\delta(\mathbf{v}-\mathbf{v}')$, etc., are Dirac delta functions; $\mathbf{v}_i^*=\mathbf{v}_i-(\mathbf{v}_{ji}\cdot\hat{\mathbf{q}}_{ji})\hat{\mathbf{q}}_{ji}$ represents postcollisional velocity of the ith molecule, with $\mathbf{v}_{ji}=\mathbf{v}_j-\mathbf{v}_i$, $\hat{\mathbf{q}}_{ji}$ being the unit vector in the direction from the center of mass of the jth molecule to the center of mass of the ith molecule; $f^H(\mathbf{q},\mathbf{q}')=\exp[-\beta\phi_H(\mathbf{q},\mathbf{q}')]-1=\theta(|\mathbf{q}-\mathbf{q}'|-\sigma)-1$ is the Mayer function of the fluid-fluid molecule hard-core interactions; $\theta(|\mathbf{q}-\mathbf{q}'|-\sigma)$ denotes the Heaviside step function. The summation on the right-hand side of Eq. (2.1) runs over all of the components of the nanofluid mixture and $\int d\hat{\boldsymbol{\sigma}}$ means integration over the surface of the sphere of the unit radius.

The kinetic equations (2.1) have been derived in the framework of the FPT approach [1] and are rigorous generalizations of the kinetic equations obtained for uniform fluid mixtures in Ref. [5] to nanofluid mixtures. The kinetic equations of Ref. [5] in turn rigorously generalize to dense fluids the Enskog-like kinetic equations describing uniform fluids of low density (see references in Refs. [1] and [5]). This family of kinetic equations may be called Enskog-like kinetic equations since they are linearized, rigorous generalizations of the heuristic kinetic equation for dense gases originally suggested by Enskog [9]. Due to the representation of the potentials of intermolecular interactions in terms of the short-range, hard-core, and long-range soft contributions (which was suggested by Sung and Dahler [5] for uniform fluids and used by the authors of this paper in Refs. [1,4]), the "collision integrals" on the right-hand side of Eq. (2.1) include the potentials of intermolecular interaction implicitly through the *equilibrium* structure factors of the nanofluid mixture.

B. Velocity distribution functions in terms of their moments

The velocity distribution functions of Eq. (2.1) may be written in terms of their velocity moments, in which case Eq. (2.1) gives rise to an infinite system of nonlocal moment equations. For this purpose we make use of the generalized Hermite polynomials [10], defined by the expressions

$$\psi_l^{(i)}(\mathbf{v})=\Psi_l^{(i)}(\boldsymbol{\xi})\equiv\Phi_i^{-1}(\xi)(l_1!l_2!l_3!)^{-1/2}\times\left(-\frac{\partial}{\partial\xi_1}\right)^{l_1}\left(-\frac{\partial}{\partial\xi_2}\right)^{l_2}\left(-\frac{\partial}{\partial\xi_3}\right)^{l_3}\Phi_i(\xi) \tag{2.3}$$

for each of $l=(l_1,l_2,l_3)$ and each of the Maxwell-Boltzmann distributions $\Phi_i(v)$ expressed in terms of the dimensionless velocity $\boldsymbol{\xi}=(m_i\beta)^{1/2}\mathbf{v}\equiv\xi_1\mathbf{i}+\xi_2\mathbf{j}+\xi_3\mathbf{k}$, so that $\Phi_i(\xi)=(2\pi)^{-3/2}\exp(-\xi^2/2)$, where $\xi^2=|\boldsymbol{\xi}|^2$ and $l_1,l_2,l_3=1,2,3,\ldots$. Also, for each of the $\Phi_i(\xi)$ the polynomials (2.3) form the basis vector set M_i satisfying the orthogonality and completeness conditions

$$\int d\xi\,\Phi_i(\xi)\Psi_l^{(i)}(\boldsymbol{\xi})\psi_k^{(i)}(\boldsymbol{\xi})=\delta_{lk},$$
$$\sum_{l=1}^{\infty}\Phi_i(\xi)\Psi_l^{(i)}(\boldsymbol{\xi})\Psi_l^{(i)}(\boldsymbol{\xi}')=\delta(\boldsymbol{\xi}-\boldsymbol{\xi}'), \tag{2.4}$$

where $\Psi_l^{(i)}(\boldsymbol{\xi})$ and $\Psi_k^{(i)}(\boldsymbol{\xi})\in M_i$.

The polynomials (2.3) can be considered as the ξ representatives of some abstract bra $\langle l^i|$ and ket $|l^i\rangle$ vectors

$$\Psi_l^{(i)}(\boldsymbol{\xi})=\langle l^i|\xi\rangle\equiv\langle l_1^i l_2^i l_3^i|\xi\rangle,$$
$$\Phi_i(\xi)\Psi_l^{(i)}(\boldsymbol{\xi})=\langle\xi|l^i\rangle\equiv\langle\xi|l_1^i l_2^i l_3^i\rangle, \tag{2.5}$$

in which case the conditions (2.4) take the form $\langle l^i|k^i\rangle=\delta_{lk}$ and $\Sigma_l|l^i\rangle\langle l^i|=1$.

For each $\delta F_i(\mathbf{q},\mathbf{v};t)$ Eq. (2.1) can be spanned by the vectors of the basis set $\langle k^i|$ to read

$$\left\langle k^i\left|\frac{\partial}{\partial t}\delta F_i\right.\right\rangle+\left\langle k^i\left|\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{q}}\delta F_i\right.\right\rangle=\sum_l^N\sum_m^\infty\int d\mathbf{q}'\langle k^i|\Gamma_{il}|m^l\rangle\langle m^l|\delta F_l\rangle, \tag{2.6}$$

where the "projections" $\langle k^i|\delta F_i\rangle$ of $\delta F_i(\mathbf{q},\mathbf{v};t)$ on its basis set vectors $\langle k^i|$ are velocity moments of $\delta F_i(\mathbf{q},\mathbf{v};t)$,

$$\langle k^i|\delta F_i\rangle=\int d\mathbf{v}'\,\psi_k^{(i)}(\mathbf{v}')\,\delta F_i(\mathbf{q},\mathbf{v}';t), \tag{2.7}$$

and

$$\left\langle k^i\middle|\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{q}}\,\delta F_i\right\rangle=\int d\mathbf{v}\;\psi_k^{(i)}(\mathbf{v})\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{q}}\,\delta F_i(\mathbf{q},\mathbf{v};t), \tag{2.8}$$

$$\langle k^i|\Gamma_{il}|m^l\rangle=\int d\mathbf{v}\,d\mathbf{v}'\,\psi_k^{(i)}(\mathbf{v})\Gamma_{il}(\mathbf{q},\mathbf{v};\mathbf{q}',\mathbf{v}')\times\Phi_l(v')\,\psi_m^{(l)}(\mathbf{v}'). \tag{2.9}$$

The basis set of $\langle l^i|$, or $\langle k^i|$, vectors consists of infinitely many vectors, which correspond to infinitely many velocity moments of the distribution function and consequently to infinitely many equations in the equation set (2.6). Since one cannot solve the entire set of equations (2.6), this set should be truncated by choosing an appropriate finite number of moments, which still have to supply a reasonably detailed description of transport processes in the nanofluid mixture. The simplest set of moments that satisfy this requirement is that supplied by the first 13 velocity moments of $\delta F_i(\mathbf{q},\mathbf{v};t)$ [9,2]. The corresponding truncation of the system (2.6) is called the 13-moment approximation. In this approximation the basis set of vectors $\langle k^i|\mathbf{v}\rangle$ is limited to the elements

$$\langle n_i|\mathbf{v}\rangle\equiv\psi_n^{(i)}(\mathbf{v})=1, \tag{2.10}$$

$$\langle\mathbf{u}_i|\mathbf{v}\rangle\equiv(m_i\beta)^{1/2}\psi_u^{(i)}(\mathbf{v})=(m_i\beta)^{1/2}\mathbf{v}, \tag{2.11}$$

$$\langle\hat{T}_i|\mathbf{v}\rangle\equiv(\tfrac{2}{3})^{1/2}\beta\psi_T^{(i)}(\mathbf{v})=(\tfrac{2}{3})^{1/2}\left(\frac{\beta m_i v^2}{2}-\frac{3}{2}\right),\quad v=|\mathbf{v}|^2 \tag{2.12}$$

$$\langle\hat{\mathbf{P}}_i^0|\mathbf{v}\rangle\equiv2^{-1/2}\beta\psi_P^{(i)}(\mathbf{v})=2^{-1/2}\beta m_i[\mathbf{vv}-\tfrac{1}{3}v^2\mathbf{I}], \tag{2.13}$$

$$\langle\hat{\mathbf{Q}}_i|\mathbf{v}\rangle\equiv(\tfrac{2}{5})^{1/2}(m_i\beta^3)^{1/2}\psi_Q^{(i)}(\mathbf{v})=(\tfrac{2}{5})^{1/2}(m_i\beta)^{1/2}\left[\frac{\beta m_i v^2}{2}-\frac{5}{2}\right]\mathbf{v}, \tag{2.14}$$

where

$$\psi_n^{(i)}(\mathbf{v})=1,\quad\psi_u^{(i)}(\mathbf{v})=\mathbf{v},$$

$$\psi_T^{(i)}(\mathbf{v})=\frac{m_i v^2}{2}-\frac{3}{2\beta}=\frac{1}{\beta}\left(\frac{\beta m_i v^2}{2}-\frac{3}{2}\right),$$

$$\psi_P^{(i)}(\mathbf{v})=m_i[\mathbf{vv}-\tfrac{1}{3}v^2\mathbf{I}],$$

$$\psi_Q^{(i)}(\mathbf{v})=\left(\frac{m_i v^2}{2}-\frac{5}{2\beta}\right)\mathbf{v}=\frac{1}{\beta}\left(\frac{\beta m_i v^2}{2}-\frac{5}{2}\right)\mathbf{v}.$$

The above basis set vectors are labeled with the quasicontinuum variables $\delta n_i(\mathbf{q},t)$, $\mathbf{u}_i(\mathbf{q},t)$, $\delta T_i(\mathbf{q},t)$, $\hat{\mathbf{P}}_i^0(\mathbf{q},t)$, and $\mathbf{Q}_i(\mathbf{q},t)$, which correspond to the expectation values of the vectors of the basis set and stand for the deviations of the quasicontinuum number density, quasihydrodynamic velocity, and temperature of the ith component of the mixture from their equilibrium values and for the kinetic contributions to the pressure tensor and the energy flux of the mixture due to its ith component, respectively; the notation $\mathbf{I}$ means the unit matrix. The above quasicontinuum variables are defined as

$$\delta n_i(\mathbf{q},t)\equiv\int d\mathbf{v}\;\psi_n^{(i)}(\mathbf{v})\,\delta F_i(\mathbf{q},\mathbf{v};t), \tag{2.15a}$$

$$\rho_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)\equiv\int d\mathbf{v}\;m_i\psi_u^{(i)}(\mathbf{v})\,\delta F_i(\mathbf{q},\mathbf{v};t);$$

$$\tfrac{3}{2}k_B n_i(\mathbf{q})\,\delta T_i(\mathbf{q},t)\equiv\int d\mathbf{v}\;\psi_T^{(i)}(\mathbf{v})\,\delta F_i(\mathbf{q},\mathbf{v};t), \tag{2.15b}$$

$$\hat{\mathbf{P}}_i^0(\mathbf{q},t)\equiv\int d\mathbf{v}\;\psi_P^{(i)}(\mathbf{v})\,\delta F_i(\mathbf{q},\mathbf{v};t);$$

$$\mathbf{Q}_i(\mathbf{q},t)\equiv\sum_{i=1}^{N}\int d\mathbf{v}\;\psi_Q^{(i)}(\mathbf{v})\,\delta F_i(\mathbf{q},\mathbf{v};t). \tag{2.15c}$$

The corresponding quasicontinuum quantities for the nanofluid mixture are

$$\delta n(\mathbf{q},t)=\sum_{i=1}^{N}\delta n_i(\mathbf{q},t), \tag{2.16a}$$

$$\rho(\mathbf{q})\mathbf{u}(\mathbf{q},t)=\sum_{i=1}^{N}m_i n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t);$$

$$\tfrac{3}{2}k_B n(\mathbf{q})\,\delta T(\mathbf{q},t)=\sum_{i=1}^{N}\tfrac{3}{2}k_B n_i(\mathbf{q})\,\delta T_i(\mathbf{q},t), \tag{2.16b}$$

$$\hat{\mathbf{P}}^0(\mathbf{q},t)=\sum_{i=1}^{N}\hat{\mathbf{P}}_i^0(\mathbf{q},t);$$

$$\mathbf{Q}(\mathbf{q},t)=\sum_{i=1}^{N}\mathbf{Q}_i(\mathbf{q},t), \tag{2.16c}$$

where $\rho(\mathbf{q})=\Sigma_{i=1}^N m_i n_i(\mathbf{q})\equiv\Sigma_{i=1}^N\rho_i(\mathbf{q})$ stands for the *equilibrium* mass density of the nanofluid mixture. The 13-moment approximation for the distributions $\delta F_i(\mathbf{q}',\mathbf{v}';t)$ reads

$$
\begin{aligned}
\delta F_i(\mathbf{q}',\mathbf{v}';t) &= \langle \mathbf{v}' | \delta F_i \rangle \\
&= \sum_{k^i=1}^{M_i} \langle \mathbf{v}' | k^i \rangle \langle k^i | \delta F_i \rangle \\
&= \Phi_i(\mathbf{v}')[\psi_n^{(i)}(\mathbf{v}')\,\delta n_i(\mathbf{q}',t) \\
&\quad + \psi_u^{(i)}(\mathbf{v}')\cdot \beta\rho_i(\mathbf{q}')\mathbf{u}_i(\mathbf{q}',t) \\
&\quad + \psi_T^{(i)}(\mathbf{v}')\beta^2 k_B n_i(\mathbf{q}')\,\delta T_i(\mathbf{q}',t) \\
&\quad + \psi_P^{(i)}(\mathbf{v}'):\tfrac{1}{2}\beta^2 \hat{\mathbf{P}}_i^0(\mathbf{q}',t) \\
&\quad + \psi_Q^{(i)}(\mathbf{v}')\cdot \tfrac{2}{5} m_i \beta^3 \mathbf{Q}_i(\mathbf{q}',t). \qquad (2.17)
\end{aligned}
$$

C. The 13-moment equations for the quasicontinuum variables

Using Eq. (2.17), calculating integrals (2.7)–(2.9), and substituting the results in Eq. (2.6), one can recover nonlocal moment equations of the 13-moment approximation. The simplest of them is the continuity equation for the deviation $\delta n_i(\mathbf{q},\omega)$ of the ith component number density from its equilibrium value

$$
\begin{aligned}
&\frac{\partial}{\partial t}\,\delta n_i(\mathbf{q},t) + \frac{\partial}{\partial \mathbf{q}}\cdot[n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)] \\
&\quad = n_i(\mathbf{q})\sum_{k=1}^{N}\sigma_{ik}^2 \int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}}) g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}}) \\
&\qquad \times \hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q},t)-\mathbf{u}_i(\mathbf{q},t)] + n_i(\mathbf{q})\sum_{k=1}^{N}\sigma_{ik}^2\int d\hat{\boldsymbol{\sigma}} \\
&\qquad \times n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}}) g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t) \\
&\qquad -\mathbf{u}_k(\mathbf{q},t)] + n_i(\mathbf{q})\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}}) \\
&\qquad \times g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot\mathbf{u}_i(\mathbf{q},t). \qquad (2.18)
\end{aligned}
$$

The evolution equation for the deviation $\rho_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},\omega)$ of the momentum of the ith component of the nanofluid mixture from the corresponding equilibrium value is

$$
\begin{aligned}
&\frac{\partial}{\partial t}[\rho_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)] + \frac{\partial}{\partial \mathbf{q}}\cdot[\hat{\mathbf{P}}_i^0(\mathbf{q},t)+k_B n_i(\mathbf{q})\,\delta T_i(\mathbf{q},t)\mathbf{I}] + \frac{1}{\beta}\frac{\partial}{\partial \mathbf{q}}\,\delta n_i(\mathbf{q},t) \\
&= \frac{1}{\beta} n_i(\mathbf{q})\sum_{k=1}^{N}\int d\mathbf{q}'\,\frac{\partial C_{ik}(\mathbf{q},\mathbf{q}')}{\partial \mathbf{q}}\,\delta n_k(\mathbf{q}',t) - \frac{1}{\beta} n_i(\mathbf{q})\sum_{k=1}^{N} 2b_{ik}^H g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\,\delta n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t) + \frac{1}{\beta}\frac{\partial n_i(\mathbf{q})}{\partial \mathbf{q}} \\
&\quad \times \sum_{k=1}^{N}\int d\mathbf{q}'\left[1+C_{ik}(\mathbf{q},\mathbf{q}')-\sum_{l=1}^{N}\int d\mathbf{q}'' n_l(\mathbf{q}'')C_{lk}(\mathbf{q}'',\mathbf{q}')\right]\delta n_k(\mathbf{q}',t) + 4\sqrt{\frac{m_i}{2\pi\beta}}\, n_i(\mathbf{q})\sum_{k=1}^{N}\frac{\sigma_{ik}^2\sqrt{m_k/m_i}}{\sqrt{1+m_k/m_i}} \\
&\quad \times \int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q},t)-\mathbf{u}_i(\mathbf{q},t)] \\
&\quad + 4\sqrt{\frac{m_i}{2\pi\beta}}\, n_i(\mathbf{q})\sum_{k=1}^{N}\frac{\sigma_{ik}^2\sqrt{m_k/m_i}}{\sqrt{1+m_k/m_i}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{u}_k(\mathbf{q},t)] \\
&\quad + 4\sqrt{\frac{m_i}{2\pi\beta}}\, n_i(\mathbf{q})\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\cdot\mathbf{u}_i(\mathbf{q},t) \\
&\quad + k_B n_i(\mathbf{q})\sum_{k=1}^{N}\frac{\sigma_{ik}^2}{1+m_k/m_i}\int d\hat{\sigma}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\delta T_k(\mathbf{q},t)-\delta T_i(\mathbf{q},t)] \\
&\quad + k_B n_i(\mathbf{q})\sum_{k=1}^{N}\frac{\sigma_{ik}^2}{1+m_k/m_i}\int d\hat{\sigma}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\delta T_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\delta T_k(\mathbf{q},t)] \\
&\quad - \frac{1}{2}\sum_{k=1}^{N}\sigma_{ik}^2\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\mathbf{I}_p:\hat{\mathbf{P}}_i^0(\mathbf{q},t) \\
&\quad + \sum_{k=1}^{N}\frac{\sigma_{ik}^2}{1+m_k/m_i}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:[n_i(\mathbf{q})\hat{\mathbf{P}}_k^0(\mathbf{q},t)-n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\mathbf{P}}_i^0(\mathbf{q},t)] \\
&\quad + \sum_{k=1}^{N}\frac{\sigma_{ik}^2}{1+m_k/m_i}\int d\hat{\boldsymbol{\sigma}}\, n_i(\mathbf{q})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:[\hat{\mathbf{P}}_k^0(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\hat{\mathbf{P}}_k^0(\mathbf{q},t)] \\
&\quad - \frac{\sigma_{iw}^2}{2}\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\mathbf{I}_p:\hat{\mathbf{P}}_i^0(\mathbf{q},t) - \frac{4}{5}\sqrt{\frac{m_i\beta}{2\pi}}\sum_{k=1}^{N}\frac{\sigma_{ik}^2[m_k/m_i-1]\sqrt{m_k/m_i}}{[1+m_k/m_i]^{3/2}} \\
&\quad \times \int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot\mathbf{Q}_i(\mathbf{q},t) + \frac{4}{5}\sqrt{\frac{m_i\beta}{2\pi}}\sum_{k=1}^{N}\frac{\sigma_{ik}^2\sqrt{m_k/m_i}}{[1+m_k/m_i]^{3/2}}
\end{aligned}
$$

$$\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot[n_i(\mathbf{q})\mathbf{Q}_k(\mathbf{q},t)-n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\mathbf{Q}_i(\mathbf{q},t)]+\frac{4}{5}\sqrt{\frac{m_i\beta}{2\pi}}\,n_i(\mathbf{q})$$
$$\times\sum_{k=1}^{N}\frac{\sigma_{ik}^2\sqrt{m_k/m_i}}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot[\mathbf{Q}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{Q}_k(\mathbf{q},t)]-\frac{4}{5}\sqrt{\frac{m_i\beta}{2\pi}}\,\sigma_{iw}^2$$
$$\times\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot\mathbf{Q}_i(\mathbf{q},t), \tag{2.19}$$

wherein $\mathbf{I}_p=\mathbf{ii}\hat{\boldsymbol{\sigma}}+\mathbf{jj}\hat{\boldsymbol{\sigma}}+\mathbf{i}\hat{\boldsymbol{\sigma}}\mathbf{i}+\mathbf{j}\hat{\boldsymbol{\sigma}}\mathbf{j}$, $b_{ik}=\frac{2}{3}\pi\sigma_{ik}^3$, $i,k=1,\ldots,N$, and quantities $\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}$, $\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}$, etc., are tensors composed of the unit vector $\hat{\boldsymbol{\sigma}}$. The energy evolution of the ith component of the nanofluid mixture is described by the equation

$$\frac{3}{2}k_Bn_i(\mathbf{q})\frac{\partial}{\partial t}\delta T_i(\mathbf{q},t)+\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{Q}_i(\mathbf{q},t)+k_BT\frac{\partial}{\partial\mathbf{q}}\cdot[n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)]$$
$$=\frac{3k_BTn_i(\mathbf{q})}{2\pi}\sum_{k=1}^{N}\frac{(m_k/m_i)b_{ik}}{[1+(m_k/m_i)]\sigma_{ik}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{u}_k(\mathbf{q},t)]$$
$$+k_BTn_i(\mathbf{q})\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{1+(m_k/m_i)}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q},t)-\mathbf{u}_i(\mathbf{q},t)]+k_BTn_i(\mathbf{q})\sigma_{iw}^2$$
$$\times\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot\mathbf{u}_i(\mathbf{q},t)+2\sqrt{2}\left(\frac{48b_i\lambda_in_i(\mathbf{q})}{25\pi^2\sigma_{ii}}\right)\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}b_{ik}}{[1+m_k/m_i]^{3/2}\sigma_{ik}}$$
$$\times\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\delta T_k(\mathbf{q},t)-\delta T_i(\mathbf{q},t)]+2\sqrt{2}\left(\frac{48b_i\lambda_in_i(\mathbf{q})}{25\pi^2\sigma_{ii}}\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}b_{ik}}{[1+m_k/m_i]^{3/2}\sigma_{ik}}\right)$$
$$\times\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\delta T_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\delta T_k(\mathbf{q},t)]+\frac{4}{\sqrt{2\pi\beta m_i}}\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}$$
$$\times\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:[n_i(\mathbf{q})\hat{\mathbf{P}}_k^0(\mathbf{q},t)-n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\mathbf{P}}_i^0(\mathbf{q},t)]$$
$$+\frac{4n_i(\mathbf{q})}{\sqrt{2\pi\beta m_i}}\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:[\hat{\mathbf{P}}_k^0(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\hat{\mathbf{P}}_k^0(\mathbf{q},t)]$$
$$+\sum_{k=1}^{N}\frac{[-5+2(m_k/m_i)-5(m_k/m_i)^2]\sigma_{ik}^2}{5[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot\mathbf{Q}_i(\mathbf{q},t)$$
$$+\sum_{k=1}^{N}\frac{9(m_k/m_i)b_{ik}}{5\pi[1+m_k/m_i]^2\sigma_{ik}}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot[n_i(\mathbf{q})\mathbf{Q}_k(\mathbf{q},t)-n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\mathbf{Q}_i(\mathbf{q},t)]$$
$$+\sum_{k=1}^{N}\frac{9(m_k/m_i)b_{ik}n_i(\mathbf{q})}{5\pi[1+m_k/m_i]^2\sigma_{ik}}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot[\mathbf{Q}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{Q}_k(\mathbf{q},t)]$$
$$+\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdot\mathbf{Q}_i(\mathbf{q},t), \tag{2.20}$$

where we have introduced the notation $\lambda_i\equiv 75k_B/64\sigma_{ii}^2\sqrt{\pi\beta m_i}$. The evolution equation for the kinetic contribution $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ to the pressure tensor due to the ith component of the mixture reads

$$\beta\frac{\partial}{\partial t}\mathbf{P}_i^0(\mathbf{q},t)+2\hat{\mathbf{S}}_{inu}(\mathbf{q},t)+\tfrac{4}{5}\beta\hat{\mathbf{S}}_{iQ}(\mathbf{q},t)$$
$$=2n_i(\mathbf{q})\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{1+m_k/m_i}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q},t)-\mathbf{u}_i(\mathbf{q},t)]$$

$$+2n_i(\mathbf{q})\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{1+m_k/m_i}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\cdot[\mathbf{u}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{u}_k(\mathbf{q},t)]$$

$$+2\sigma_{iw}^2 n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\cdot\mathbf{u}_i(\mathbf{q},t)$$

$$+4k_Bn_i(\mathbf{q})\sqrt{\frac{2\beta}{\pi m_i}}\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}][\delta T_k(\mathbf{q},t)-\delta T_i(\mathbf{q},t)]$$

$$+4k_Bn_i(\mathbf{q})\sqrt{\frac{2\beta}{\pi m_i}}\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}][\delta T_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)$$

$$-\delta T_k(\mathbf{q},t)]+4\sqrt{\frac{2\beta}{\pi m_i}}\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\mathbf{u}}\boldsymbol{\sigma})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:[n_i(\mathbf{q})\hat{\mathbf{P}}_k^0(\mathbf{q},t)$$

$$-n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\mathbf{P}}_i^0(\mathbf{q},t)]+4\sqrt{\frac{2\beta}{\pi m_i}}\,n_i(\mathbf{q})\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}$$

$$\times\hat{\boldsymbol{\sigma}}:[\hat{\mathbf{P}}_k^0(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\hat{\mathbf{P}}_i^0(\mathbf{q},t)]$$

$$-6\sqrt{\frac{2\beta}{\pi m_i}}\sum_{k=1}^{N}\frac{\sqrt{m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:\hat{\mathbf{P}}_i^0(\mathbf{q},t)$$

$$-6\sqrt{\frac{2\beta}{\pi m_i}}\,\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}}n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:\hat{\mathbf{P}}_i^0(\mathbf{q},t)$$

$$+\tfrac{2}{5}\beta\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{1+m_k/m_i}\int d\hat{\boldsymbol{\sigma}}n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\cdot\mathbf{Q}_i(\mathbf{q},t)$$

$$+\tfrac{8}{5}\beta\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\cdot[n_i(\mathbf{q})\mathbf{Q}_k(\mathbf{q},t)-n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\mathbf{Q}_i(\mathbf{q},t)]$$

$$+\tfrac{8}{5}\beta n_i(\mathbf{q})\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\cdot[\mathbf{Q}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{Q}_i(\mathbf{q},t)]$$

$$+\tfrac{4}{5}\beta\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\cdot\mathbf{Q}_i(\mathbf{q},t), \tag{2.21}$$

where we introduced tensors

$$\hat{\mathbf{S}}_{inu}(\mathbf{q},t)=\frac{1}{2}\left\{\left[\frac{\partial[n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)]}{\partial\mathbf{q}}+\left(\frac{\partial[n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)]}{\partial\mathbf{q}}\right)^{\dagger}\right]-\frac{2}{3}\,\mathbf{I}\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)]\right]\right\}, \tag{2.22}$$

$$\hat{\mathbf{S}}_{iQ}(\mathbf{q},t)=\frac{1}{2}\left\{\left[\frac{\partial\mathbf{Q}_i(\mathbf{q},t)}{\partial\mathbf{q}}+\left(\frac{\partial\mathbf{Q}_i(\mathbf{q},t)}{\partial\mathbf{q}}\right)^{\dagger}\right]-\frac{2}{3}\,\mathbf{I}\left[\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{Q}_i(\mathbf{q},t)\right]\right\}, \tag{2.23}$$

and the dagger denotes tensorial transposition. At constant $n_i(\mathbf{q})$ the second-rank Cartesian tensor $\hat{\mathbf{S}}_{inu}(\mathbf{q},t)$ reduces to $n_i\hat{\mathbf{S}}_{iu}(\mathbf{q},t)$, where $\hat{\mathbf{S}}_{iu}(\mathbf{q},t)$ is the contribution to the ''shear rate'' tensor $\hat{\mathbf{S}}_u(\mathbf{q},t)$ of the system due to the ith component of the mixture. The second-rank Cartesian tensor $\hat{\mathbf{S}}_{iQ}(\mathbf{q},t)$ reflects the idea of $\hat{\mathbf{S}}_{iu}(\mathbf{q},t)$ in the case of the energy flux. The ''shear rate'' tensors (2.22) and (2.23) can also be represented in the form

$$\hat{\mathbf{S}}_{inu}(\mathbf{q},t)=\tfrac{1}{2}\left[2\mathbf{I}_4+\mathbf{I}_\delta-\frac{5}{3}\,\mathbf{II}\right]:\frac{\partial[n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},t)]}{\partial\mathbf{q}},\quad \hat{\mathbf{S}}_{iQ}(\mathbf{q},t)=\tfrac{1}{2}[2\mathbf{I}_4+\mathbf{I}_\delta-\tfrac{5}{3}\mathbf{II}]:\frac{\partial\mathbf{Q}_i(\mathbf{q},t)}{\partial\mathbf{q}},$$

which is more convenient technically. The only nonzero components of the above fourth-rank Cartesian tensor $\mathbf{I}_4$ are **iiii**, **jjjj**, and **kkkk**. The fourth-rank Cartesian tensor $\mathbf{I}_\delta$ has 21 nonzero components

iiii, **iijj**, **iikk**, **ijij**, **ijji**, **ikik**, **ikki**,

jiij, **jiji**, **jjii**, **jjjj**, **jjkk**, **jkjk**, **jkkj**,

kiik, **kiki**, **kjjk**, **kjkj**, **kkii**,**kkjj**, **kkkk**,

and the fourth-rank Cartesian tensor **II** is the tensorial product of the unit matrices. The above tensors satisfy conditions $\mathbf{I}_\delta \cdot \mathbf{I} = \mathbf{II}$ and $\mathbf{I}_4 \cdot \mathbf{I} = \mathbf{I}_4$.

The evolution of the kinetic contribution $\mathbf{Q}_i(\mathbf{q},\omega)$ to the energy flux due to the ith component of the nanofluid mixture is described by the equation

$$\frac{\partial}{\partial t}\mathbf{Q}_i(\mathbf{q},t) + \frac{1}{\beta m_i}\frac{\partial}{\partial \mathbf{q}}\cdot \hat{\mathbf{P}}_i^0(\mathbf{q},t) + \frac{5k_B}{2\beta m_i}\frac{\partial}{\partial \mathbf{q}}[n_i(\mathbf{q})\,\delta T_i(\mathbf{q},t)]$$

$$= \frac{2n_i(\mathbf{q})}{\beta\sqrt{2\pi\beta m_i}}\sum_{k=1}^{N}\frac{\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}} n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot[\mathbf{u}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{u}_k(\mathbf{q},t)]$$

$$+ \frac{2n_i(\mathbf{q})}{\beta\sqrt{2\pi\beta m_i}}\sum_{k=1}^{N}\frac{\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot[\mathbf{u}_k(\mathbf{q},t)-\mathbf{u}_i(\mathbf{q},t)]$$

$$+ \frac{2n_i(\mathbf{q})}{\beta\sqrt{2\pi\beta m_i}}\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}} n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot\mathbf{u}_i(\mathbf{q},t)$$

$$+ \frac{3k_Bn_i(\mathbf{q})}{\beta m_i}\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}} n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\delta T_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\delta T_k(\mathbf{q},t)]$$

$$+ \frac{3k_Bn_i(\mathbf{q})}{\beta m_i}\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}} n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\delta T_k(\mathbf{q},t)-\delta T_i(\mathbf{q},t)]$$

$$- \frac{5k_Bn_i(\mathbf{q})}{2\beta m_i}\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}} n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\delta T_i(\mathbf{q},t)$$

$$+ \frac{3n_i(\mathbf{q})}{\beta m_i}\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}} g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:[\hat{\mathbf{P}}_k^0(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\hat{\mathbf{P}}_k^0(\mathbf{q},t)]$$

$$+ \frac{3}{\beta m_i}\sum_{k=1}^{N}\frac{(m_k/m_i)\sigma_{ik}^2}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}} g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:[n_i(\mathbf{q})\hat{\mathbf{P}}_k^0(\mathbf{q},t)$$

$$- n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\mathbf{P}}_i^0(\mathbf{q},t)] - \frac{1}{2\beta m_i}\sum_{k=1}^{N}\sigma_{ik}^2\int d\hat{\boldsymbol{\sigma}} n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\mathbf{I}-\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}]\hat{\boldsymbol{\sigma}}:\hat{\mathbf{P}}_i^0(\mathbf{q},t)$$

$$+ \frac{2\sigma_{iw}^2}{\beta m_i}\int d\hat{\boldsymbol{\sigma}} n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\mathbf{I}-\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}]\hat{\boldsymbol{\sigma}}:\hat{\mathbf{P}}_i^0(\mathbf{q},t)$$

$$+ \frac{27\sqrt{2}n_i(\mathbf{q})}{5\sqrt{\pi\beta m_i}}\sum_{k=1}^{N}\frac{(m_k/m_i)^{3/2}\sigma_{ik}^2}{[1+m_k/m_i]^{5/2}}\int d\hat{\boldsymbol{\sigma}} g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot[\mathbf{Q}_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)-\mathbf{Q}_k(\mathbf{q},t)]$$

$$+ \frac{27\sqrt{2}}{5\sqrt{\pi\beta m_i}}\sum_{k=1}^{N}\frac{(m_k/m_i)^{3/2}\sigma_{ik}^2}{[1+m_k/m_i]^{5/2}}\int d\hat{\boldsymbol{\sigma}} g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot[n_i(\mathbf{q})\mathbf{Q}_k(\mathbf{q},t)-n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\mathbf{Q}_k(\mathbf{q},t)]$$

$$
-\frac{1}{5}\sqrt{\frac{2}{\pi\beta m_i}}\sum_{k=1}^{N}\sigma_{ik}^2\int d\hat{\boldsymbol{\sigma}}n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})
\times\left\{\frac{4}{[1+m_k/m_i]^{3/2}}\mathbf{I}+\frac{\sqrt{m_k/m_i}}{[1+m_k/m_i]^{5/2}}\left[18-23\frac{m_k}{m_i}+13\left(\frac{m_k}{m_i}\right)^2\right]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\right\}\cdot\mathbf{Q}_i(\mathbf{q},t)
+\frac{13}{5}\sqrt{\frac{2}{\pi\beta m_i}}\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}}n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\cdot\mathbf{Q}_i(\mathbf{q},t). \quad (2.24)
$$

The coupled integro-differential equations (2.18)–(2.21) and (2.24) form a closed system of equations that can be reduced further to obtain a ''quasihydrodynamic'' (or ''quasimacroscopic'') description of evolution of the nanofluid mixture (Sec. III). Also, this system itself can be used to obtain a detailed description of the quasihydrodynamic velocity and temperature fields. In this way, Eqs. (2.18)–(2.21) and (2.24) can be solved numerically, which may be easier than solving the resulting quasihydrodynamic equations. This can be seen from the structure of the right-hand sides of these equations, which do not contain any spatial derivatives of the quasicontinuum variables. The coefficients coming with the quasicontinuum variables can be calculated numerically, provided the dimensionless data on the equilibrium values of the number densities and contact values of the pair correlation functions are known from theory, equilibrium NEMD simulations, or experiment. Such calculations would embrace classes of nanofluid mixtures (say, Lennard-Jones ones) for each given geometry of the confinement. However, some extra care is needed to calculate integrals of combinations of the quasicontinuum variables with the equilibrium structure factors over the surface of the unit sphere $\int d\hat{\boldsymbol{\sigma}}$. Equations (2.18)–(2.21) and (2.24) generalize to inhomogeneous fluid mixtures Eqs. (A1)–(A5) of Ref. [2] derived for a pure inhomogeneous fluid.

III. LINEARIZED NAVIER-STOKES EQUATIONS FOR NANOFLUID MIXTURES

A. Kinetic contributions to the pressure tensor and energy flux

The right-hand sides of the integro-differential equations (2.18)–(2.21) and (2.24) include deviations in nonequilibrium values of the quasicontinuum variables from equilibrium, assigned both to spatial points $\mathbf{q}$ and to their σ_{ik} neighborhoods. It has already been noted (see also [11]) that if a nanofluid mixture is in a nonequilibrium state that is not far from equilibrium, such deviations are small for real confined fluid systems, even at high pressures and temperatures. Thus, in the σ_{ik} vicinity of $\mathbf{q}$ the quasicontinuum variables of Eqs. (2.18)–(2.21) and (2.24) can be expanded in a Taylor series

$$
\mathbf{A}_i(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}},t)=\mathbf{A}_i(\mathbf{q},t)-\sigma_{ik}\hat{\boldsymbol{\sigma}}\cdot\frac{\partial}{\partial\mathbf{q}}\mathbf{A}_i(\mathbf{q},t)
+\frac{1}{2}\sigma_{ik}^2\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}:\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}\mathbf{A}_i(\mathbf{q},t)+\cdots,
$$

where the $\mathbf{A}_i(\mathbf{q},t)$ are defined by Eqs. (2.15a)–(2.15c). For example, by their definitions, the variables $\mathbf{A}_i(\mathbf{q},t)$ *do not include* the nonequilibrium number densities $n_i(\mathbf{q},t)$ or temperatures $T_i(\mathbf{q},t)$, nor the differences between these quantities and their equilibrium values specific to uniform fluids; instead, they include the differences $\delta n_i(\mathbf{q},t)$ and $\delta T_i(\mathbf{q},t)$ in these quantities between the nonequilibrium and equilibrium systems, both of which are inhomogeneous. Such differences are not large, even near walls in the case of confined systems, because the departure from equilibrium is assumed to be small.

Using the above Taylor expansions for the quasicontinuum variables (2.15a)–(2.15c) in Eqs. (2.18)–(2.21) and (2.24), one can recover the differential form of these equations. Further Fourier transformation of those differential equations with respect to the time variable t supplies differential equations for Fourier transforms of the quasicontinuum variables (2.15a)–(2.15c). The next step in reduction of the differential equations for the Fourier transforms of the quasicontinuum variables to the linearized Navier-Stokes form includes recovering the kinetic contributions $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ and $\mathbf{Q}_i(\mathbf{q},\omega)$ from their corresponding differential equations (here ω stands for the frequency, which substitutes for the time variable t in the Fourier-transformed equations) and substitution of the values so obtained into the differential equations for the Fourier transforms $\delta n_i(\mathbf{q},\omega)$, $\mathbf{u}_i(\mathbf{q},\omega)$, and $\delta T_i(\mathbf{q},\omega)$ of the rest of the quasicontinuum variables. For this purpose the differential equations for $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ and $\mathbf{Q}_i(\mathbf{q},\omega)$ should be simplified. Such a simplification may be performed upon consideration that the deviations of the nonequilibrium temperatures and quasihydrodynamic velocities of the mixture components from their equilibrium values do not vary appreciably in mean free paths (which are proportional to the σ_{ik}), because the nanofluid mixture is not far from equilibrium. This validates the neglect of terms proportional to the second spatial gradients of $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ and

$\mathbf{Q}_i(\mathbf{q},\omega)$ and terms with $\hat{\mathbf{S}}_{iQ}(\mathbf{q},\omega)$ in the differential equations for these kinetic contributions, and indicates the smallness of the first spatial gradients of $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ and $\mathbf{Q}_i(\mathbf{q},\omega)$. Moreover, since $|\sigma_x|$, $|\sigma_y|$, and $|\sigma_z|\leqslant 1$, the conditions (3.1) and (3.2) of Ref. [2] hold for any integrable, positively defined function $f(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})$:

$$\int d\hat{\sigma} f(\mathbf{q}-\sigma_{ik}\hat{\sigma})\underbrace{\sigma_\alpha\cdots\sigma_\gamma}_{m}\leqslant\int d\hat{\sigma} f(\mathbf{q}-\sigma_{ik}\hat{\sigma})\underbrace{\sigma_\alpha\cdots\sigma_\beta}_{m-1},\quad m=1,3,\ldots$$

$$\int d\hat{\sigma} f(\mathbf{q}-\sigma_{ik}\hat{\sigma})\sigma_\alpha^2>\int d\hat{\sigma} f(\mathbf{q}-\sigma_{ik}\hat{\sigma})\sigma_\alpha^2\sigma_\gamma^2>\cdots>\int d\hat{\sigma} f(q-\sigma_{ik}\hat{\sigma})\underbrace{\sigma_\beta\cdots\sigma_\rho}_{m},\quad m=3,4,\ldots, \tag{3.1}$$

where $\alpha,\beta,\gamma,\rho=x,y,z$ and m signifies a number of $\hat{\sigma}$ components $\sigma_\alpha\cdots\sigma_\gamma$. The first spatial gradients of $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ and $\mathbf{Q}_i(\mathbf{q},\omega)$ (which are small themselves) come into the differential equations for $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ and $\mathbf{Q}_i(\mathbf{q},\omega)$ with multipliers that are proportional to the integrals of odd sets of $\hat{\boldsymbol{\sigma}}$ over the domain of $\hat{\boldsymbol{\sigma}}$. Using the approximation

$$\int d\hat{\boldsymbol{\sigma}}\, f(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}\cong\frac{1}{4\pi}\int d\hat{\boldsymbol{\sigma}}\, f(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\int d\hat{\boldsymbol{\sigma}}\,\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}} \tag{3.2}$$

and the first condition of Eqs. (3.1), one can prove that the multipliers of the first spatial gradients of $\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)$ and $\mathbf{Q}_i(\mathbf{q},\omega)$ in the differential equations for these kinetic contributions tend to zero, so such terms should be neglected. The remaining coupling terms in these equations can be estimated upon usage of the above conditions (3.1) and the approximation (3.2). The solutions of the differential equations for the Fourier transforms of the kinetic contributions into the pressure tensor and the energy flux due to the ith component of the mixture are

$$\begin{aligned}\hat{\mathbf{P}}_i^0(\mathbf{q},\omega)=&-2\sum_{k=1}^N\hat{\boldsymbol{\eta}}_{ik}^{(2)}(\mathbf{q},\omega):\frac{\partial\mathbf{u}_k(\mathbf{q},\omega)}{\partial\mathbf{q}}\\&-8\pi\eta_i\tau_{i\eta}^*(\mathbf{q},\omega)\hat{\mathbf{S}}_{u\Delta n}^{(i)}(\mathbf{q},\omega)\\&+4\pi\eta_i\tau_{i\eta}^*(\mathbf{q},\omega)n_i(\mathbf{q})\sum_{k=1}^N\sigma_{ik}^4\\&\times\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(i)}(\mathbf{q},\omega)\cdot:\frac{\partial^2\mathbf{u}_k(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}\\&+8\pi\eta_i\tau_{i\eta}^*(\mathbf{q},\omega)n_i(\mathbf{q},\omega)\\&\times\sum_{k=1}^N\sigma_{ik}^2\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(i)}(\mathbf{q},\omega)\cdot\mathbf{u}_k(\mathbf{q},\omega)\\&-\tfrac{32}{15}\sqrt{\pi\beta m_i}\lambda_i\tau_{i\eta}^*(\mathbf{q},\omega)n_i(\mathbf{q})\\&\times\sum_{k=1}^N\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(i)}(\mathbf{q},\omega)\cdot\frac{\partial\delta T_k(\mathbf{q},\omega)}{\partial\mathbf{q}}\\&+\tfrac{16}{15}\sqrt{\pi\beta m_i}\lambda_i\tau_{i\eta}^*(\mathbf{q},\omega)n_i(\mathbf{q})\sum_{k=1}^N\\&\times\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(i)}(\mathbf{q},\omega):\frac{\partial^2\delta T_k(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}\\&+2\pi\sqrt{\pi\beta m_i}\lambda_i\tau_{i\eta}^*(\mathbf{q},\omega)\tau_{i\lambda}^*(\mathbf{q},\omega)n_i(\mathbf{q})\\&\times\sum_{k=1}^N\hat{\boldsymbol{\mathcal{P}}}_{Tk}^{(i)}(\mathbf{q},\omega)\delta T_k(\mathbf{q},\omega),\end{aligned} \tag{3.3}$$

$$\begin{aligned}\mathbf{Q}_i(\mathbf{q},\omega)=&-\sum_{k=1}^N\hat{\boldsymbol{\lambda}}_{ik}^{(2)}(\mathbf{q},\omega)\cdot\frac{\partial\delta T_k(\mathbf{q},\omega)}{\partial\mathbf{q}}\\&-4\pi\lambda_i\tau_{i\lambda}^*(\mathbf{q},\omega)\sum_{k=1}^N\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(i)}(\mathbf{q},\omega)\delta T_k(\mathbf{q},\omega)\\&+\tfrac{12}{5}\pi\lambda_i\tau_{i\lambda}^*(\mathbf{q},\omega)n_i(\mathbf{q})\\&\times\sum_{k=1}^N\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(i)}(\mathbf{q},\omega):\frac{\partial^2\delta T_k(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}\\&-3\sqrt{\frac{\pi}{\beta m_i}}\eta_i\tau_{i\lambda}^*(\mathbf{q},\omega)\sum_{k=1}^N\\&\times\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(i)}(\mathbf{q},\omega):\frac{\partial\mathbf{u}_k(\mathbf{q},\omega)}{\partial\mathbf{q}}\\&+3\sqrt{\frac{\pi}{\beta m_i}}\eta_i\tau_{i\lambda}^*(\mathbf{q},\omega)n_i(\mathbf{q})\\&\times\sum_{k=1}^N\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(i)}(\mathbf{q},\omega)\cdot:\frac{\partial^2\mathbf{u}_k(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}\\&+6\sqrt{\frac{2\pi}{\beta m_i}}\sigma_{iw}^2\eta_i\tau_{i\lambda}^*(\mathbf{q},\omega)n_i(\mathbf{q})\\&\times\sum_{k=1}^N\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(i)}(\mathbf{q},\omega)\cdot\mathbf{u}_k(\mathbf{q},\omega)\\&-\tfrac{15}{4}\pi\sqrt{\frac{\pi}{\beta m_i}}\eta_i\tau_{i\lambda}^*(\mathbf{q},\omega)\tau_{i\eta}^*(\mathbf{q},\omega)\\&\times\hat{\boldsymbol{\mathcal{C}}}_P^{(i)}(\mathbf{q}):\hat{\mathbf{S}}_{u\nabla n}^{(i)}(\mathbf{q},\omega).\end{aligned} \tag{3.4}$$

In the above equations the quantities

$$\hat{\boldsymbol{\mathcal{P}}}^{(i)}(\mathbf{q},\omega),\hat{\boldsymbol{\mathcal{Q}}}^{(i)}(\mathbf{q},\omega),\text{ and }\hat{\boldsymbol{\mathcal{C}}}_P^{(i)}(\mathbf{q},\omega)$$

are coefficients that depend upon various smoothed (i.e., integrated over the domain of $\hat{\sigma}$) values of *the equilibrium structure functions* $n_i(\mathbf{q})$ and $g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})$ of the nanofluid mixture; the corresponding explicit expressions for these quantities are given in Appendix A. The notations $\cdot$, :, and $\cdot$: refer to tensorial convolutions; the tensor $\hat{\mathbf{S}}_{u\nabla n}^{(i)}(\mathbf{q},\omega)$ is defined as

$$\hat{\mathbf{S}}_{u\nabla n}^{(i)}(\mathbf{q})=\tfrac{1}{2}[2\mathbf{I}_4+\mathbf{I}_\delta-\tfrac{5}{3}\mathbf{II}]:\mathbf{u}_i(\mathbf{q},\omega)\frac{\partial n_i(\mathbf{q})}{\partial\mathbf{q}}.$$

The contributions to the shear viscosity tensor due to the kinetic contribution of the ith component of the mixture to the pressure tensor are

$$\hat{\boldsymbol{\eta}}_{ik}^{(2)}(\mathbf{q},\omega)=4\pi\eta_i n_i(\mathbf{q})\tau_{i\eta}^{*}(\mathbf{q},\omega)\Big\{\delta_{ik}\tfrac{1}{2}[2\mathbf{I}_4+\mathbf{I}_\delta-\tfrac{5}{3}\mathbf{II}] + \frac{3b_{ik}m_k/m_i}{2\pi[1+m_k/m_i]}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}} + \frac{3b_{ik}\sqrt{2}}{8\pi[1+m_k/m_i]^{3/2}}\tau_{i\lambda}^{*}(\mathbf{q},\omega) \times\hat{\boldsymbol{\mathcal{C}}}_Q^{(i)}(\mathbf{q},\omega)\cdot\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}}) \times g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\hat{\sigma}\Big\}. \tag{3.5}$$

The explicit expressions for the quantities $\hat{\boldsymbol{\mathcal{C}}}_Q^{(i)}(\mathbf{q},\omega)$ are listed in Appendix A.

The contributions to the thermal conductivity tensor due to the kinetic contribution of the ith component of the mixture into the energy flux read

$$\hat{\boldsymbol{\lambda}}_{ik}^{(2)}(\mathbf{q},\omega)=4\pi\lambda_i\tau_{i\lambda}^{*}(\mathbf{q},\omega)n_i(\mathbf{q})\Big\{\delta_{ik}\mathbf{I}+\frac{9b_{ik}m_k/m_i}{5\pi[1+m_k/m_i]^2} \times\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}} + \frac{1}{4}\tau_{ik}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{C}}}_P^{(i)}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(i)}(\mathbf{q},\omega)\Big\}. \tag{3.6}$$

The relaxation times of molecular ''friction'' processes (or the viscorelaxation times) are given by

$$\tau_{i\eta}^{*}(\mathbf{q},\omega)=\frac{\tau_{i\eta}(\mathbf{q})}{[1-i\omega\overline{\tau_{i\eta}(\mathbf{q})}]}, \tag{3.7}$$

where in the denominator $i=\sqrt{-1}$ and other notations include

$$\tau_{i\eta}^{-1}(\mathbf{q})\equiv\sum_{k=1}^{N}\frac{2\sigma_{ik}^2\sqrt{m_k/m_i}}{\sqrt{2}\sigma_{ii}^2\sqrt{1+m_k/m_i}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})+\frac{1}{3}\int d\hat{\boldsymbol{\sigma}}\, g_{ii}(\mathbf{q},\mathbf{q}-\sigma_{ii}\hat{\boldsymbol{\sigma}})[n_i(\mathbf{q}-\sigma_{ii}\hat{\boldsymbol{\sigma}})-n_i(\mathbf{q})]+\frac{\sqrt{2}\sigma_{iw}^2}{\sigma_{ii}^2}\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}});$$

$$[\tau_{i\eta}]_0^{-1}\equiv\frac{16\sigma_{ii}^2}{5}\sqrt{\frac{\pi}{\beta m_i}},\quad \eta_i\equiv\frac{5}{16\sigma_{ii}^2}\sqrt{\frac{m_i}{\pi\beta}},$$

$$\overline{\tau_{i\eta}(\mathbf{q})}\equiv\frac{5\sqrt{\pi\beta m_i}}{4\sigma_{ii}^2}\tau_{i\eta}(\mathbf{q}).$$

We note that $[\tau_{i\eta}]_0^{-1}\eta_i=1/\beta$. Thermal processes are characterized by the relaxation times

$$\tau_{i\lambda}^{*}(\mathbf{q},\omega)=\frac{\tau_{i\lambda}(\mathbf{q})}{1-i\omega\overline{\tau_{i\lambda}(\mathbf{q})}}, \tag{3.8}$$

where

$$\tau_{i\lambda}^{-1}(\mathbf{q})\equiv\sum_{k=1}^{N}\frac{3\sqrt{2}}{8}\left(\frac{\sigma_{ik}}{\sigma_{ii}}\right)^2\Bigg\{\frac{4}{[1+m_k/m_i]^{3/2}}+\frac{\sqrt{m_k/m_i}}{3[1+m_k/m_i]^{5/2}}\left[18-23\frac{m_k}{m_i}+13\left(\frac{m_k}{m_i}\right)^2\right]\Bigg\}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})+\frac{27}{32}\int d\hat{\boldsymbol{\sigma}}\, g_{ii}(\mathbf{q},\mathbf{q}-\sigma_{ii}\hat{\boldsymbol{\sigma}})[n_i(\mathbf{q})-n_i(\mathbf{q}-\sigma_{ii}\hat{\boldsymbol{\sigma}})]+\frac{13\sqrt{2}}{8}\left(\frac{\sigma_{iw}}{\sigma_{ii}}\right)^2\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}});$$

$$[\tau_{i\lambda}]_0^{-1}\equiv\frac{32\sigma_{ii}^2}{15}\sqrt{\frac{\pi}{m_i\beta}},\quad \lambda_i=\frac{75k_B}{64\sigma_{ii}^2\sqrt{\pi\beta m_i}},$$

$$\overline{\tau_{i\lambda}(\mathbf{q})}\equiv\frac{15\sqrt{\pi\beta m_i}}{8\sigma_{ii}^2}\tau_{i\lambda}(\mathbf{q}),$$

and $[\tau_{i\lambda}]_0^{-1}\lambda_i=5k_B/2\beta_i m_i$.

Equations (3.3) and (3.4) generalize to inhomogeneous fluid mixtures expressions derived in Refs. [2] and [4] for pure inhomogeneous fluids. They also contain terms proportional to the second spatial gradients of the deviations in nonequilibrium values of the quasihydrodynamic velocities and temperatures of the mixture components from equilibrium, which have been neglected in the corresponding expressions for pure inhomogeneous fluids.

Substituting the expressions (3.3) and (3.4) into the differential equations for the Fourier transforms $\delta n_i(\mathbf{q},\omega)$, $\delta T_i(\mathbf{q},\omega)$, and $\mathbf{u}_i(\mathbf{q},\omega)$, one can recover for these Fourier transforms a system of differential equations in partial derivatives that is a generalization of the conventional Navier-Stokes system of equations valid for uniform fluid mixtures (see, e.g., Ref. [5]) to the nanofluid mixtures. Also, this system generalizes that of Ref. [2] derived for pure inhomogeneous fluids.

B. Continuity equations

Fourier transformation of the continuity equations for the components of the nanofluid mixture leads to the equations

$$-i\omega\delta n_i(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\mathcal{N}}_i(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\mathcal{N}}_R^{(ik)}(\mathbf{q})\cdot\mathbf{u}_k(\mathbf{q},\omega), \tag{3.9}$$

where the flux $\boldsymbol{\mathcal{N}}_i(\mathbf{q},\omega)$ of the ith species particle number and the Cartesian three-vectors $\boldsymbol{\mathcal{N}}_R^{(ik)}(\mathbf{q})$, which are included in ‘‘thermodynamic sources’’ on the right-hand side of Eq. (3.9), are given by the expressions

$$\boldsymbol{\mathcal{N}}_i(\mathbf{q},\omega)=\sum_{k=1}^{N}\left[\boldsymbol{\mathcal{N}}_{i1}^{k}(\mathbf{q})\cdot\mathbf{u}_k(\mathbf{q},\omega)-\frac{1}{2}\,\sigma_{ik}^4\times\boldsymbol{\Phi}_{13}^{(ik)}(\mathbf{q})\colon\frac{\partial\mathbf{u}_k(\mathbf{q},\omega)}{\partial\mathbf{q}}\right],$$

$$\boldsymbol{\mathcal{N}}_{i1}^{k}(\mathbf{q})=\delta_{ik}n_i(q)\mathbf{I}+\sigma_{ik}^3\boldsymbol{\Phi}_{12}^{(ik)}(\mathbf{q})+\frac{1}{2}\,\sigma_{ik}^4\,\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Phi}_{13}^{(ik)}(\mathbf{q}),$$

$$\boldsymbol{\mathcal{N}}_{R}^{(ik)}(\mathbf{q})=-\delta_{ik}\sum_{l=1}^{N}\sigma_{il}^2\boldsymbol{\Phi}_{01}^{(il)}(\mathbf{q})+\sigma_{ik}^2\boldsymbol{\Phi}_{01}^{(ik)}(\mathbf{q})+\sigma_{ik}^3\,\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Phi}_{12}^{(ik)}(\mathbf{q})+\frac{1}{2}\,\sigma_{ik}^4\,\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}\colon\boldsymbol{\Phi}_{13}^{(ik)}(\mathbf{q})+\delta_{ik}\sigma_{iw}^2\boldsymbol{\Phi}_{01}^{(iw)}(\mathbf{q}). \tag{3.10}$$

In the above expressions the Cartesian tensors $\boldsymbol{\Phi}^{(ik)}(\mathbf{q})$ have resulted from smoothing of the values of equilibrium structure factors of the nanofluid mixture (i.e., integration of the structure factors over the domain of $\hat{\boldsymbol{\sigma}}$) and are inherited from the integro-differential equations (2.18)–(2.21) and (2.24). The explicit expressions for these quantities in terms of the structure factors of the nanofluid mixture are given in Appendix B.

C. Momentum conservation equations and tensorial viscosities

Conservation of the momentum specific to the ith component of the nanofluid mixture is described by the equation

$$-i\omega m_in_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}_i(\mathbf{q},\omega)=\sum_{k=1}^{N}\{\boldsymbol{\mathcal{R}}_u^{(ik)}(\mathbf{q},\omega)\cdot\mathbf{u}_k(\mathbf{q},\omega)+\boldsymbol{\mathcal{R}}_S^{(ik)}(\mathbf{q},\omega)\colon\hat{\mathbf{S}}_{u\nabla n}^{(k)}(\mathbf{q},\omega)+\boldsymbol{\mathcal{R}}_T^{(ik)}(\mathbf{q},\omega)\,\delta T_k(\mathbf{q},\omega)\}, \tag{3.11}$$

where the momentum fluxes $\boldsymbol{\Pi}_i(\mathbf{q},\omega)$ are defined as

$$\boldsymbol{\Pi}_i(\mathbf{q},\omega)\equiv\sum_{\alpha=1}^{9}\boldsymbol{\Pi}_{i\alpha}(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i1}(\mathbf{q},\omega)=\frac{1}{\beta}\,\mathbf{I}\left\{\delta n_i(\mathbf{q},\omega)-n_i(\mathbf{q},\omega)\sum_{k=1}^{N}\int d\mathbf{q}'\,C_{ik}(\mathbf{q},\mathbf{q}')\,\delta n_k(\mathbf{q}',\omega)-n_i(\mathbf{q})\sum_{k=1}^{N}\int d\mathbf{q}'\left[1-\sum_{l=1}^{N}\int d\mathbf{q}''n_l(\mathbf{q}'')\times C_{lk}(\mathbf{q}'',\mathbf{q}')\right]\delta n_k(\mathbf{q}',\omega)\right\},$$

$$\boldsymbol{\Pi}_{i2}(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\Pi}_{i2}^{(k)}(\mathbf{q},\omega)\,\delta T_k(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i3}(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\Pi}_{i3}^{(k)}(\mathbf{q},\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\,\delta T_k(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i4}(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\Pi}_{i4}^{(k)}(\mathbf{q},\omega)\colon\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}\,\delta T_k(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i5}(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\Pi}_{i5}^{(k)}(\mathbf{q},\omega)\cdot\mathbf{u}_k(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i6}(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\Pi}_{i6}^{(k)}(\mathbf{q},\omega)\colon\hat{\mathbf{S}}_{u\nabla n}^{(k)}(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i7}(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\Pi}_{i7}^{(k)}(\mathbf{q},\omega)\cdot\colon\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}\,\mathbf{u}_k(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i8}(\mathbf{q},\omega)=-\sum_{k=1}^{N}\boldsymbol{\Pi}_{i8}^{(k)}(\mathbf{q},\omega)\colon\frac{\partial}{\partial\mathbf{q}}\,\mathbf{u}_k(\mathbf{q},\omega),$$

$$\boldsymbol{\Pi}_{i9}(\mathbf{q},\omega)=\sum_{k=1}^{N}\boldsymbol{\Pi}_{i9}^{(k)}(\mathbf{q},\omega)\cdot\colon\frac{\partial}{\partial\mathbf{q}}\,\hat{\mathbf{S}}_{u\nabla n}^{(k)}(\mathbf{q},\omega). \tag{3.12}$$

The Cartesian tensors $\boldsymbol{\Pi}_{in}^{(k)}(\mathbf{q},\omega)$, $n=1,\ldots,9$, from Eq. (3.12) and the tensorial coefficients $\boldsymbol{\mathcal{R}}^{(ik)}(\mathbf{q},\omega)$ on the right-hand side of Eq. (3.11) are complicated combinations of tensorial quantities involving various tensorial functions of the smoothed structure factors of the mixture. Regarding Eq. (3.11), our major concern is the Cartesian tensors of the diffusion coefficients and viscosities, which are defined below in terms of the tensors $\boldsymbol{\Pi}_{i1}^{(k)}(\mathbf{q},\omega)$, $\boldsymbol{\Pi}_{i8}^{(k)}(\mathbf{q},\omega)$, and $\boldsymbol{\Pi}_{i7}^{(k)}(\mathbf{q},\omega)$, respectively. Thus we list these quantities here and leave the expressions for the remaining tensors $\boldsymbol{\Pi}_{in}^{(k)}(\mathbf{q},\omega)$, $n=2,\ldots,6,9$, and the tensors $\boldsymbol{\mathcal{R}}^{(ik)}(\mathbf{q},\omega)$ to Appendix C,

$$\boldsymbol{\Pi}_{i7}^{(k)}(\mathbf{q},\omega)=\sum_{l=1}^{N}\Bigg\{4\pi\eta_l\sigma_{lk}^4n_l(\mathbf{q})\,\tau_{l\eta}^{*}(\mathbf{q},\omega)\left[\delta_{ik}\hat{\mathbf{1}}_4+\frac{\sigma_{il}^3}{1+m_l/m_i}\,\mathbf{F}_4^{(il)}(\mathbf{q})\right]\colon\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)+\frac{\sigma_{il}^4}{1+m_l/m_i}\,\mathbf{F}_{05}^{(il)}(\mathbf{q})\colon\odot\,\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega)\colon\hat{\mathbf{1}}_6-\frac{2\pi\sigma_{il}^4\sigma_{lk}^4}{1+m_l/m_i}\,\mathbf{F}_{05}^{(il)}(\mathbf{q})\colon\odot\,\frac{\partial}{\partial\mathbf{q}}\times[n_l(\mathbf{q})\,\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]+\frac{6\sqrt{2m_k/m_l}\sigma_{il}^3\eta_l}{5[1+m_l/m_i]^{3/2}}\,n_l(\mathbf{q})\,\tau_{l\lambda}^{*}(\mathbf{q},\omega)\times\boldsymbol{\Xi}^{(il)}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)+\frac{3\sqrt{2m_k/m_l}\sigma_{il}^4\eta_l}{5[1+m_l/m_i]^{3/2}}$$

$$\times\tau^*_{l\lambda}(\mathbf{q},\omega)\mathbf{\Xi}^{(il)}_0(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{Q}}}^{(l)}_{\nabla uk}(\mathbf{q},\omega):\hat{\mathbf{1}}_6 - \frac{3\sqrt{2m_k/m_l}\sigma^4_{il}\eta_l}{5[1+m_l/m_i]^{3/2}}\mathbf{\Xi}^{(il)}_0(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}} \times[n_l(\mathbf{q})\tau^*_{l\lambda}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}^{(l)}_{\Delta uk}(\mathbf{q},\omega)]\Bigg\}, \quad (3.13)$$

$$\mathbf{\Pi}^{(k)}_{i8}(\mathbf{q},\omega)=\sum_l\Bigg\{2\left[\delta_{il}\hat{\mathbf{1}}_4+\frac{\sigma^3_{il}}{1+m_l/m_i}\mathbf{F}^{(il)}_4(\mathbf{q})\right]:\hat{\boldsymbol{\eta}}^{(2)}_{lk}(\mathbf{q},\omega) + \sqrt{\frac{2m_k}{\pi\beta}}\frac{\sigma^4_{ik}}{\sqrt{1+m_k/m_i}}\delta_{kl}\mathbf{\Psi}^{(ik)}_0(\mathbf{q}) - \frac{\sigma^4_{il}}{1+m_l/m_i}\mathbf{F}^{(il)}_{05}(\mathbf{q}):\odot\frac{\partial}{\partial\mathbf{q}}\hat{\boldsymbol{\eta}}^{(2)}_{lk}(\mathbf{q},\omega) + \frac{4\pi\sigma^2_{lk}\sigma^4_{il}}{1+m_l/m_i}\eta_l n_l(\mathbf{q})\tau^*_{l\eta}(\mathbf{q},\omega)\mathbf{F}^{(il)}_{05}(\mathbf{q}):\odot \times\hat{\boldsymbol{\mathcal{P}}}^{(l)}_{uk}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4+\frac{6\sqrt{2}\sigma^3_{il}}{5[1+m_l/m_i]^{3/2}}\eta_l\tau^*_{l\lambda}(\mathbf{q},\omega) \times\mathbf{\Xi}^{(il)}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}^{(l)}_{\nabla uk}(\mathbf{q},\omega)-\frac{3\sqrt{2}\sigma^4_{il}}{5[1+m_l/m_i]^{3/2}}\eta_l \times\mathbf{\Xi}^{(il)}_0(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}}[\tau^*_{l\lambda}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}^{(l)}_{\nabla uk}(\mathbf{q},\omega)] + \frac{12\sigma^2_{lw}\sigma^4_{il}}{5[1+m_l/m_i]^{3/2}}\eta_l n_l(\mathbf{q})\tau^*_{l\lambda}(\mathbf{q},\omega) \times\mathbf{\Xi}^{(il)}_0(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{Q}}}^{(l)}_{uk}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4 + \frac{4\pi\sigma^2_{il}\sigma^4_{lk}}{1+m_l/m_k}\eta_l[\tau^*_{l\eta}(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}): \times\hat{\boldsymbol{\mathcal{P}}}^{(l)}_{\Delta uk}(\mathbf{q},\omega)]_1 - 2\pi\sigma^2_{iw}\sigma^4_{ik}\eta_i\Big[n_i(\mathbf{q})\tau^*_{i\eta}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}^0_{ii}(\mathbf{q},\omega): \times\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\Delta uk}(\mathbf{q},\omega)]_1\delta_{kl} + \frac{3}{5}\sqrt{\frac{m_i}{m_l}}\sigma^2_{il}\eta_l[n_l(\mathbf{q})\tau^*_{l\lambda}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot \times\hat{\boldsymbol{\mathcal{Q}}}^{(l)}_{\nabla uk}(\mathbf{q},\omega)]_1-\frac{3}{5}\sigma^2_{iw}\eta_i[n_i(\mathbf{q})\tau^*_{i\lambda}(\mathbf{q},\omega) \times\hat{\boldsymbol{\mathcal{B}}}^0_{ii}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}^{(k)}_{\nabla uk}(\mathbf{q},\omega)]_1\delta_{kl}\Bigg\}, \quad (3.14)$$

$$\mathbf{\Pi}^{(k)}_{i9}(\mathbf{q},\omega)=\frac{4\pi\sigma^4_{ik}\eta_k}{1+m_k/m_i}\tau^*_{k\eta}(\mathbf{q},\omega)\mathbf{F}^{(ik)}_{05}(\mathbf{q}) + \frac{3\pi\sigma^4_{ik}\eta_k}{2\sqrt{2}[1+m_k/m_i]^{3/2}}\tau^*_{k\eta}(\mathbf{q},\omega)\tau^*_{k\lambda}(\mathbf{q},\omega) \times\mathbf{\Xi}^{(ik)}_0(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{C}}}^{(k)}_P(\mathbf{q}):\hat{\mathbf{1}}_6. \quad (3.14')$$

In terms of ith contributions to the shear rate and vorticity tensors [2,4], the quasihydrodynamic velocity of the ith mixture component can be written as

$$\frac{\partial\mathbf{u}_i(\mathbf{q},\omega)}{\partial\mathbf{q}}=\hat{\mathbf{S}}_{iu}(\mathbf{q},\omega)+\hat{\mathbf{W}}_i(\mathbf{q},\omega)+\frac{1}{3}\mathbf{I}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}_i(\mathbf{q},\omega), \quad (3.15)$$

where the ith contribution to the shear rate tensor is

$$\hat{\mathbf{S}}_{iu}(\mathbf{q},\omega)=\frac{1}{2}\left[\left(\frac{\partial\mathbf{u}_i(\mathbf{q},\omega)}{\partial\mathbf{q}}\right)+\left(\frac{\partial\mathbf{u}_i(\mathbf{q},\omega)}{\partial\mathbf{q}}\right)^{\dagger}\right] -\frac{1}{3}\mathbf{I}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}_i(\mathbf{q},\omega) \quad (3.16)$$

and the corresponding contribution to the vorticity tensor reads

$$\mathbf{W}_{iu}(\mathbf{q},\omega)=\frac{1}{2}\left[\left(\frac{\partial\mathbf{u}_i(\mathbf{q},\omega)}{\partial\mathbf{q}}\right)-\left(\frac{\partial\mathbf{u}_i(\mathbf{q},\omega)}{\partial\mathbf{q}}\right)^{\dagger}\right]. \quad (3.17)$$

Expressing the first and second spatial gradients of $\mathbf{u}_i(\mathbf{q},\omega)$ and the tensor $\hat{\mathbf{S}}^{(k)}_{u\nabla n}(\mathbf{q},\omega)$ in terms of the above shear rate and vorticity tensors, one can rewrite the momentum conservation equation (3.11) for the ith mixture component in the form

$$-i\omega m_i n_i(\mathbf{q})\mathbf{u}_i(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\sum_{\alpha=1}^{6}\mathbf{\Pi}_{i\alpha}(\mathbf{q},\omega)+\mathbf{\Pi}''_i(\mathbf{q},\omega) =\sum_{k=1}^{N}\{\boldsymbol{\mathcal{R}}^{(ik)}_u(\mathbf{q},\omega)\cdot\mathbf{u}_k(\mathbf{q},\omega)+\boldsymbol{\mathcal{R}}^{(ik)}_S(\mathbf{q},\omega):\hat{\mathbf{S}}^{(k)}_{u\nabla n}(\mathbf{q},\omega) +\boldsymbol{\mathcal{R}}^{(ik)}_T(\mathbf{q},\omega)\delta T_k(\mathbf{q},\omega)\}, \quad (3.18)$$

where the vector $\mathbf{\Pi}''_i(\mathbf{q},\omega)$ is

$$\mathbf{\Pi}''_i(\mathbf{q},\omega)=-2\sum_{k=1}^{N}\hat{\boldsymbol{\eta}}_{ik}(\mathbf{q},\omega):\cdot\frac{\partial}{\partial\mathbf{q}}\hat{\mathbf{S}}_{ku}(\mathbf{q},\omega) -\sum_{k=1}^{N}\hat{\boldsymbol{\mathcal{W}}}_{ik}(\mathbf{q},\omega):\cdot\frac{\partial}{\partial\mathbf{q}}\mathbf{W}_{ku}(\mathbf{q},\omega) -\sum_{k=1}^{N}\hat{\boldsymbol{\mathcal{K}}}_{ik}(\mathbf{q},\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}_k(\mathbf{q},\omega)\right) +\sum_{k=1}^{N}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}^{(k)}_{i8}(\mathbf{q},\omega)\right):\frac{\partial u_k(\mathbf{q},\omega)}{\partial\mathbf{q}} +\frac{\partial}{\partial\mathbf{q}}\cdot\left[\sum_{k=1}^{N}\mathbf{\Pi}^{(k)}_{i9}(\mathbf{q},\omega):\cdot\left.\frac{\partial}{\partial\mathbf{q}}\right|_u\hat{\mathbf{S}}^{(k)}_{u\nabla n}(\mathbf{q},\omega)\right] +\sum_{k=1}^{N}\left[\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}^{(k)}_{i9}(\mathbf{q},\omega)\right]:\cdot\left.\frac{\partial}{\partial\mathbf{q}}\right|_{\nabla n}\hat{\mathbf{S}}^{(k)}_{u\nabla n}(\mathbf{q},\omega). \quad (3.19)$$

In this expression notations $\partial/\partial\mathbf{q}|_u$ and $\partial/\partial\mathbf{q}|_{\nabla n}$ mean differentiation at constant $\mathbf{u}_i(\mathbf{q},\omega)$ and $\nabla n(\mathbf{q})$, respectively, and the contributions to the viscosity tensors are as follows.

''Molecular friction'' of the ith and kth component molecules is described by the fourth-rank Cartesian tensor $\hat{\boldsymbol{\eta}}_{ik}(\mathbf{q},\omega)$, which is the tensorial ik contribution to the shear viscosity tensor of the mixture,

$$\hat{\boldsymbol{\eta}}_{ik}(\mathbf{q},\omega)\equiv\frac{1}{2}\left\{\mathbf{\Pi}_{i8}^{(k)}(\mathbf{q},\omega):\odot\hat{\mathbf{1}}_6-\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_{i7}^{(k)}(\mathbf{q},\omega)-\mathbf{G}_S^{(k)}(\mathbf{q},\omega):\odot\hat{\mathbf{1}}_6\right\}, \tag{3.20}$$

where the Cartesian tensor $\mathbf{G}_S^{(k)}(\mathbf{q},\omega)$ is given in Appendix E. The tensorial ik contribution to the turbulent viscosity tensor of the mixture is

$$\hat{\boldsymbol{\mathcal{W}}}_{ik}(\mathbf{q},\omega)\equiv\left\{\mathbf{\Pi}_{i8}^{(k)}(\mathbf{q},\omega):\odot\hat{\mathbf{1}}_6-\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_{i7}^{(k)}(\mathbf{q},\omega)+\mathbf{G}_T^{(k)}(\mathbf{q},\omega):\odot\hat{\mathbf{1}}_6\right\}, \tag{3.21}$$

with the Cartesian tensor $\mathbf{G}_T^{(k)}(\mathbf{q},\omega)$ listed in Appendix E.

The bulk viscosity tensor of the mixture has the ikth tensorial contribution, the second-rank Cartesian tensor, defined as

$$\hat{\boldsymbol{\mathcal{K}}}_{ik}(\mathbf{q},\omega)\equiv\frac{1}{3}\left\{\mathbf{\Pi}_{i8}^{(k)}(\mathbf{q},\omega):\mathbf{I}-\left[\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_{i7}^{(k)}(\mathbf{q},\omega)\right]:\mathbf{I}-\mathbf{G}_B^{(k)}(\mathbf{q},\omega)\right\}, \tag{3.22}$$

where the expression for the Cartesian tensor $\mathbf{G}_B^{(k)}(\mathbf{q},\omega)$ can be found in Appendix E.

The above contributions to the viscosity tensors of the nanofluid mixture are complicated tensorial combinations of quantities composed of smoothed values of the equilibrium structure factors of the mixture. These contributions are ''flow independent'' because they do not depend on the particular type of fluid flow. However, for different flow types, the role of different components of these tensors can vary dramatically (this depends on the interplay of components of the spatial gradients of the quasihydrodynamic velocity, which should be convoluted with the components of the viscosity tensors), so the gross result would look as if the viscosities of the fluid mixture are flow dependent. This feature of the viscosity tensors is exactly the same as that for the viscosity tensors of a pure nanofluid and is discussed in Refs. [2–4] in great detail, including theoretical and numerical calculations of the viscosities for several particular cases.

Comparing Eqs. (3.20) and (3.21), one can see that the major contributions [the first two terms in Eq. (3.21)] to the ik turbulent viscosity tensor is twice as large as that to the ik shear viscosity tensor. However, in the momentum conservation equation for the ith mixture component, Eq. (3.18) [see also Eq. (3.19)], the ik shear viscosity tensor convolutes with the gradient of the k contribution to the shear rate tensor and the ik turbulent viscosity tensor convolutes with the gradient of the kth contribution to the vorticity tensor. The latter is the antisymmetric component of the gradient of the i contribution to the quasihydrodynamic velocity, Eq. (3.17), which for laminar flows is an order of magnitude smaller than the symmetric component, the ith contribution to the shear rate tensor. This accounts for neglect of the turbulent viscosity in the case of laminar flows.

As follows from Eq. (3.18), inhomogeneity in fluid density would cause instability of the laminar type of fluid flow and would lead to various types of turbulent flows in the general case of large-scale inhomogeneous fluid systems (which also are described by our theory). In this respect fluid flows in nanopores of several molecular diameters in width are a lucky exception, because turbulence cannot develop in such narrow channels. Thus we note that in the case of nanofluids the turbulent viscosity tensor is not of much importance.

The viscosity tensors for the nanofluid mixture can be recovered from Eq. (3.18) upon representation of the quasihydrodynamic velocity of the ith mixture component in terms of the quasihydrodynamic velocity of the nanofluid mixture $\mathbf{u}(\mathbf{q},\omega)$ and the diffusion velocity of the ith component of the mixture, $\mathbf{V}_i(\mathbf{q},\omega)$ [9],

$$\mathbf{u}_i(\mathbf{q},\omega)=\mathbf{u}(\mathbf{q},\omega)+\mathbf{V}_i(\mathbf{q},\omega), \tag{3.23}$$

substitution of Eq. (3.23) into Eq. (3.15), substitution of the obtained result into Eq. (3.18), and summation of Eq. (3.18) over the index i running through the mixture components. The viscosity tensors of the nanofluid mixture emerge in the simple form

$$\hat{\boldsymbol{\eta}}(\mathbf{q},\omega)=\sum_{i=1}^{N}\sum_{k=1}^{N}\hat{\boldsymbol{\eta}}_{ik}(\mathbf{q},\omega), \tag{3.24}$$

$$\hat{\boldsymbol{\mathcal{W}}}(\mathbf{q},\omega)=\sum_{i=1}^{N}\sum_{k=1}^{N}\hat{\boldsymbol{\mathcal{W}}}_{ik}(\mathbf{q},\omega), \tag{3.25}$$

$$\hat{\boldsymbol{\mathcal{K}}}(\mathbf{q},\omega)=\sum_{i=1}^{N}\sum_{k=1}^{N}\hat{\boldsymbol{\mathcal{K}}}_{ik}(\mathbf{q},\omega). \tag{3.26}$$

We note that even for homogeneous (bulk) fluid mixtures Eqs. *(3.24)–(3.26) do not reduce to a single summation of the tensorial viscosities of the mixture components*.

D. Energy conservation equations and tensorial thermal conductivities

Upon substitution of the results (3.3) and (3.4), and usage of approximations (3.1), (3.2) one can recover from Eq. (2.20) the energy conservation equation for the ith component of the mixture in the form

$$-\frac{3}{2}k_Bn_i(\mathbf{q})i\omega\delta T_i(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{J}_i(\mathbf{q},\omega)=\sum_{k=1}^{N}\{\mathfrak{R}_u^{(ik)}(\mathbf{q},\omega)\cdot\mathbf{u}_k(\mathbf{q},\omega)+\mathfrak{R}_T^{(ik)}(\mathbf{q},\omega)\delta T_k(\mathbf{q},\omega)+\mathfrak{R}_S^{(ik)}(\mathbf{q},\omega):\hat{\mathbf{S}}_{u\nabla n}^{(k)}(\mathbf{q},\omega)\}, \tag{3.27}$$

where the thermodynamic sources $\boldsymbol{\mathcal{R}}^{(ik)}(\mathbf{q},\omega)$ are listed in Appendix D and the fluxes $\mathbf{J}_i(\mathbf{q},\omega)$ are given by the expressions

$$\mathbf{J}_i(\mathbf{q},\omega)=\sum_{\alpha=1}^{8}\mathbf{J}_{i\alpha}(\mathbf{q},\omega),$$

$$\mathbf{J}_{i6}(\mathbf{q},\omega)=\sum_{k=1}^{N}\mathbf{J}_{i6}^{(k)}(\mathbf{q},\omega)\,\delta T_k(\mathbf{q},\omega),$$

$$\mathbf{J}_{i7}(\mathbf{q},\omega)=\sum_{k=1}^{N}\mathbf{J}_{i7}^{(k)}(\mathbf{q},\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\,\delta T_k(\mathbf{q},\omega),$$

$$\mathbf{J}_{i8}(\mathbf{q},\omega)=-\sum_{k=1}^{N}\mathbf{J}_{i8}^{(k)}(\mathbf{q},\omega):\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}\,\delta T_k(\mathbf{q},\omega),$$

$$\mathbf{J}_{i1}(\mathbf{q},\omega)=\sum_{k=1}^{N}\mathbf{J}_{i1}^{(k)}(\mathbf{q},\omega)\cdot\mathbf{u}_k(\mathbf{q},\omega),$$

$$\mathbf{J}_{i2}(\mathbf{q},\omega)=\sum_{k=1}^{N}\mathbf{J}_{i2}^{(k)}(\mathbf{q},\omega):\hat{\mathbf{S}}_{u\nabla n}^{(k)}(\mathbf{q},\omega),$$

$$\mathbf{J}_{i5}(\mathbf{q},\omega)=\sum_{k=1}^{N}\mathbf{J}_{i5}^{(k)}(\mathbf{q},\omega)\cdot:\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}\,\mathbf{u}_k(\mathbf{q},\omega),$$

$$\mathbf{J}_{i4}(\mathbf{q},\omega)=\sum_{k=1}^{N}\mathbf{J}_{i4}^{(k)}(\mathbf{q},\omega):\frac{\partial}{\partial\mathbf{q}}\,\mathbf{u}_k(\mathbf{q},\omega),$$

$$\mathbf{J}_{i3}(\mathbf{q},\omega)=\sum_{k=1}^{N}\mathbf{J}_{i3}^{(k)}(\mathbf{q},\omega)\cdot:\frac{\partial}{\partial\mathbf{q}}\,\hat{\mathbf{S}}_{u\nabla n}^{(k)}(\mathbf{q},\omega). \tag{3.28}$$

The Cartesian tensors $\mathbf{J}_{\gamma}^{(k)}(\mathbf{q},\omega)$, $\gamma=1,\ldots,6$, from Eq. (3.28) are listed in Appendix D, and the Cartesian tensors $\mathbf{J}_{i7}^{(k)}(\mathbf{q},\omega),\mathbf{J}_{i8}^{(k)}(\mathbf{q},\omega)$ of the second and the third ranks, respectively, are

$$\begin{aligned}\mathbf{J}_{i7}^{(k)}(\mathbf{q},\omega)=\sum_{l=1}^{N}\Bigg\{&\left[\delta_{il}\mathbf{I}+\frac{9(m_l/m_i)b_{il}}{5\pi[1+m_l/m_i]^2}\,\mathbf{F}_2^{(il)}(\mathbf{q})\right]\cdot\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\mathbf{q},\omega)+\frac{48\sqrt{2m_k/m_i}b_{ii}\sigma_{ik}\lambda_i b_{ik}}{25\pi^2\sigma_{ii}[1+m_k/m_i]^{3/2}}\,\delta_{kl}\boldsymbol{\Phi}_{02}^{(ik)}(\mathbf{q})\\&+\frac{16}{15}\sqrt{\pi\beta m_l}\lambda_l\tau_{l\eta}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})[\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1+\frac{12}{5}\,\pi\lambda_l\tau_{l\lambda}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})[\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1\\&-\frac{9(m_l/m_i)\sigma_{il}b_{il}}{10\pi[1+m_l/m_i]^2}\,\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\,\frac{\partial\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\mathbf{q},\omega)}{\partial\mathbf{q}}-\frac{18(m_l/m_i)\sigma_{il}\lambda_l b_{il}}{5[1+m_l/m_i]^2}\,\tau_{l\lambda}^{*}(\mathbf{q},\omega)\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(l)}(\mathbf{q},\omega)\mathbf{I}\\&+\frac{64\sqrt{2m_l/m_i}\sigma_{il}^3\lambda_l}{15[1+m_l/m_i]^{3/2}}\,\tau_{l\eta}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\mathbf{F}_3^{(il)}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)-\frac{32\sqrt{2m_l/m_i}\sigma_{il}^4\lambda_l}{15[1+m_l/m_i]^{3/2}}\\&\times\mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\,\frac{\partial}{\partial\mathbf{q}}\,[\tau_{l\eta}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)]+\frac{2\pi\sqrt{2m_l/m_i}\sigma_{il}^4\lambda_l}{[1+m_l/m_i]^{3/2}}\,\tau_{l\eta}^{*}(\mathbf{q},\omega)\tau_{l\lambda}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\\&\times\mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\hat{\boldsymbol{\mathcal{P}}}_{Tk}^{(l)}(\mathbf{q},\omega)\mathbf{I}\Bigg\},\end{aligned} \tag{3.29}$$

$$\begin{aligned}\mathbf{J}_{i8}^{(k)}(\mathbf{q},\omega)=\sum_{l=1}^{N}\Bigg\{&-\frac{12}{5}\,\pi\lambda_l\tau_{l\lambda}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\left[\delta_{il}\mathbf{I}+\frac{9(m_l/m_i)b_{il}}{5\pi[1+m_l/m_i]^2}\,\mathbf{F}_2^{(il)}(\mathbf{q})\right]\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)-\frac{9(m_l/m_i)b_{il}\sigma_{il}}{10\pi[1+m_l/m_i]^2}\,\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\\&\times\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4+\frac{54(m_l/m_i)b_{il}\sigma_{il}\lambda_l}{25[1+m_l/m_i]^2}\,\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\,\frac{\partial}{\partial\mathbf{q}}\,[\tau_{l\lambda}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]\\&-\frac{32\sqrt{2m_l/m_i}\sigma_{il}^3\lambda_l}{15[1+m_l/m_i]^{3/2}}\,\tau_{l\eta}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\mathbf{F}_3^{(il)}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)-\frac{32\sqrt{2m_l/m_i}\sigma_{il}^4\lambda_l}{15[1+m_l/m_i]^{3/2}}\,\tau_{l\eta}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\\&\times\mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4-\frac{16\sqrt{2m_l/m_i}\sigma_{il}^4\lambda_l}{15[1+m_l/m_i]^{3/2}}\,\mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\,\frac{\partial}{\partial\mathbf{q}}\,[\tau_{l\eta}^{*}(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]\Bigg\}.\end{aligned} \tag{3.30}$$

The ik contribution to the second-rank Cartesian tensor of thermal conductivity immediately follows from Eq. (3.27),

$$\hat{\lambda}_{ik}(\mathbf{q},\omega)=\mathbf{J}_{i7}^{(k)}(\mathbf{q},\omega):\hat{\mathbf{1}}_4+\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{J}_{i8}^{(k)}(\mathbf{q},\omega), \quad (3.31)$$

and the second-rank Cartesian tensor of thermal conductivity of the mixture is

$$\hat{\boldsymbol{\lambda}}(\mathbf{q},\omega)=\sum_{i=1}^{N}\sum_{k=1}^{N}\hat{\boldsymbol{\lambda}}_{ik}(\mathbf{q},\omega). \quad (3.32)$$

The analysis of flow dependence of the tensorial thermal conductivity of the nanofluid mixture is qualitatively the same as that of the above tensorial viscosities. We note that on letting $\omega\to0$, one can easily obtain the values of these tensorial transport coefficients in the low-frequency limit from Eqs. (3.24)–(3.26) and (3.32).

The above expressions for tensorial viscosities (3.24)–(3.26) and thermal conductivity (3.32) generalize those for bulk fluids [5] and pure inhomogeneous fluids [2,4]. The complicated structure of these coefficients reduces to relatively simple expressions if there is any spatial symmetry in the system (see examples in Refs. [1,2,4]).

IV. DIFFUSION IN NANOFLUID MIXTURES

A. Diffusion velocities of the components

Together with Eq. (3.23), Eq. (3.11) provides a recurrence relation for the diffusion velocities of the components of the nanofluid mixture. Further usage of the relations (3.1) and (3.2) for approximation of terms on the right-hand side of Eq. (3.11) and evaluation of the terms with the spatial gradients of the diffusion velocities on the left-hand side of Eq. (3.11) lead to the following form of this recurrence relation:

$$\begin{aligned}\mathbf{V}_i(\mathbf{q},\omega)=&-\frac{3\tau_{id}^{*}(\mathbf{q},\omega)}{2\sigma_{ii}^2 n_i(\mathbf{q})}\sqrt{\frac{\pi\beta}{m_i}}\left\{\left[\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}_{i1}(\mathbf{q},\omega)+\sum_{k\neq i}^{N}\frac{3\sqrt{2}\sigma_{ik}^2\tau_{kd}^{*}(\mathbf{q},\omega)}{[1+m_k/m_i]^{1/2}\sigma_{kk}^2 n_k(\mathbf{q})}\boldsymbol{\Phi}_2^{ik}(\mathbf{q})\cdot\left(\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}_{k1}(\mathbf{q},\omega)\right)\right]\right.\\&+\left[\sum_{k=1}^{N}\left(\boldsymbol{\Pi}_{i2}^{(k)}(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}_{i3}^{(k)}(\mathbf{q},\omega)\right)\cdot\frac{\partial}{\partial\mathbf{q}}\delta T_k(\mathbf{q},\omega)+\sum_{k\neq i}^{N}\frac{3\sqrt{2}\sigma_{ik}^2\tau_{kd}^{*}(\mathbf{q},\omega)}{[1+m_k/m_i]^{1/2}\sigma_{kk}^2 n_k(\mathbf{q})}\right.\\&\left.\times\boldsymbol{\Phi}_2^{ik}(\mathbf{q})\cdot\sum_{l=1}^{N}\left(\boldsymbol{\Pi}_{k2}^{(l)}(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}_{k3}^{(l)}(\mathbf{q},\omega)\right)\cdot\frac{\partial}{\partial\mathbf{q}}\delta T_l(\mathbf{q},\omega)\right]\\&+\left[\sum_{k=1}^{N}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}_{i2r}^{(k)}(\mathbf{q},\omega)\right)\delta T_k(\mathbf{q},\omega)+\sum_{k\neq i}^{N}\frac{3\sqrt{2}\sigma_{ik}^2\tau_{kd}^{*}(\mathbf{q},\omega)}{[1+m_k/m_i]^{1/2}\sigma_{kk}^2 n_k(\mathbf{q})}\boldsymbol{\Phi}_2^{ik}(\mathbf{q})\cdot\sum_{l=1}^{N}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}_{k2r}^{(l)}(\mathbf{q},\omega)\right)\delta T_l(\mathbf{q},\omega)\right]\\&-\left[\sum_{k=1}^{N}\boldsymbol{\mathcal{R}}_{Tr}^{(ik)}(\mathbf{q},\omega)\delta T_k(\mathbf{q},\omega)+\sum_{k\neq i}^{N}\frac{3\sqrt{2}\sigma_{ik}^2\tau_{kd}^{*}(\mathbf{q},\omega)}{[1+m_k/m_i]^{1/2}\sigma_{kk}^2 n_k(\mathbf{q})}\boldsymbol{\Phi}_2^{ik}(\mathbf{q})\cdot\sum_{l=1}^{N}\boldsymbol{\mathcal{R}}_{Tr}^{(lk)}(\mathbf{q},\omega)\delta T_l(\mathbf{q},\omega)\right]\\&\left.-\left[\sum_{k\neq i}^{N}\frac{2\sqrt{2m_k m_i}\sigma_{ik}^2\tau_{kd}^{*}(\mathbf{q},\omega)}{[1+m_k/m_i]^{1/2}n_k(\mathbf{q})}\sqrt{\frac{m_i}{\pi\beta}}\boldsymbol{\Phi}_2^{(ik)}(\mathbf{q})\cdot\sum_{l\neq k}^{N}\frac{3\sqrt{2}\sigma_{lk}^2 m_l}{[1+m_l/m_k]^{1/2}\sigma_{kk}^2}\boldsymbol{\Phi}_2^{(kl)}(\mathbf{q})\cdot\mathbf{V}_l(\mathbf{q},\omega)\right]\right\}. \quad (4.1)\end{aligned}$$

In this expression the tensorial coefficients are those defined by Eqs. (3.12), (C1)–(C3), (C9), and (B1), and the added subscript r means reduction of some of these coefficients. Thus $\boldsymbol{\Pi}_{i2r}^{(k)}(\mathbf{q},\omega)$ contains the first five lines of Eq. (C4) and $\boldsymbol{\mathcal{R}}_{Tr}^{(ik)}(\mathbf{q},\omega)$ consists of lines 1, 4, 6, 10, and 12 of Eq. (C9). The diffusion relaxation times are defined as

$$\overline{\tau_{id}(\mathbf{q})}\equiv\frac{3\sqrt{\pi\beta m_i}}{2\sigma_{ii}^2}\tau_{id}(\mathbf{q}), \quad (4.2a)$$

$$\begin{aligned}\tau_{id}^{-1}(\mathbf{q},\omega)\equiv&\sum_{k\neq i}^{N}\frac{\sqrt{2m_k/m_i}\sigma_{ik}^2}{[1+m_k/m_i]^{1/2}\sigma_{ii}^2}\int d\hat{\boldsymbol{\sigma}}\,n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})-\frac{\sqrt{2}\sigma_{iw}^2}{\sigma_{ii}^2}\\&\times\int d\hat{\boldsymbol{\sigma}}\,n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}}),\end{aligned} \quad (4.2b)$$

$$\tau_{id}^{*}(\mathbf{q},\omega)=\frac{\tau_{id}(\mathbf{q})}{1-i\omega\overline{\tau_{id}(\mathbf{q})}}. \quad (4.2c)$$

B. Diffusion coefficients of the nanofluid mixture

In Eq. (4.1) the first term in square brackets contains the major contribution to the diffusion coefficients. The additional contributions can be found upon solving Eq. (4.1) by iteration methods. The simplest trial solution of this equation is the same expression as Eq. (4.1), but without the last term on the right-hand side. Such a zero approximation for the diffusion velocity of the ith component $\mathbf{V}_i^0(\mathbf{q},\omega)$ can be substituted into the last term on the right-hand side of Eq. (4.1) and supplies the first approximation for the diffusion velocity. Carrying on such step-by-step approximations, one can obtain a solution of Eq. (4.1) of any desirable accuracy. Upon the nth step of this iteration procedure the term containing the diffusion coefficient reads

$$-\frac{3\tau_{id}^*(\mathbf{q},\omega)}{2\sigma_{ii}^2 n_i(\mathbf{q})}\sqrt{\frac{\pi\beta}{m_i}}\Bigg\{\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_{i1}(\mathbf{q},\omega)+\sum_{k\neq i}^{N}\Omega_{ik}(\mathbf{q},\omega)\hat{\mathbf{\Omega}}_{ik}(\mathbf{q})\cdot\left[\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_{k1}(\mathbf{q},\omega)\right]+\cdots+\underbrace{\sum_{k\neq i}^{N}\sum_{l\neq k}^{N}\cdots\sum_{j\neq s}^{N}}_{n}\Omega_{ik}(\mathbf{q},\omega)\Omega_{kl}(\mathbf{q},\omega)\cdots\Omega_{sj}(\mathbf{q},\omega)\times\hat{\mathbf{\Omega}}_{ik}(\mathbf{q})\cdot\hat{\mathbf{\Omega}}_{kl}(\mathbf{q})\cdot\cdots\cdot\hat{\mathbf{\Omega}}_{sj}(\mathbf{q})\cdot\left[\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_{j1}(\mathbf{q},\omega)\right]\Bigg\}, \tag{4.3}$$

where there are n terms with sums on the right-hand side of Eq. (4.3), and

$$\Omega_{ik}(\mathbf{q},\omega)=\frac{3\sqrt{2}m_i\sigma_{ik}^2 n_i(\mathbf{q})}{[1+m_k/m_i]^{1/2}\sigma_{kk}^2 n_k(\mathbf{q})}\tau_{kd}^*(\mathbf{q},\omega), \tag{4.4}$$

$$\hat{\mathbf{\Omega}}_{ik}(\mathbf{q})=\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]. \tag{4.5}$$

To extract an explicit expression for the diffusion tensor from the term (4.3), $(\partial/\partial\mathbf{q})\cdot\mathbf{\Pi}_{k1}(\mathbf{q},\omega)$ must be related to the gradients of the nonequilibrium densities of the components. Such a representation follows immediately from the definition of these quantities [see the second expression in Eq. (3.12)], but the result obtained is not very useful because it expresses the diffusion coefficients in terms of the direct correlation functions, which are not well known for inhomogeneous fluids. Another possibility is to rewrite the definition of $\mathbf{\Pi}_{i1}(\mathbf{q},\omega)$ from Eq. (3.12) in terms of the equilibrium pressure of the inhomogeneous fluid mixture. Using a generalization to inhomogeneous fluid mixtures of expression (21) from Ref. [12] for the functional of the pressure tensor of an inhomogeneous fluid, one can derive the expression

$$\mathbf{\Pi}_{i1}(\mathbf{q},\omega)=\int d\mathbf{q}'\sum_{k=1}^{N}\left\{\left[\left.\frac{\delta\mathbf{P}(\mathbf{q})}{\delta n_k(\mathbf{q}')}\right|_{\beta,n}\right]_{(i)}-\frac{1}{3\beta}n_i(\mathbf{q})\mathrm{Tr}\Lambda_{ik}(\mathbf{q},\mathbf{q}')\right\}\delta n_k(\mathbf{q}',\omega)\mathbf{I}-n_i(\mathbf{q})\int d\mathbf{q}'\int d\mathbf{q}''\sum_{l=1}^{N}\sum_{k=1}^{N}\left\{\left[\left.\frac{\delta\mathbf{P}(\mathbf{q}'')}{\delta n_k(\mathbf{q}')}\right|_{\beta,n}\right]_{(l)}-\frac{1}{3\beta}n_l(\mathbf{q}'')\mathrm{Tr}\Lambda_{lk}(\mathbf{q}'',\mathbf{q}')\right\}\delta n_k(\mathbf{q}',\omega)\mathbf{I}. \tag{4.6}$$

In this expression $[\delta\mathbf{P}(\mathbf{q})/\delta n_k(\mathbf{q})|_{\beta,n}]_{(i)}$ denotes the ith contribution to the Frechet derivative of the equilibrium pressure of the inhomogeneous fluid mixture with respect to the equilibrium density of the kth component at fixed temperature and the equilibrium densities of the remaining components of the mixture. The notation Tr means the trace of a matrix and the quantity $\Lambda_{ik}(\mathbf{q},\mathbf{q}')$ is a complicated functional of the equilibrium densities of the components, which depends upon the equilibrium free-energy density and the structure factors of the nanofluid mixture (see Ref. [12]). Expression (4.6) reduces further in the case of weakly inhomogeneous fluid mixtures. For such mixtures the quantities $\Lambda_{ik}(\mathbf{q},\mathbf{q}')$ can be neglected, the Frechet derivative of the pressure with respect to the kth component density reduces to $[\partial\mathbf{P}(\mathbf{q})/\partial n_k(\mathbf{q})]\delta(\mathbf{q}-\mathbf{q}')$, the second term in Eq. (4.6) becomes negligibly small, and the pressure itself can be written in the form

$$\mathbf{P}(\mathbf{q})=\sum_{i=1}^{N}\sum_{j=1}^{N}\Bigg\{n_i(\mathbf{q})k_BT\left[\delta_{ij}+\frac{1}{4\pi}b_{ij}n_j(\mathbf{q})\times\int d\hat{\boldsymbol{\sigma}}\,g_{ij}(\mathbf{q},\mathbf{q}-\sigma_{ij}\hat{\boldsymbol{\sigma}})\right]-\frac{1}{6}n_i(\mathbf{q})n_j(\mathbf{q})\times\int_{\sigma_{ij}\hat{\boldsymbol{\sigma}}}^{\infty}d\mathbf{r}\,g_{ij}(\mathbf{q},\mathbf{q}+\mathbf{r})\left[\frac{\partial\phi_{ij}(\mathbf{r})}{\partial\mathbf{r}}\cdot\mathbf{r}\right]|\mathbf{r}|^2\Bigg\}, \tag{4.7}$$

where $\phi_{ij}(\mathbf{r})$ is the attractive part of the intermolecular interaction potential specific to i and j components.

Using Eq. (4.7) in Eq. (4.6), substituting the result into Eq. (4.3), and extracting from Eq. (4.3) the contribution proportional to the gradients of the nonequilibrium densities of the components, one can derive the following expression for the contribution to the diffusion velocity of the ith component $\mathbf{V}_{i\nabla n}(\mathbf{q},\omega)$ due to the gradients of the nonequilibrium densities:

$$\mathbf{V}_{i\nabla n}(\mathbf{q},\omega)=-\frac{3}{2\sigma_{ii}^2}\sqrt{\frac{\pi\beta}{m_i}}\frac{\tau_{id}^*(\mathbf{q},\omega)}{n_i(\mathbf{q})}\times\sum_{\alpha=1}^{N}\hat{\mathbf{D}}_{i\alpha}(\mathbf{q},\omega)\cdot\frac{\partial\delta n_\alpha(\mathbf{q})}{\partial\mathbf{q}}, \tag{4.8}$$

where the second-rank Cartesian tensor $\hat{\mathbf{D}}_{i\alpha}(\mathbf{q},\omega)$, $\alpha=1,2,\ldots,N$, is given by the expression

$$\hat{\mathbf{D}}_{i\alpha}(\mathbf{q},\omega)=\Bigg\{E_{i\alpha}(\mathbf{q})+\sum_{k\neq i}^{N}\Omega_{ik}(\mathbf{q},\omega)E_{k\alpha}(\mathbf{q})\hat{\mathbf{\Omega}}_{ik}(\mathbf{q})+\sum_{k\neq i}^{N}\sum_{l\neq k}^{N}\cdots\sum_{j\neq s}^{N}\Omega_{ik}(\mathbf{q},\omega)\times\Omega_{lk}(\mathbf{q},\omega)\cdots\Omega_{js}(\mathbf{q},\omega)E_{j\alpha}(\mathbf{q})\times\hat{\mathbf{\Omega}}_{ik}(\mathbf{q})\cdot\hat{\mathbf{\Omega}}_{lk}(\mathbf{q})\cdot\cdots\cdot\hat{\mathbf{\Omega}}_{js}(\mathbf{q})\Bigg\}\mathbf{I} \tag{4.9}$$

and $E_{il}(\mathbf{q})$ is

$$E_{il}(\mathbf{q})=\frac{1}{\beta}\Bigg\{\delta_{il}+\frac{1}{2\pi}n_i(\mathbf{q})b_{il}\int d\hat{\boldsymbol{\sigma}}\,g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})$$

$$+\frac{1}{4\pi}\sum_j n_i(\mathbf{q})n_j(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\,\frac{\partial g_{ij}(\mathbf{q},\mathbf{q}-\sigma_{ij}\hat{\boldsymbol{\sigma}})}{\partial n_l(\mathbf{q})}$$
$$-\frac{\beta}{3}\,n_i(\mathbf{q})\int_{\sigma_{il}\hat{\boldsymbol{\sigma}}+\mathbf{q}}^{\infty} d\mathbf{q}''|\mathbf{q}''|^2\mathbf{q}''\cdot\frac{d\phi_{il}(\mathbf{q}'')}{d\mathbf{q}''}\,g_{il}(\mathbf{q},\mathbf{q}'')$$
$$-\frac{\beta}{6}\sum_j n_i(\mathbf{q})n_j(\mathbf{q})\int_{\sigma_{ij}\hat{\boldsymbol{\sigma}}+\mathbf{q}}^{\infty} d\mathbf{q}''|\mathbf{q}''|^2$$
$$\left.\times\mathbf{q}''\cdot\frac{d\phi_{ij}(\mathbf{q}'')}{d\mathbf{q}}\,\frac{\partial g_{ij}(\mathbf{q},\mathbf{q}'')}{\partial n_l(\mathbf{q})}\right\}. \quad (4.10)$$

The expression (4.9) defines the tensorial diffusion coefficients of the N-component nanofluid mixture. The deviations of the number densities of the components from the corresponding equilibrium values, featured in Eq. (4.8), are linearly dependent and related by the equation of state. The latter is unknown for a nonequilibrium state of the system. However, as we already noted, near equilibrium the structure properties of the mixture do not differ significantly from those at equilibrium. Thus we can use the equilibrium equation of state to express the linear dependent quantity $\delta n_m(\mathbf{q},\omega)$ in terms of the rest of the densities, pressure, and temperature of the mixture. Thus it follows from Eq. (4.8) that

$$\mathbf{V}_{i\nabla n}(\mathbf{q},\omega)=-\frac{3}{2\sigma_{ii}^2}\sqrt{\frac{\pi\beta}{m_i}}\frac{\tau_{id}^*(\mathbf{q},\omega)}{n_i(\mathbf{q})}\sum_{l\neq m}^{N}\left\{\hat{\mathbf{D}}_{il}(\mathbf{q},\omega)-\frac{P_l(\mathbf{q},\omega)}{P_m(\mathbf{q},\omega)}\hat{\mathbf{D}}_{im}(\mathbf{q},\omega)\right\}\cdot\frac{\rho_l(\mathbf{q})}{\rho(\mathbf{q})}\frac{\partial\delta n_\alpha(\mathbf{q})}{\partial\mathbf{q}}, \quad (4.11)$$

where

$$P_l(\mathbf{q})=\sum_{i=1}^{N}E_{il}(\mathbf{q}), \quad (4.12)$$

and m is the index of the linearly dependent density.

From Eq. (4.11) it follows that the theoretical diffusion coefficients of the nanofluid mixture are

$$[\hat{\mathbf{D}}_{il}(\mathbf{q},\omega)]_T=\frac{3\tau_{id}^*(\mathbf{q},\omega)\rho_l(\mathbf{q})}{2\sigma_{ii}^2 n_i(\mathbf{q})\rho(\mathbf{q})}\sqrt{\frac{\pi\beta}{m_i}}\times\left[\hat{\mathbf{D}}_{il}(\mathbf{q},\omega)-\frac{P_l(\mathbf{q})}{P_m(\mathbf{q})}\hat{\mathbf{D}}_{im}(\mathbf{q},\omega)\right]. \quad (4.13)$$

The above diffusion coefficients are not linearly independent and satisfy the condition

$$\sum_i m_i n_i(\mathbf{q})[\hat{\mathbf{D}}_{il}(\mathbf{q},\omega)]_T=0, \quad (4.14)$$

which follows from $\Sigma_{i=1}^{N} m_i n_i(\mathbf{q})\mathbf{V}_i(\mathbf{q},\omega)=0$. At $\omega=0$ from Eqs. (4.13) and (4.14) one can derive the frequency-independent diffusion coefficients of the nanofluid mixture.

C. Phenomenological definition of the diffusion coefficients

The phenomenological diffusion coefficients $\hat{\mathbf{D}}_{il}^{p}(\mathbf{q})$ are defined by the expression for the mass flux of the ith component, $\mathbf{J}_i^p(\mathbf{q})$,

$$\mathbf{J}_i^p(\mathbf{q})=m_i n_i(\mathbf{q})\mathbf{V}_i(\mathbf{q})=-\sum_{l\neq m}\hat{\mathbf{D}}_{il}^{p}(\mathbf{q})m_l\cdot\frac{\partial n_l(\mathbf{q})}{\partial\mathbf{q}}-\hat{\mathbf{D}}_l^{T}(\mathbf{q})\left(\frac{\partial\ \ln T(\mathbf{q})}{\partial\mathbf{q}}\right),$$

where $\hat{\mathbf{D}}_l^{T}(\mathbf{q})$ is the thermal diffusion coefficient. A comparison of this expression and Eq. (4.11) at $\omega=0$ leads to the relation

$$\hat{\mathbf{D}}_{il}^{p}(\mathbf{q})=\frac{m_i}{m_l}\,n_i(\mathbf{q})[\hat{\mathbf{D}}_{il}(\mathbf{q})]_T, \quad (4.15)$$

where the definition (4.13) has been taken into account.

D. Diffusion coefficients for binary mixtures of nanofluids

In the case of weak inhomogeneity of the nanofluid mixture the terms with sums on the right-hand side of Eq. (4.9) can be neglected, and from Eqs. (4.9), (4.13), (4.2b), (4.2c), and (4.14) it follows that the theoretical diffusion coefficient of the binary mixture $[\hat{\mathbf{D}}_{12}(\mathbf{q})]_T$ at $\omega=0$ is

$$[\hat{\mathbf{D}}_{12}(\mathbf{q})]_T=\frac{4D_{12}^*(\mathbf{q})n(\mathbf{q})\beta m_2 n_2(\mathbf{q})}{n_1(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\,n_2(\mathbf{q}-\sigma_{12}\hat{\boldsymbol{\sigma}})g_{12}(\mathbf{q},\mathbf{q}-\sigma_{12}\hat{\boldsymbol{\sigma}})\rho(\mathbf{q})}\times\left[E_{12}(\mathbf{q})-\frac{P_2(\mathbf{q})}{P_1(\mathbf{q})}E_{11}(\mathbf{q})\right]\mathbf{I}, \quad (4.16)$$

where

$$D_{12}^*(\mathbf{q})=\frac{3\sqrt{2\pi k_B T}}{16\pi\sigma_{12}^2 n(\mathbf{q})\sqrt{m_{12}}},\qquad m_{12}=\frac{m_1 m_2}{m_1+m_2}.$$

From Eqs. (4.16) and (4.15) one can derive the following relation between the phenomenological diffusion coefficients of the inhomogeneous binary mixture:

$$\hat{\mathbf{D}}_{12}^{p}(\mathbf{q})=\left[\frac{m_1P_2(\mathbf{q})}{m_2P_1(\mathbf{q})}\right]\times\left[\frac{n_2(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\,n_1(\mathbf{q}-\sigma_{12}\hat{\boldsymbol{\sigma}})g_{12}(\mathbf{q},\mathbf{q}-\sigma_{12}\hat{\boldsymbol{\sigma}})}{n_1(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\,n_2(\mathbf{q}-\sigma_{12}\hat{\boldsymbol{\sigma}})g_{12}(\mathbf{q},\mathbf{q}-\sigma_{12}\hat{\boldsymbol{\sigma}})}\right]\hat{\mathbf{D}}_{21}^{p}(\mathbf{q}). \quad (4.17)$$

In the particular case of a homogeneous binary mixture this expression reduces to

$$\hat{\mathbf{D}}_{12}^{p}=\left[\frac{m_1P_2}{m_2P_1}\right]\hat{\mathbf{D}}_{21}^{p},$$

where $\hat{\mathbf{D}}_{12}^{p}$ is the homogeneous reduction of the corresponding phenomenological coefficient (4.15) expressed in terms of the theoretical diffusion coefficient (4.16) calculated for the homogeneous mixture. This relation has been originally derived in Ref. [13] for a homogeneous binary mixture of hard spheres in the framework of the Chapman-Enskog method [9]. Here we have shown that the same relation also holds for a binary mixture of any homogeneous fluids provided their intermolecular interaction potentials can be represented as a sum of hard-core repulsive and soft attractive contributions.

From Eqs. (4.9), (4.6), and (4.3) it follows that the diffusion coefficients of the nanofluid mixture depend strongly on the equilibrium pressure of the mixture, which in the above case depends explicitly on the attractive part of the intermolecular interaction potentials [see, for example, Eq. (4.7)]. It follows that the values of the diffusion coefficients are very sensitive to the approximation made for the equilibrium pressure of the nanofluid mixture. In this respect the diffusion coefficients differ significantly from the viscosities and thermal conductivity coefficients of such mixtures [Eqs. (3.24)–(3.26) and (3.32)], which do not depend on the equilibrium pressure explicitly.

V. SUMMARY

The transport theory presented above is a rigorous generalization to nanofluid mixtures of the approach [1–4] suggested by the authors for pure inhomogeneous fluids and based on the rigorous development [1] of the Mori-Zwanzig projection operator method. Although rigorous, this theory remains tractable due to an advantage of dividing the potentials of intermolecular interactions into hard-core repulsive and soft attractive contributions, suggested originally by Sung and Dahler [5] for homogeneous fluids. The transport coefficients derived in the framework of this theory have a simple and tractable structure that permits their further investigation and evaluation.

The theory incorporates two basic assumptions. The major one is the neglect of the dynamic memory effects in the generalized Langevin equations (GLEs) used to derive the kinetic equations (2.1). The main contribution to the dynamic memory effects comes from repeated core collisions and is important for dense bulk fluids [5]. Nevertheless, the success of the theory in calculating the shear viscosity of a pure dense fluid confined in slit pores of several molecular diameters in width [3] suggests that such effects are not important for fluids confined in narrow capillary pores. The physical reason for this is that the confinement suppresses repeated core collisions of the fluid molecules, reducing their mobility. However, in other applications such reduction of molecular mobility may not occur. Examples include systems often considered in fluid mechanics (flow of colloid mixtures, flows containing macroscopic and/or mesoscopic particles, and flows of fine solid particles), fluid-fluid interfaces, relatively large pores filled with colloid mixtures, and membranes of living cells. In such cases the neglect of the dynamic memory effects may be approximately corrected for by adjusting the theoretical results to match simulation data for mixtures of hard spheres of the same hard-sphere diameters [5]. Analytic corrections for this effect can also be derived by incorporating the dynamic memory effects (which are included into the GLEs of Ref. [1]) in the kinetic equations (2.1) and developing the transport theory close to the lines presented above.

The second basic assumption of the theory is the use of the 13-moment approximation in deriving the quasihydrodynamic equations (Sec. III). This can be alleviated, in principle, by expanding the basis set beyond the first 13 velocity moments of the singlet dynamic distribution functions of the mixture components. However, it is well known that for homogeneous fluids more accurate estimates of the transport coefficients at zero frequency, both in the conventional Chapman-Enskog procedure and in the 21-moment approximation [9,14], lead to negligibly small modifications of the numerical values of the transport coefficients and these are proportional to $n^2b^2g(\sigma)$; the corresponding correction factors are $(1.016)^{-1}$ for the shear viscosity and $(1.025)^{-1}$ for the thermal conductivity. There is no physical reason for these correction factors to become much larger in the case of inhomogeneous fluids. Thus we do not expect the use of the 13-moment approximation to lead to large errors.

Calculation of the transport coefficients based on Eqs. (3.24)–(3.26), (4.9), and (4.13) requires data on equilibrium distribution functions of the nanofluid mixtures, in particular the number densities $n_i(\mathbf{q})$, the contact values of their pair-correlation functions $g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\sigma})$, and the effective hard-core diameters σ_{il} calculated for the composite intermolecular interaction potentials. Such intermolecular interaction potentials have to be obtained from more realistic intermolecular interaction potentials (e.g., the Lennard-Jones model potentials) by means of the Weeks-Chandler-Andersen (WCA) [7] or Barker-Henderson (BH) [8] methods. The WCA method supplies hard-core diameters $\sigma_{il}^{\mathrm{WCA}}$ that depend on the equilibrium number densities of the components and the temperature of the mixture, whereas the BH procedure leads to $\sigma_{il}^{\mathrm{BH}}$ that depend only on temperature. From a dynamical point of view the differences between collisional encounters described by the model potentials of this theory and more realistic ones are small, so that it is reasonable to account for such differences in the potentials by choosing the hard-core diameters to be functionals of the equilibrium number densities and temperature of the mixture, as has been suggested in Ref. [5].

In the case of the WCA choice of hard-core diameters, the present theory includes an assumption that the hard-core diameter $\sigma_{il}^{\mathrm{WCA}}$ is the same for the local densities $n_i(\mathbf{q}),n_l(\mathbf{q})$ and $n_i(\mathbf{q}+\mathbf{q}'),n_l(\mathbf{q}+\mathbf{q}')$ when $\mathbf{q}'\ll\sigma_{il}^{\mathrm{WCA}}$. Since the density dependence of $\sigma_{il}^{\mathrm{WCA}}$ is weak [7], we believe this is a good approximation. This consideration is also supported by the results of Ref. [3]. However, from a rigorous theoretical point of view the above transport theory should be regarded as a zeroth-order theory with respect to the density dependence of $\sigma_{il}^{\mathrm{WCA}}$, provided the WCA choice of the hard-core diameters has been used.

In order to avoid calculation of σ_{il} for every local set of values of $n_i(\mathbf{q})$, $i=1,\ldots,N$, one can use the BH choice of hard-core diameters, which do not depend on the densities of the components or the density of the mixture. In the case of nanofluid mixtures confined in narrow capillary pores this seems to be the best choice of the hard-core diameters. However, for other systems, where the neglect of dynamic memory effects may require alleviation, the treatment becomes more complicated because it is not clear that the main contribution to such memory effects is from repeated hard-core collisions only.

The above equilibrium distribution functions of the nanofluid mixtures can be obtained by direct equilibrium computer simulations. These results may be expressed in dimensionless form and as such are valid for any σ_{il} and $n_i(\mathbf{q})$. Another possibility is to determine the distribution functions by analytical means, using integral equations of equilibrium statistical mechanics or the density-functional theory. For practical purposes direct computer simulation data seem to be more useful, as they should reflect the structure of a particular nanofluid system in greater detail.

Calculations of the diffusion coefficients given by Eqs. (4.9), (4.13), (4.15), and (4.16) also require data on the derivatives of the equilibrium pair-correlation functions with respect to the component densities. These data can be obtained from the equilibrium molecular-dynamic simulations mentioned above. The spatial integrals on the right-hand side of Eq. (4.10) can also be evaluated analytically upon determination of the pair-correlation functions of the components.

Several important aspects of the above theory have been left for further investigations. This includes detailed studies of the diffusion coefficients of nanofluid mixtures by nonequilibrium molecular-dynamics simulation. We also plan to consider further theoretical investigation of the pressure dependence of the diffusion coefficients in the framework of Eqs. (4.6) and (4.8) for several particular cases. Finally, in future studies we plan to derive analytic expressions for the thermal diffusion coefficients of nanofluid mixtures and to analyze the properties of the remaining transport coefficients in the quasihydrodynamic equations (3.11), (3.27), and (4.1), which do not have their immediate counterparts for bulk fluid mixtures.

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APPENDIX A: COEFFICIENTS IN EQS. (3.3)–(3.5)

The quantity $\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{uk}(\mathbf{q},\omega)$ is the following Cartesian tensor of the third rank:

$$\begin{aligned}\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{uk} \equiv{}& \frac{m_k/m_i}{1+m_k/m_i}\int d\hat{\boldsymbol{\sigma}}\; n_k(\mathbf{q}-\sigma_{ik}\hat{\sigma})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}-\delta_{ik}\sum_{l=1}^{N}\frac{m_l/m_i}{1+m_l/m_i}\\ &\times\int d\hat{\boldsymbol{\sigma}}\; n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}+\delta_{ik}\left(\frac{\sigma_{iw}}{\sigma_{ik}}\right)^2\int d\hat{\boldsymbol{\sigma}}\; n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\\ &\times[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}+\frac{3\sqrt{2}\,\tau^*_{i\lambda}(\mathbf{q},\omega)}{8[1+m_k/m_i]^{3/2}}\,\hat{\boldsymbol{\mathcal{C}}}^{(i)}_Q(\mathbf{q},\omega)\cdot\int d\hat{\boldsymbol{\sigma}}\; n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\\ &+\delta_{ik}\frac{3\sqrt{2}\,\tau^*_{i\lambda}(\mathbf{q},\omega)}{8}\left(\frac{\sigma_{iw}}{\sigma_{ik}}\right)^2\hat{\boldsymbol{\mathcal{C}}}^{(i)}_Q(\mathbf{q},\omega)\cdot\int d\hat{\boldsymbol{\sigma}}\; n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\\ &-\delta_{ik}\frac{3\sqrt{2}\,\tau^*_{i\lambda}(\mathbf{q},\omega)}{8}\,\hat{\boldsymbol{\mathcal{C}}}^{(i)}_Q(\mathbf{q},\omega)\cdot\sum_{l=1}^{N}\int d\hat{\boldsymbol{\sigma}}\; n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}].\end{aligned}\tag{A1}$$

The fifth-rank Cartesian tensor $\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\Delta uk}(\mathbf{q},\omega)$ is defined by the equation

$$\begin{aligned}\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\Delta uk}\equiv{}&\frac{m_k/m_i}{1+m_k/m_i}\int d\hat{\boldsymbol{\sigma}}\; n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\\ &+\frac{3\sqrt{2}\,\tau^*_{i\lambda}(\mathbf{q},\omega)}{4[1+m_k/m_i]^{3/2}}\,\hat{\boldsymbol{\mathcal{C}}}^{(i)}_Q\cdot\int d\hat{\boldsymbol{\sigma}}\; n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}.\end{aligned}\tag{A2}$$

The expression for the second-rank Cartesian tensor $\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{Tk}(\mathbf{q},\omega)$ is

$$\begin{aligned}\hat{\mathbf{P}}^{(i)}_{Tk}(\mathbf{q},\omega)\equiv{}&\frac{32\sqrt{2m_k/m_i}\,\sigma^2_{ik}n_i(\mathbf{q})}{15\pi\tau^*_{i\lambda}[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\; n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\\ &+\frac{6(m_k/m_i)\sigma^2_{ik}n_i(\mathbf{q})}{5[1+m_k/m_i]^2}\,\hat{\boldsymbol{\mathcal{C}}}^{(i)}_Q(\mathbf{q},\omega)\cdot\int d\hat{\boldsymbol{\sigma}}\; n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\\ &-\delta_{ik}\hat{\boldsymbol{\mathcal{C}}}^{(i)}_Q(\mathbf{q},\omega)\cdot\left[\frac{\partial n_i(\mathbf{q})}{\partial\mathbf{q}}+\sigma^2_{iw}n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\; n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\right]\\ &-\frac{6}{5}\,\delta_{ik}n_i(\mathbf{q})\hat{\boldsymbol{\mathcal{C}}}^{(i)}_Q(\mathbf{q},\omega)\cdot\sum_{l=1}^{N}\frac{\sigma^2_{il}(m_l/m_i)}{[1+m_l/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\; n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\end{aligned}$$

$$-\delta_{ik}\frac{32\sqrt{2}n_i(\mathbf{q})}{15\pi\tau^*_{i\lambda}(\mathbf{q},\omega)}\sum_{l=1}^{N}\frac{\sigma_{il}^2\sqrt{m_l/m_i}}{[1+m_l/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]. \quad \text{(A3)}$$

The remaining Cartesian tensors $\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\nabla Tk}(\mathbf{q},\omega)$ and $\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\Delta Tk}(\mathbf{q},\omega)$ are of the third and the fourth ranks, respectively, and are given by the expressions

$$\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\nabla Tk}(\mathbf{q},\omega)\equiv\frac{3\sqrt{2m_k/m_i}b_{ik}}{\pi[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}+\frac{15}{16}\pi\tau^*_{i\lambda}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{Q}(\mathbf{q},\omega)\cdot\Bigg[\delta_{ik}\mathbf{I}$$
$$+\frac{9(m_k/m_i)b_{ik}}{5\pi[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\Bigg], \quad \text{(A4)}$$

$$\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\Delta Tk}(\mathbf{q},\omega)\equiv\frac{2\sqrt{2m_k/m_i}\sigma_{ik}^4}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}+\frac{9\pi(m_k/m_i)\sigma_{ik}^4\tau^*_{i\lambda}(\mathbf{q},\omega)}{8[1+m_k/m_i]^2}$$
$$\times\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{Q}(\mathbf{q},\omega)\cdot\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}. \quad \text{(A5)}$$

In the above expressions and in Eq. (3.5) the coefficient $\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{Q}(\mathbf{q},\omega)$ is the third-rank Cartesian tensor

$$\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{Q}(\mathbf{q},\omega)\equiv\sum_{l=1}^{N}\frac{(m_l/m_i)\sigma_{il}^2}{[1+m_l/m_i]\sigma_{ii}^2}\int d\hat{\boldsymbol{\sigma}}\, n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}+\int d\hat{\boldsymbol{\sigma}}\, g_{ii}(\mathbf{q},\mathbf{q}-\sigma_{ii}\hat{\boldsymbol{\sigma}})[n_i(\mathbf{q})-n_i(\mathbf{q}$$
$$-\sigma_{ii}\hat{\boldsymbol{\sigma}})][\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}+2\left(\frac{\sigma_{iw}}{\sigma_{ii}}\right)^2\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}. \quad \text{(A6)}$$

The quantity $\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{Tk}(\mathbf{q},\omega)$ is the Cartesian three-vector

$$\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{Tk}\equiv\delta_{ik}\frac{\partial n_i(\mathbf{q})}{\partial\mathbf{q}}+\delta_{ik}\sigma_{iw}^2 n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}-\frac{6(m_k/m_i)\sigma_{ik}^2 n_i(\mathbf{q})}{5[1+m_k/m_i]^2}$$
$$\times\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}+\tfrac{5}{6}\delta_{ik}n_i(\mathbf{q})\sum_{l=1}^{N}\frac{(m_l/m_i)\sigma_{il}^2}{[1+m_l/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}$$
$$-\tfrac{15}{64}\pi\tau^*_{i\eta}(\mathbf{q},\omega)\tau^*_{i\lambda}(\mathbf{q},\omega)n_i(\mathbf{q})\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{P}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{Tk}(\mathbf{q},\omega). \quad \text{(A7)}$$

The third-rank Cartesian tensor $\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{\Delta Tk}(\mathbf{q},\omega)$ is

$$\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{\Delta Tk}(\mathbf{q},\omega)\equiv\frac{(m_k/m_i)\sigma_{ik}^4}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}+\tfrac{5}{24}\tau^*_{i\eta}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{P}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{\Delta Tk}(\mathbf{q},\omega). \quad \text{(A8)}$$

The quantity $\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{uk}(\mathbf{q},\omega)$ is the Cartesian tensor of the second rank defined by the expression

$$\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{uk}(\mathbf{q},\omega)\equiv-\delta_{ik}\sum_{l=1}^{N}\frac{\sigma_{il}^2}{\sigma_{iw}^2[1+m_l/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]+\frac{\sigma_{ik}^2}{\sigma_{iw}^2[1+m_k/m_i]^{3/2}}$$
$$\times\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]+\delta_{ik}\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]$$
$$+\frac{5\sqrt{2}\pi\sigma_{ik}^2}{16\sigma_{iw}^2}\tau^*_{i\eta}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{P}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}^{(i)}_{uk}(\mathbf{q},\omega). \quad \text{(A9)}$$

The third-rank Cartesian tensor $\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{\nabla uk}(\mathbf{q},\omega)$ is defined as

$$\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{\nabla uk}(\mathbf{q},\omega)\equiv\frac{3\sqrt{2}b_{ik}n_i(\mathbf{q})}{\pi[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}+\frac{5}{16\eta_i}\hat{\boldsymbol{\mathcal{C}}}^{(i)}_{P}(\mathbf{q}):\hat{\boldsymbol{\eta}}^{(2)}_{ik}(\mathbf{q},\omega). \quad \text{(A10)}$$

Finally, the fourth-rank Cartesian tensor $\hat{\boldsymbol{\mathcal{Q}}}^{(i)}_{\Delta uk}(\mathbf{q},\omega)$ is given by the expression

$$\hat{\mathcal{Q}}^{(i)}_{\Delta uk}(\mathbf{q},\omega)\equiv\frac{\sqrt{2}\sigma_{ik}^2}{[1+m_k/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}+\tfrac{5}{8}\pi\sigma_{ik}^4\tau^*_{i\eta}(\mathbf{q},\omega)\hat{\mathcal{C}}^{(i)}_P(\mathbf{q}):\hat{\mathcal{P}}^{(i)}_{\Delta uk}(\mathbf{q},\omega). \tag{A11}$$

In the above definitions of the tensors $\hat{\mathcal{Q}}^{(i)}(\mathbf{q},\omega)$ we have used the third-rank Cartesian tensor $\hat{\mathcal{C}}^{(i)}_P(\mathbf{q})$, which is given by the expression

$$\hat{\mathcal{C}}^{(i)}_P(\mathbf{q})\equiv 3\int d\hat{\boldsymbol{\sigma}}\, g_{ii}(\mathbf{q},\mathbf{q}-\sigma_{ii}\hat{\boldsymbol{\sigma}})[n_i(\mathbf{q})-n_i(\mathbf{q}-\sigma_{ii}\hat{\boldsymbol{\sigma}})]\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-2\sum_{l=1}^{N}\left(\frac{\sigma_{il}}{\sigma_{ii}}\right)^2\int d\hat{\boldsymbol{\sigma}}\, n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})[\mathbf{I}-\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}]\hat{\boldsymbol{\sigma}}. \tag{A12}$$

APPENDIX B: DESCRIPTION OF ‘‘SMOOTHING’’ PROCEDURES

The following Cartesian tensors, vectors, and scalars have emerged upon derivation of the quasihydrodynamic equations for the Fourier transforms of the quasicontinuum variables from Eqs. (2.18)–(2.24) and (2.24):

$$\boldsymbol{\Phi}^{(ik)}_m(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}} n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\underbrace{\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}}_{m}+\frac{\sigma_{ik}}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\left[\int d\hat{\boldsymbol{\sigma}} n_i(\mathbf{q})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\underbrace{\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}}_{m+1}\right],$$

$$\boldsymbol{F}^{(ik)}_m(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}} g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\underbrace{\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}}_{m}+\frac{\sigma_{ik}}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\left[\int n_i(\mathbf{q})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\underbrace{\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}}_{m+1}\right],$$

$$\boldsymbol{\Xi}^{(ik)}(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]+\frac{\sigma_{ik}}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\left[\int d\hat{\boldsymbol{\sigma}}\, n_i(\mathbf{q})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\right],$$

$$\boldsymbol{F}^{(ik)}_{0m}(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}} g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\underbrace{\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}}_{m},$$

$$\boldsymbol{\Xi}^{(ik)}_0(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}},$$

$$\boldsymbol{\Phi}^{(ik)}_{0m}(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}} g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\underbrace{\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}}_{m},$$

$$\boldsymbol{\Psi}^{(ik)}(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]$$
$$+\frac{\sigma_{ik}}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\left[\int d\hat{\boldsymbol{\sigma}}\, n_i(\mathbf{q})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\right],$$

$$\boldsymbol{\Psi}^{(ik)}_0(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}]\hat{\boldsymbol{\sigma}},$$

$$\boldsymbol{\Psi}^{(ik)}_2(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}],$$

$$\boldsymbol{\Phi}^{(ik)}_{12}(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}],$$

$$\boldsymbol{\Phi}^{(ik)}_{13}(\mathbf{q})=n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I}]. \tag{B1}$$

In these expressions the $\hat{\boldsymbol{\sigma}}\cdots\hat{\boldsymbol{\sigma}}$ mean tensorial products of the unit vector $\hat{\boldsymbol{\sigma}}$ by itself; m means the number of $\hat{\boldsymbol{\sigma}}$ components in these products; the index k runs through the components of the mixture, $k=1,\dots,N$, and the confinement (walls) w; and the index i runs through the components of the mixture, $i=1,\dots,N$.

APPENDIX C: COEFFICIENTS IN EQS. (3.11) AND (3.12)

The tensorial coefficients $\mathbf{\Pi}_{i\alpha}^{(k)}(\mathbf{q},\omega)$, $\alpha=2,\ldots,6,9$, which are included in the fluxes $\mathbf{\Pi}_{i\alpha}(\mathbf{q},\omega)$ on the left-hand side of Eq. (3.11), respectively, can be expressed as follows. The second-rank Cartesian tensor $\mathbf{\Pi}_{i2}^{(k)}(\mathbf{q},\omega)$ is

$$\begin{aligned}
\mathbf{\Pi}_{i2}^{(k)}(\mathbf{q},\omega) \equiv \sum_{l=1}^{N} \Bigg\{ & k_B n_i(\mathbf{q})\delta_{ik}\delta_{kl}\mathbf{I} + \frac{k_B\sigma_{ik}^3}{1+m_k/m_i}\,\delta_{kl}\mathbf{\Phi}_2^{(ik)}(\mathbf{q}) + 2\pi\sqrt{\pi\beta m_l}\lambda_l n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\tau_{l\lambda}^*(\mathbf{q},\omega) \\
& \times\left[\delta_{il}\hat{\mathbf{1}}_4 + \frac{\sigma_{il}^3}{1+m_l/m_i}\,\mathbf{F}_4^{(il)}(\mathbf{q})\right]:\hat{\mathcal{P}}_{Tk}^{(l)}(\mathbf{q},\omega) - \pi\sqrt{\pi\beta m_l}\lambda_l\,\frac{\sigma_{il}^4}{1+m_l/m_i}\,\mathbf{F}_{05}^{(il)}(\mathbf{q}):\odot\,\frac{\partial}{\partial\mathbf{q}} \\
& \times[\tau_{l\eta}^*(\mathbf{q},\omega)\tau_{l\lambda}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\mathcal{P}}_{Tk}^{(l)}(\mathbf{q},\omega)] - \frac{8\sqrt{2\beta m_l\pi}\sigma_{il}^3\lambda_l}{5[1+m_l/m_i]^{3/2}}\,\tau_{l\lambda}^*(\mathbf{q},\omega)\mathbf{\Xi}^{(il)}(\mathbf{q})\cdot\hat{\mathcal{Q}}_{Tk}^{(l)}(\mathbf{q},\omega) + \frac{4\sqrt{2\pi\beta m_l}\sigma_{il}^4\lambda_l}{5[1+m_l/m_i]^{3/2}} \\
& \times\mathbf{\Xi}_0^{(il)}(\mathbf{q})\cdot\odot\,\frac{\partial}{\partial\mathbf{q}}[\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\mathcal{Q}}_{Tk}^{(l)}(\mathbf{q})] + \frac{32\sqrt{\pi\beta m_l}\sigma_{il}^2\lambda_l}{15[1+m_l/m_i]}[\tau_{l\eta}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\mathcal{A}}_{il}(q):\hat{\mathcal{P}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)]_1 + \frac{16\sqrt{\pi\beta m_l}\sigma_{il}^2\lambda_l}{15[1+m_l/m_i]} \\
& \times\left[\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_{l\eta}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\mathcal{A}}_{il}(\mathbf{q}):\hat{\mathcal{P}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1\right]_1 - \delta_{kl}\,\frac{16}{15}\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i[\tau_{i\eta}^*(\mathbf{q},\omega)n_i(\mathbf{q})\hat{\mathcal{A}}_{ii}^0(q):\hat{\mathcal{P}}_{\nabla Tk}^{(i)}(\mathbf{q},\omega)]_1 \\
& -\delta_{kl}\,\frac{8}{15}\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i\left[\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_{i\eta}^*(\mathbf{q},\omega)n_i(\mathbf{q})\hat{\mathcal{A}}_{ii}^0(\mathbf{q}):\hat{\mathcal{P}}_{\Delta Tk}^{(i)}(\mathbf{q},\omega)]_1\right]_1 + \frac{\sigma_{il}^2}{5}\sqrt{\frac{\beta m_i}{\pi}}[\hat{\mathcal{B}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\hat{\mathbf{q}},\omega)]_1 \\
& -\delta_{kl}\,\frac{\sigma_{iw}^2}{5}\sqrt{\frac{\beta m_i}{\pi}}[\hat{\mathcal{B}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\lambda}}_{ik}^{(2)}(\mathbf{q},\omega)]_1 + \frac{12}{25}\sqrt{\pi\beta m_i}\sigma_{il}^2\lambda_l\left[\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_{l\lambda}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\mathcal{B}}_{il}(\mathbf{q})\cdot\hat{\mathcal{Q}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1\right]_1 \\
& -\delta_{lk}\,\frac{12}{25}\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i\left[\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_{i\lambda}^*(\mathbf{q},\omega)n_i(\mathbf{q})\hat{\mathcal{B}}_{ii}^0(\mathbf{q})\cdot\hat{\mathcal{Q}}_{\Delta Tk}^{(i)}(\mathbf{q},\omega)]_1\right]_1\Bigg\},
\end{aligned} \tag{C1}$$

where $[\mathbf{T}\cdots\mathbf{T}]_1$ means that the left index of the tensor $\mathbf{T}\cdots\mathbf{T}$ has to be convoluted with the nearest $\partial/\partial\mathbf{q}$ to the left; the notation $\odot$ means that the right index of the nearest tensor to the left of $\odot$ has to be convoluted with the nearest $\partial/\partial\mathbf{q}$ to the right of this sign. The explicit expressions for the Cartesian tensors $\mathbf{\Phi}^{ik}$, $\mathbf{\Xi}^{ik}$, and $\mathbf{F}^{ik}$ can be found in Appendix B. The $2m$th rank Cartesian tensors $\hat{\mathbf{1}}_{2m}$ are defined and discussed in Appendix D of Ref. [2],

$$(\hat{\mathbf{1}}_{2m})_{\underbrace{ijk\cdots\alpha\beta\gamma}_{2m}} = \underbrace{\delta_{i\alpha}\delta_{j\beta}\cdots\delta_{k\gamma}}_{m}, \quad m=1,2\ \ldots\ .$$

The Cartesian tensors $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ are defined by the expressions

$$\hat{\mathcal{A}}_{ik}(\mathbf{q}) = \mathbf{F}_{03}^{(ik)}(\mathbf{q}) + \sigma_{ik}\,\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{F}_{04}^{(ik)}(\mathbf{q}) + \frac{1}{2}\,\sigma_{ik}^2\,\frac{\partial}{\partial\mathbf{q}}:\mathbf{F}_{05}^{(ik)}(\mathbf{q}),$$

$$\hat{\mathcal{A}}_{ii}^{(0)}(\mathbf{q}) = \int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\mathbf{I}_P + \sum_{k=1}^{N}\frac{2\sigma_{ik}^2}{\sigma_{iw}^2}\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\left[\frac{1}{1+m_k/m_i}\,\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}} + \frac{1}{2}\,\mathbf{I}_P\right],$$

$$\hat{\mathcal{B}}_{ik}(\mathbf{q}) = \frac{\sqrt{2m_k/m_i}}{[1+m_k/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[n_i(\mathbf{q})-(1-m_k/m_i)n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})][\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}] + \sigma_{ik}\,\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Xi}^{(ik)}(\mathbf{q}),$$

$$\begin{aligned}
\hat{\mathcal{B}}_{ii}^0(\mathbf{q}) = \sum_{k=1}^{N}\frac{\sigma_{ik}^2\sqrt{2m_k/m_i}}{\sigma_{iw}^2[1+m_k/m_i]^{3/2}}&\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}] \\
&+\sqrt{2}\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})[\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I}].
\end{aligned} \tag{C2}$$

The second-rank Cartesian tensor $\mathbf{\Pi}_{i3}^{(k)}(\mathbf{q})$ has the form

$$\mathbf{\Pi}_{i3}^{(k)}(\mathbf{q})=\sum_{l=1}^{N}\Bigg\{-\delta_{kl}\frac{k_B\sigma_{ik}^4}{2[1+m_k/m_i]}\mathbf{\Phi}_{03}^{(ik)}(\mathbf{q})-\frac{32}{15}\sqrt{\pi\beta m_l}\lambda_l\tau_{l\eta}^*(\mathbf{q},\omega)n_l(\mathbf{q})\left[\delta_{il}\hat{\mathbf{1}}_4+\frac{\sigma_{il}^3}{1+m_l/m_i}\mathbf{F}_4^{(il)}(\mathbf{q})\right]:\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)$$
$$+\frac{16\sqrt{\pi\beta m_l}\lambda_l\sigma_{il}^4}{15[1+m_l/m_i]}\mathbf{F}_{05}^{(il)}(\mathbf{q}):\odot\frac{\partial}{\partial\mathbf{q}}[\tau_{l\eta}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\mathcal{P}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)]-\frac{2\sigma_{il}^3}{5[1+m_l/m_i]^{3/2}}\sqrt{\frac{2\beta m_l}{\pi}}\mathbf{\Xi}^{(il)}(\mathbf{q})\cdot$$
$$\times\hat{\lambda}_{lk}^{(2)}(\mathbf{q},\omega)+\frac{\sigma_{il}^4}{5[1+m_l/m_i]^{3/2}}\sqrt{\frac{2\beta m_l}{\pi}}\mathbf{\Xi}_0^{(il)}(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}}[\hat{\lambda}_{il}^{(2)}(\mathbf{q},\omega)]-\frac{4\sigma_{il}^4\lambda_l}{5[1+m_l/m_i]^{3/2}}\sqrt{2\pi\beta m_l}\tau_{l\lambda}^*(\mathbf{q},\omega)$$
$$\times\mathbf{\Xi}_0^{(il)}(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(l)}(\mathbf{q},\omega)\mathbf{I}-\frac{\pi\sigma_{il}^4\lambda_l}{1+m_l/m_i}\sqrt{\pi\beta m_l}\tau_{l\eta}^*(\mathbf{q},\omega)\tau_{l\lambda}^*(\mathbf{q},\omega)n_l(\mathbf{q})\mathbf{F}_{05}^{(il)}(\mathbf{q}):\odot\bar{\boldsymbol{\mathcal{P}}}_{Tk}^{(l)}(\mathbf{q},\omega)\mathbf{I}$$
$$-\frac{16\sigma_{il}^2\lambda_l\sqrt{\pi\beta m_l}}{15[1+m_l/m_i]}[\tau_{l\eta}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1$$
$$+\tfrac{8}{15}\delta_{kl}\sigma_{iw}^2\lambda_i\sqrt{\pi\beta m_i}[\tau_{i\eta}^*(\mathbf{q},\omega)n_i(\mathbf{q})\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(i)}(\mathbf{q},\omega)]_1-\tfrac{12}{25}\sigma_{il}^2\lambda_l\sqrt{\pi\beta m_l}[\tau_{l\lambda}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1$$
$$+\tfrac{12}{25}\delta_{kl}\sigma_{iw}^2\lambda_i\sqrt{\pi\beta m_i}[\tau_{i\lambda}^*(\mathbf{q},\omega)n_i(\mathbf{q})\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(i)}(\mathbf{q},\omega)]_1\Bigg\}. \tag{C3}$$

The quantity $\mathbf{\Pi}_{i4}^{(k)}(\mathbf{q},\omega)$ is the fourth-rank Cartesian tensor of the form

$$\mathbf{\Pi}_{i4}^{(k)}(\mathbf{q},\omega)=\frac{1}{5}\sum_{l=1}^{N}\Bigg\{\frac{16}{3}\sqrt{\pi\beta m_l}\lambda_l n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\left[\delta_{il}\hat{\mathbf{1}}_4+\frac{\sigma_{il}^3}{1+m_l/m_i}\mathbf{F}_4^{(il)}(\mathbf{q})\right]:\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)-\frac{8\sigma_{il}^4\lambda_l\sqrt{\pi\beta m_l}}{3[1+m_l/m_i]}$$
$$\times\mathbf{F}_{05}^{(il)}(\mathbf{q}):\odot\frac{\partial}{\partial\mathbf{q}}[\tau_{l\eta}^*(\mathbf{q},\omega)n_l(\mathbf{q})\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]+\frac{16\sigma_{il}^4\lambda_l\sqrt{\pi\beta m_l}}{3[1+m_l/m_i]}n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\mathbf{F}_{05}^{(il)}(\mathbf{q}):\odot\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4$$
$$+\frac{24\sigma_{il}^3\lambda_l\sqrt{2\pi\beta m_l}}{5[1+m_l/m_i]^{3/2}}n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\mathbf{\Xi}^{(il)}(\mathbf{q})\cdot\boldsymbol{\mathcal{Q}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)+\frac{\sigma_{il}^4\sqrt{2\beta m_l/\pi}}{[1+m_l/m_i]^{3/2}}\mathbf{\Xi}_0^{(il)}(\mathbf{q})\cdot\odot\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4$$
$$-\frac{12\sigma_{il}^4\lambda_l\sqrt{2\pi\beta m_i}}{5[1+m_l/m_i]^{3/2}}\mathbf{\Xi}_0^{(il)}(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}}[n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]\Bigg\}. \tag{C4}$$

The third-rank Cartesian tensor $\mathbf{\Pi}_{i5}^{(k)}(\mathbf{q},\omega)$ is

$$\mathbf{\Pi}_{i5}^{(k)}(\mathbf{q},\omega)=\sum_{l=1}^{N}\Bigg\{\delta_{kl}\frac{2\sigma_{ik}^3\sqrt{2m_k/(\pi\beta)}}{[1+m_k/m_i]^{1/2}}\mathbf{\Psi}^{(ik)}(\mathbf{q})+8\pi\sigma_{lk}^2\eta_l n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\left[\delta_{il}\hat{\mathbf{1}}_4+\frac{\sigma_{il}^3}{1+m_l/m_i}\mathbf{F}_4^{(il)}(\mathbf{q})\right]:\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(l)}(\mathbf{q},\omega)$$
$$-\frac{4\pi\sigma_{il}^4\sigma_{lk}^2\eta_l}{1+m_l/m_i}\mathbf{F}_{05}^{(il)}(\mathbf{q}):\odot\frac{\partial}{\partial\mathbf{q}}[n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(l)}(\mathbf{q},\omega)]+\frac{24\sigma_{il}^3\sigma_{lw}^2\eta_l}{5[1+m_l/m_i]^{3/2}}n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\mathbf{\Xi}^{(il)}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(l)}(\mathbf{q},\omega)$$
$$-\frac{12\sigma_{il}^4\sigma_{lw}^2\eta_l}{5[1+m_l/m_i]^{3/2}}\mathbf{\Xi}_0^{(il)}(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}}[n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(l)}(\mathbf{q},\omega)]+\frac{2\sigma_{il}^2}{1+m_l/m_i}[\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega)]_1$$
$$-\sigma_{iw}^2\delta_{kl}[\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):\hat{\boldsymbol{\eta}}_{ik}^{(2)}(\mathbf{q},\omega)]_1+\frac{4\pi\sigma_{il}^2\sigma_{lk}^4\eta_l}{1+m_l m_i}\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_1\right]_1$$
$$-2\pi\sigma_{iw}^2\sigma_{ik}^4\eta_l\delta_{kl}\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_i(\mathbf{q})\tau_{i\eta}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(i)}(\mathbf{q},\omega)]_1\right]_1+\tfrac{3}{5}\sqrt{(m_i/m_l)}\sigma_{il}^2\eta_l[\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(l)}(\mathbf{q})]_1$$
$$-\tfrac{3}{5}\sigma_{iw}^2\eta_i\delta_{kl}[\tau_{i\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(i)}(\mathbf{q})]_1+\tfrac{3}{5}\sqrt{(m_i/m_l)}\sigma_{il}^2\eta_l\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q})]_1\right]_1$$
$$-\tfrac{3}{5}\sigma_{iw}^2\eta_i\delta_{kl}\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_i(\mathbf{q})\tau_{i\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(i)}(\mathbf{q})]_1\right]_1\Bigg\}. \tag{C5}$$

The fourth-rank Cartesian tensor $\mathbf{\Pi}_{i6}^{(k)}(\mathbf{q},\omega)$ is given by the expression

$$\mathbf{\Pi}_{i6}^{(k)}(\mathbf{q},\omega)=-8\pi\eta_k\tau_{k\eta}^{*}(\mathbf{q},\omega)\left[\delta_{ik}\hat{\mathbf{1}}_4+\frac{\sigma_{ik}^3}{1+m_k/m_i}\mathbf{F}_4^{(ik)}(\mathbf{q})\right]+\frac{4\pi\sigma_{ik}^4\eta_k}{1+m_k/m_i}\mathbf{F}_{05}^{(ik)}(\mathbf{q})\odot\frac{\partial}{\partial\mathbf{q}}[\tau_{k\eta}^{*}(\mathbf{q},\omega)]$$
$$-\frac{3\pi\sigma_{ik}^3\eta_k}{\sqrt{2}[1+m_k/m_i]^{3/2}}\tau_{k\eta}^{*}(\mathbf{q},\omega)\tau_{k\lambda}^{*}(\mathbf{q},\omega)\mathbf{\Xi}^{(ik)}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})$$
$$+\frac{3\pi\sigma_{ik}^4\eta_k}{2\sqrt{2}[1+m_k/m_i]^{3/2}}\mathbf{\Xi}_0^{(ik)}(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}}[\tau_{k\eta}^{*}(\mathbf{q},\omega)\tau_{k\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})]. \tag{C6}$$

Finally, the fifth-rank Cartesian tensor $\mathbf{\Pi}_{i9}^{(k)}(\mathbf{q},\omega)$ is

$$\mathbf{\Pi}_{i9}^{(k)}(\mathbf{q},\omega)=\frac{4\pi\sigma_{ik}^4\eta_k}{1+m_k/m_i}\tau_{k\eta}^{*}(\mathbf{q},\omega)\mathbf{F}_{05}^{(ik)}(\mathbf{q})+\frac{3\pi\sigma_{ik}^4\eta_k}{2\sqrt{2}[1+m_k/m_i]^{3/2}}\tau_{k\eta}^{*}(\mathbf{q},\omega)\tau_{k,\lambda}^{*}(\mathbf{q},\omega)\mathbf{\Xi}_0^{(ik)}(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q}):\hat{\mathbf{1}}_6. \tag{C7}$$

The tensorial coefficients $\boldsymbol{\mathcal{R}}^{(ik)}(\mathbf{q},\omega)$ on the right-hand side of Eq. (3.11) are given by the expressions

$$\boldsymbol{\mathcal{R}}_u^{(ik)}(\mathbf{q},\omega)=\frac{2\sigma_{ik}^2\sqrt{2m_k}}{\sqrt{\pi\beta}[1+m_k/m_i]^{1/2}}\left[\mathbf{\Phi}_{02}^{(ik)}(\mathbf{q})+\sigma_{ik}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Psi}^{(ik)}(\mathbf{q})\right]-2\sqrt{\frac{2}{\pi\beta}}\delta_{ik}\sum_{l=1}^{N}\frac{\sigma_{il}^2\sqrt{m_l}}{[1+m_l/m_i]^{1/2}}\mathbf{\Phi}_{02}^{(il)}(\mathbf{q})$$
$$+2\sqrt{\frac{2m_i}{\pi\beta}}\sigma_{iw}^2\delta_{ik}\mathbf{\Phi}_{02}^{(iw)}(\mathbf{q})-\sigma_{iw}^2\frac{\partial}{\partial\mathbf{q}}\cdot[\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):\hat{\boldsymbol{\eta}}_{ik}^{(2)}(\mathbf{q},\omega)]_1-2\pi\sigma_{iw}^2\sigma_{ik}^4\eta_i\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_i(\mathbf{q})\tau_{i\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):$$
$$\times\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(i)}(\mathbf{q},\omega)]_{12}-4\pi\sigma_{iw}^2\sigma_{ik}^4\eta_i n_i(\mathbf{q})\tau_{i\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(i)}(\mathbf{q},\omega)-\frac{3}{5}\sigma_{iw}^2\eta_i\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_{i\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(i)}(\mathbf{q},\omega)]_1$$
$$-\frac{3}{5}\sigma_{iw}^2\eta_i\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_i(\mathbf{q})\tau_{i\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(i)}(\mathbf{q},\omega)]_{12}-\frac{6\sqrt{2}}{5}\sigma_{iw}^4\eta_i n_i(\mathbf{q})\tau_{i\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(i)}(\mathbf{q},\omega)$$
$$+\sum_{l=1}^{N}\left\{\frac{2\sigma_{il}^2}{1+m_l/m_i}\frac{\partial}{\partial\mathbf{q}}\cdot[\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega)]_1+\frac{4\pi\sigma_{il}^2\sigma_{lk}^4\eta_l}{1+m_l/m_i}\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_{12}\right.$$
$$+\frac{8\pi\sigma_{il}^2\sigma_{lk}^2\eta_l}{1+m_l/m_i}n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(l)}(\mathbf{q},\omega)+\frac{3}{5}\sqrt{\frac{m_i}{m_l}}\sigma_{il}^2\eta_l\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(l)}(\mathbf{q},\omega)]_1$$
$$+\frac{3}{5}\sqrt{\frac{m_i}{m_l}}\sigma_{il}^2\eta_l\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_{12}$$
$$\left.+\frac{6}{5}\sqrt{\frac{2m_i}{m_l}}\sigma_{il}^2\sigma_{lw}^2\eta_l n_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(l)}(\mathbf{q},\omega)\right\}, \tag{C8}$$

$$\hat{\boldsymbol{\mathcal{R}}}_T^{(ik)}(\mathbf{q},\omega)=\frac{k_B\sigma_{ik}^2}{1+m_k/m_i}\left[\mathbf{\Phi}_{01}^{(ik)}(\mathbf{q})+\sigma_{ik}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Phi}_2^{(ik)}(\mathbf{q})\right]-\delta_{ik}\sum_{l=1}^{N}\frac{k_B\sigma_{il}^2}{1+m_l/m_i}\mathbf{\Phi}_{01}^{(il)}(\mathbf{q})-\tfrac{16}{15}\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i\frac{\partial}{\partial\mathbf{q}}$$
$$\cdot[n_i(\mathbf{q})\tau_{i\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(i)}(\mathbf{q},\omega)]_1-\tfrac{8}{15}\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_i(\mathbf{q})\tau_{i\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(i)}(\mathbf{q},\omega)]_{12}$$
$$-\pi\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i n_i(\mathbf{q})\tau_{i\eta}^{*}(\mathbf{q},\omega)\tau_{i\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(q):\hat{\boldsymbol{\mathcal{P}}}_{Tk}^{(i)}(\mathbf{q},\omega)-\frac{1}{5}\sqrt{\frac{\beta m_i}{\pi}}\sigma_{iw}^2\frac{\partial}{\partial\mathbf{q}}\cdot[\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\lambda}}_{ik}^{(2)}(\mathbf{q},\omega)]_1$$
$$+\tfrac{4}{5}\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i\tau_{i\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(i)}(\mathbf{q},\omega)-\tfrac{12}{25}\sqrt{\pi\beta m_i}\sigma_{iw}^2\lambda_i\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_i(\mathbf{q})\tau_{i\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(i)}(\mathbf{q},\omega)]_{12}$$
$$+\sum_{l=1}^{N}\left\{\frac{32\sqrt{\pi\beta m_l}\sigma_{il}^2\lambda_l}{15[1+m_l/m_i]}\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)]_1\right.$$
$$+\frac{16\sqrt{\pi\beta m_l}\sigma_{il}^2\lambda_l}{15[1+m_l/m_i]}\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_{12}$$

$$+\frac{2\pi\sqrt{\pi\beta m_l}\sigma_{il}^2\lambda_l}{1+m_l/m_i}\,n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{Tk}^{(l)}(\mathbf{q},\omega)+\frac{1}{5}\sqrt{\frac{\beta m_i}{\pi}}\,\sigma_{il}^2\,\frac{\partial}{\partial\mathbf{q}}\cdot[\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\mathbf{q},\omega)]_1$$
$$-\tfrac{4}{5}\sqrt{\pi\beta m_i}\sigma_{il}^2\lambda_l\tau_{i\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(l)}(\mathbf{q},\omega)+\tfrac{12}{25}\sqrt{\pi\beta m_i}\sigma_{il}^2\lambda_l\,\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{il}(\mathbf{q})\cdot$$
$$\times\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_{12}, \quad \text{(C9)}$$

$$\boldsymbol{\mathcal{R}}_S^{(ik)}(\mathbf{q},\omega)=-\frac{8\pi\sigma_{ik}^2\eta_k}{1+m_k/m_i}\,\tau_{k\eta}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ik}(\mathbf{q})+4\pi\sigma_{iw}^2\eta_i\delta_{ik}\tau_{i\eta}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{A}}}_{ii}^0(\mathbf{q})$$
$$-\tfrac{3}{4}\pi\sigma_{ik}^2\eta_k\sqrt{m_i/m_k}\tau_{k\eta}^*(\mathbf{q},\omega)\tau_{k\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ik}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})+\tfrac{3}{4}\pi\sigma_{iw}^2\eta_i\delta_{ik}\tau_{i\eta}^*(\mathbf{q},\omega)\tau_{i\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{B}}}_{ii}^0(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{C}}}_P^{(i)}(\mathbf{q}). \quad \text{(C10)}$$

In the above definitions the notation $[\mathbf{T}\cdots\mathbf{T}]_{12}$ means that the two left indices of the tensor $\mathbf{T}\cdots\mathbf{T}$ are convoluted with the indices of the spatial gradients to the left of this tensor [either in the above expressions themselves or in Eqs. (3.11) and (3.12)], which are separated from $[\mathbf{T}\cdots\mathbf{T}]_{12}$ with the convolution sign(s). The Cartesian tensors $\mathbf{F}^{(ik)}$, $\boldsymbol{\Xi}^{(ik)}$, $\boldsymbol{\Phi}^{(ik)}$, and $\boldsymbol{\Psi}^{(ik)}$ are defined in Appendix B.

APPENDIX D: COEFFICIENTS IN EQS. (3.27) AND (3.28)

The coefficient $\mathbf{J}_{i1}^{(k)}(\mathbf{q},\omega)$ is the second-rank Cartesian tensor

$$\mathbf{J}_{i1}^{(k)}(\mathbf{q},\omega)=k_BTn_i(\mathbf{q})\delta_{ik}\mathbf{I}+\frac{3k_BT(m_k/m_i)b_{ik}}{2\pi[1+m_k/m_i]}\,\boldsymbol{\Phi}_2^{(ik)}(\mathbf{q})+\sum_{l=1}^{N}\Bigg\{2[\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega)]_1$$
$$+4\pi\sigma_{lk}^4\eta_l\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_1\right]_1+3\sqrt{\frac{\pi}{\beta m_l}}\,\eta_l\tau_{l\lambda}^*(\mathbf{q},\omega)[\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(l)}(\mathbf{q},\omega)]_1$$
$$+3\sqrt{\frac{\pi}{\beta m_l}}\,\eta_l\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_1\right]_1$$
$$+6\sqrt{\frac{2\pi}{\beta m_l}}\,\sigma_{lw}^2\eta_ln_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\left[\delta_{il}\mathbf{I}+\frac{9(m_l/m_i)b_{il}}{5\pi[1+m_l/m_i]^2}\,\mathbf{F}_2^{(il)}(\mathbf{q})\right]\cdot\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(l)}(\mathbf{q},\omega)$$
$$-\sqrt{\frac{2\pi}{\beta m_l}}\frac{27(m_l/m_i)\sigma_{il}b_{il}\sigma_{lw}^2\eta_l}{5\pi[1+m_l/m_i]^2}\,\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\,\frac{\partial}{\partial\mathbf{q}}[n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(l)}(\mathbf{q},\omega)]$$
$$+\sqrt{\frac{2\pi}{\beta m_i}}\frac{16\sqrt{m_l/m_i}\sigma_{il}^3\sigma_{lk}^2\eta_l}{[1+m_l/m_i]^{3/2}}\,\eta_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\mathbf{F}_3^{(il)}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(l)}(\mathbf{q},\omega)$$
$$-\sqrt{\frac{2\pi}{\beta m_i}}\frac{8\sqrt{m_l/m_i}\sigma_{il}^4\sigma_{lk}^2\eta_l}{[1+m_l/m_i]^{3/2}}\,\mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\,\frac{\partial}{\partial\mathbf{q}}[n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(l)}(\mathbf{q},\omega)]\Bigg\}, \quad \text{(D1)}$$

where the second-rank Cartesian tensor $\hat{\boldsymbol{\mathcal{L}}}_{ik}(q)$ is defined as

$$\hat{\boldsymbol{\mathcal{L}}}_{ik}(\mathbf{q})=\frac{2\sqrt{2m_k/m_i}\sigma_{ik}^2}{\sqrt{\pi\beta m_i}[1+m_k/m_i]^{3/2}}\left[n_i(\mathbf{q})\int d\hat{\sigma}\;g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}+\sigma_{ik}\,\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{F}_3^{(ik)}(\mathbf{q})\right]$$
$$-\delta_{ik}\sum_{l=1}^{N}\frac{\sigma_{il}^2\sqrt{m_l/m_i}[1+m_k/m_i]^{3/2}}{\sigma_{ik}^2\sqrt{m_k/m_i}[1+m_l/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\;n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}, \quad \text{(D2)}$$

and the Cartesian three-vector $\hat{\boldsymbol{\mathcal{M}}}_{ik}(\mathbf{q})$ is

$$\hat{\boldsymbol{M}}_{ik}(\mathbf{q}) = \frac{\sigma_{ik}^2}{5[1+m_k/m_i]^2}\left[-5+2\left(\frac{m_k}{m_i}\right)-5\left(\frac{m_k}{m_i}\right)^2\right]\int d\hat{\boldsymbol{\sigma}}\, n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}$$
$$+\delta_{ik}\sigma_{iw}^2\int d\hat{\boldsymbol{\sigma}}\, n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}+\frac{6(m_k/m_i)\sigma_{ik}^2}{5[1+m_k/m_i]^2}\left[n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\, g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\right.$$
$$\left.+\sigma_{ik}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{F}_2^{(ik)}(\mathbf{q})-\delta_{ik}\sum_{l=1}^{N}\frac{\sigma_{il}^2(m_l/m_i)[1+m_k/m_i]^2}{\sigma_{ik}^2(m_k/m_i)[1+m_l/m_i]^2}\int d\hat{\boldsymbol{\sigma}}\, n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\right]. \tag{D3}$$

The third-rank Cartesian tensor $\mathbf{J}_{i2}^{(k)}(\mathbf{q})$ is defined by the expression

$$\mathbf{J}_{i2}^{(k)}(\mathbf{q}) = -\frac{15\pi\eta_k}{4}\sqrt{\frac{\pi}{\beta m_k}}\,\tau_{k\eta}^*(\mathbf{q},\omega)\tau_{k\lambda}^*(\mathbf{q},\omega)\left[\delta_{ik}\mathbf{I}+\frac{9(m_k/m_i)b_{ik}}{5\pi[1+m_k/m_i]^2}\mathbf{F}_2^{(ik)}(\mathbf{q})\right]\cdot\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})$$
$$+\frac{27(m_k/m_i)\sigma_{ik}b_{ik}\eta_k}{8[1+m_k/m_i]^2}\sqrt{\frac{\pi}{\beta m_k}}\,\mathbf{F}_{03}^{(ik)}(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}}[\tau_{k\eta}^*(\mathbf{q},\omega)\tau_{k\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})]$$
$$-\frac{16\sqrt{2m_k/m_i}\,\sigma_{ik}^3\eta_k}{[1+m_k/m_i]^{3/2}}\sqrt{\frac{\pi}{\beta m_i}}\,\tau_{k\eta}^*(\mathbf{q},\omega)\mathbf{F}_3^{(ik)}(\mathbf{q})+\frac{8\sqrt{2m_k/m_i}\,\sigma_{ik}^4\eta_k}{[1+m_k/m_i]^{3/2}}\sqrt{\frac{\pi}{\beta m_i}}\,\mathbf{F}_{04}^{(ik)}(\mathbf{q}):\odot\frac{\partial}{\partial\mathbf{q}}[\tau_{k\eta}^*(\mathbf{q},\omega)]\hat{\mathbf{1}}_4. \tag{D4}$$

The definition of the fourth-rank Cartesian tensor $\mathbf{J}_{i3}^{(k)}(\mathbf{q},\omega)$ is

$$\mathbf{J}_{i3}^{(k)}(\mathbf{q},\omega) = \frac{27(m_k/m_i)\sigma_{ik}b_{ik}\eta_k}{8[1+m_k/m_i]^2}\sqrt{\frac{\pi}{\beta m_k}}\,\tau_{k\lambda}^*(\mathbf{q},\omega)\tau_{k\eta}^*(\mathbf{q},\omega)\mathbf{F}_{03}^{(ik)}(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q}):\hat{\mathbf{1}}_6$$
$$+\frac{8\sqrt{2m_k/m_i}\,\sigma_{ik}^4\eta_k}{[1+m_k/m_i]^{3/2}}\sqrt{\frac{\pi}{\beta m_i}}\,\tau_{k\eta}^*(\mathbf{q},\omega)\mathbf{F}_{04}^{(ik)}(\mathbf{q}). \tag{D5}$$

The third-rank Cartesian tensor $\mathbf{J}_{i4}^{(k)}(\mathbf{q},\omega)$ is given by the expression

$$\mathbf{J}_{i4}^{(k)}(\mathbf{q},\omega) = \sum_{l=1}^{N}\left\{-\frac{3k_BT(m_k/m_i)\sigma_{ik}b_{ik}}{4\pi[1+m_k/m_i]}\delta_{kl}\boldsymbol{\Phi}_{03}^{(ik)}(\mathbf{q})-4\pi\sigma_{lk}^4\eta_l n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)[\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_1\right.$$
$$-3\eta_l\sqrt{\frac{\pi}{\beta m_l}}\,n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)[\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_1-3\eta_l\sqrt{\frac{\pi}{\beta m_l}}\,\tau_{l\lambda}^*(\mathbf{q},\omega)\left[\delta_{il}\mathbf{I}+\frac{9(m_l/m_i)b_{il}}{5\pi[1+m_l/m_i]^2}\right.$$
$$\left.\times\mathbf{F}_2^{(il)}(\mathbf{q})\right]\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(l)}(\mathbf{q},\omega)+\frac{27(m_l/m_i)\sigma_{il}b_{il}}{10\sqrt{\pi\beta m_l}[1+m_l/m_i]^2}\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\frac{\partial}{\partial\mathbf{q}}[\tau_{l\lambda}^*(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(l)}(\mathbf{q},\omega)]$$
$$-\frac{27\sqrt{2}(m_l/m_i)\sigma_{il}\sigma_{lw}^2b_{il}\eta_l}{5\sqrt{\pi\beta m_l}[1+m_l/m_i]^2}n_l(\mathbf{q})\tau_{l\lambda}^*(\mathbf{q},\omega)\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(l)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4-\frac{4\sqrt{2m_l/m_i}\,\sigma_{il}^3}{\sqrt{\pi\beta m_i}[1+m_l/m_i]^{3/2}}\mathbf{F}_3^{(il)}(\mathbf{q}):\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega)$$
$$+\frac{2\sqrt{2m_l/m_i}\,\sigma_{il}^4}{\sqrt{\pi\beta m_i}[1+m_l/m_i]^{3/2}}\mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\frac{\partial}{\partial\mathbf{q}}\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega)$$
$$\left.-\frac{8\sqrt{2m_l/m_i}\,\sigma_{il}^4\sigma_{lk}^2\eta_l}{\sqrt{\pi\beta m_i}[1+m_l/m_i]^{3/2}}n_l(\mathbf{q})\tau_{l\eta}^*(\mathbf{q},\omega)\mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(l)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4\right\}. \tag{D6}$$

The third-rank Cartesian tensor $\mathbf{J}_{i5}^{(k)}(\mathbf{q},\omega)$ has the form

$$\mathbf{J}_{i5}^{(k)}(\mathbf{q},\omega)=\sum_{l=1}^{N}\left\{3\sqrt{\frac{\pi}{\beta m_l}}\ \eta_l\eta_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\left[\delta_{il}\mathbf{I}+\frac{9(m_l/m_i)b_{il}}{5\pi[1+m_l/m_i]^2}\ \mathbf{F}_2^{(il)}(\mathbf{q})\right]\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)\right.$$
$$+\frac{27(m_l/m_i)\sigma_{il}b_{il}\eta_l}{10\sqrt{\pi\beta m_l}[1+m_l/m_i]^2}\ \tau_{l\lambda}^{*}(\mathbf{q},\omega)\mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(l)}(\mathbf{q},\omega):\hat{\mathbf{1}}_6$$
$$-\frac{27(m_l/m_i)\sigma_{il}b_{il}\eta_l}{10\sqrt{\pi\beta m_l}[1+m_l/m_i]^2}\ \mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\ \frac{\partial}{\partial\mathbf{q}}\left[n_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)\right]$$
$$+\frac{8\sqrt{m_l/m_i}\sigma_{il}^3\sigma_{lk}^4\eta_l}{[1+m_l/m_i]^{3/2}}\ \sqrt{\frac{2\pi}{\beta m_i}}\ n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\mathbf{F}_3^{(il)}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)+\frac{2\sqrt{2m_l/m_i}\sigma_{il}^4}{\sqrt{\pi\beta m_i}[1+m_l/m_i]^{3/2}}\ \mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot$$
$$\left.\times\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega):\hat{\mathbf{1}}_6-\frac{4\sqrt{m_l/m_i}\sigma_{il}^4\sigma_{lk}^4\eta_l}{[1+m_l/m_i]^{3/2}}\ \sqrt{\frac{2\pi}{\beta m_i}}\ \mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\ \frac{\partial}{\partial\mathbf{q}}\left[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)\right].\right. \quad \text{(D7)}$$

The expression for the Cartesian three-vector $\mathbf{J}_{i6}^{(k)}(\mathbf{q},\omega)$ is

$$\mathbf{J}_{i6}^{(k)}(\mathbf{q},\omega)=\frac{96\sqrt{2m_k/m_i}b_{ii}b_{ik}\lambda_i}{25\pi^2\sigma_{ii}[1+m_k/m_i]^{3/2}}\ \boldsymbol{\Phi}_1^{(ik)}(\mathbf{q})+\sum_{l=1}^{N}\left\{\frac{32}{15}\ \sqrt{\pi\beta m_l}\lambda_l n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)[\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q},\omega):\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)]_1\right.$$
$$+\frac{16}{15}\ \sqrt{\pi\beta m_l}\lambda_l\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q},\omega):\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1\right]_1+[\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\mathbf{q},\omega)]_1$$
$$+\frac{12}{15}\ \pi\lambda_l\left[\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q},\omega)\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_1\right]_1$$
$$-4\pi\lambda_l\tau_{l\lambda}^{*}(\mathbf{q},\omega)\left[\delta_{il}\mathbf{I}+\frac{9(m_l/m_i)b_{il}}{5\pi[1+m_l/m_i]^2}\ \mathbf{F}_2^{(il)}(\mathbf{q})\right]\cdot\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(l)}(\mathbf{q},\omega)$$
$$+\frac{18(m_l/m_i)\sigma_{il}b_{il}\lambda_l}{5[1+m_l/m_i]^2}\ \mathbf{F}_{03}^{(il)}(\mathbf{q})\cdot\odot\ \frac{\partial}{\partial\mathbf{q}}\left[\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(l)}(\mathbf{q},\omega)\right]$$
$$+\frac{4\pi\sqrt{2m_l/m_i}\sigma_{il}^3\lambda_l}{[1+m_l/m_i]^{3/2}}\ n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\tau_{l\lambda}^{*}(\mathbf{q},\omega)\mathbf{F}_3^{(il)}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{Tk}^{(l)}(\mathbf{q},\omega)$$
$$\left.-\frac{2\pi\sqrt{2m_l/m_i}\sigma_{il}^4\lambda_l}{[1+m_l/m_i]^{3/2}}\ \mathbf{F}_{04}^{(il)}(\mathbf{q}):\odot\ \frac{\partial}{\partial\mathbf{q}}\left[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{P}}}_{Tk}^{(l)}(\mathbf{q},\omega)\right]\right\}. \quad \text{(D8)}$$

The coefficients $\mathfrak{R}^{(ik)}(\mathbf{q})$ on the right-hand side of Eq. (3.27) are given by the expressions

$$\mathfrak{R}_u^{(ik)}(\mathbf{q},\omega)=\frac{3k_BT(m_k/m_i)b_{ik}}{2\pi[1+m_k/m_i]}\ \frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Phi}_2^{(ik)}(\mathbf{q})+\delta_{ik}\sigma_{iw}^2k_BTn_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\ n_w(\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})g_{iw}(\mathbf{q},\mathbf{q}-\sigma_{iw}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}$$
$$+\frac{k_BT(m_k/m_i)\sigma_{ik}^2}{1+m_k/m_i}\ \boldsymbol{\Phi}_{01}^{(ik)}(\mathbf{q})-k_BT\delta_{ik}\sum_{l=1}^{N}\ \frac{(m_l/m_i)\sigma_{il}^2}{1+m_l/m_i}\ \boldsymbol{\Phi}_{01}^{(il)}(\mathbf{q})+\sum_{l=1}^{N}\left[2\ \frac{\partial}{\partial\mathbf{q}}\cdot[\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\eta}}_{lk}^{(2)}(\mathbf{q},\omega)]_1\right.$$
$$+4\pi\sigma_{lk}^4\eta_l\ \frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_{12}+8\pi\sigma_{lk}^2\eta_l n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{uk}^{(l)}(\mathbf{q},\omega)$$
$$+3\sqrt{\frac{\pi}{\beta m_l}}\ \eta_l\ \frac{\partial}{\partial\mathbf{q}}\cdot[\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\nabla uk}^{(l)}(\mathbf{q},\omega)]_1+3\sqrt{\frac{\pi}{\beta m_l}}\ \eta_l\ \frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot$$
$$\left.\times\hat{\boldsymbol{\mathcal{Q}}}_{\Delta uk}^{(l)}(\mathbf{q},\omega)]_{12}+6\sqrt{\frac{2\pi}{\beta m_l}}\ \sigma_{lw}^2\eta_l n_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{uk}^{(l)}(\mathbf{q},\omega)\right], \quad \text{(D9)}$$

$$\mathfrak{R}_T^{(ik)}(\mathbf{q},\omega)=\frac{96\sqrt{2}b_{ii}\lambda_i}{25\pi^2\sigma_{ii}}\left[\frac{\sqrt{m_k/m_i}b_{ik}}{\sigma_{ik}[1+m_k/m_i]^{3/2}}\,n_i(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}\,n_k(\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})g_{ik}(\mathbf{q},\mathbf{q}-\sigma_{ik}\hat{\boldsymbol{\sigma}})\right.$$
$$\left.-\delta_{ik}n_i(\mathbf{q})\sum_{l=1}^{N}\frac{\sqrt{m_l/m_i}b_{il}}{\sigma_{il}[1+m_l/m_i]^{3/2}}\int d\hat{\boldsymbol{\sigma}}\,n_l(\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})g_{il}(\mathbf{q},\mathbf{q}-\sigma_{il}\hat{\boldsymbol{\sigma}})\right]+\frac{96\sqrt{2}b_{ii}\lambda_i}{25\pi^2\sigma_{ii}}\frac{\sqrt{m_k/m_i}b_{ik}}{[1+m_k/m_i]^{3/2}}\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Phi}_1^{(ik)}(\mathbf{q})$$
$$+\sum_{l=1}^{N}\left[\frac{32}{15}\sqrt{\pi\beta m_l}\lambda_l\frac{\partial}{\partial\mathbf{q}}\cdot[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{il}(q):\hat{\boldsymbol{\mathcal{P}}}_{\nabla Tk}^{(l)}(\mathbf{q},\omega)]_1\right.$$
$$+\frac{16}{15}\sqrt{\pi\beta m_l}\lambda_l\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{il}(\mathbf{q}):\hat{\boldsymbol{\mathcal{P}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_{12}$$
$$+2\pi\sqrt{\pi\beta m_l}\lambda_l n_l(\mathbf{q})\tau_{l\eta}^{*}(\mathbf{q},\omega)\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{il}(q):\hat{\boldsymbol{\mathcal{P}}}_{Tk}^{(l)}(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot[\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\lambda}}_{lk}^{(2)}(\mathbf{q},\omega)]_1$$
$$\left.-4\pi\lambda_l\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{Tk}^{(l)}(\mathbf{q},\omega)+\frac{12}{5}\pi\lambda_l\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:[n_l(\mathbf{q})\tau_{l\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{M}}}_{il}(\mathbf{q})\cdot\hat{\boldsymbol{\mathcal{Q}}}_{\Delta Tk}^{(l)}(\mathbf{q},\omega)]_{12}\right],\tag{D10}$$

$$\mathfrak{R}_S^{(ik)}(\mathbf{q},\omega)=-8\pi\eta_k\tau_{k\eta}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{L}}}_{ik}(\mathbf{q})-\frac{15}{4}\pi\sqrt{\frac{\pi}{\beta m_k}}\eta_k\tau_{k\eta}^{*}(\mathbf{q},\omega)\tau_{k\lambda}^{*}(\mathbf{q},\omega)\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q}).\tag{D11}$$

All notations in the above expressions are those of Appendixes B and C and of Secs. II and III. We note that the quantities $\mathfrak{R}_u^{(ik)}(\mathbf{q},\omega)$, $\mathfrak{R}_T^{(ik)}(\mathbf{q},\omega)$, and $\mathfrak{R}_S^{(ik)}(\mathbf{q},\omega)$ are the Cartesian three-vector, scalar, and the Cartesian second-rank tensor, respectively.

APPENDIX E: *G* TERMS IN EQS. (3.20)–(3.22)

The terms $\mathbf{G}_S^{(k)}(\mathbf{q},\omega)$, $\mathbf{G}_T^{(k)}(\mathbf{q},\omega)$, and $\mathbf{G}_B^{(k)}(\mathbf{q},\omega)$ are the Cartesian tensors of the fourth and second ranks, respectively, and are defined by the expressions

$$\mathbf{G}_S^{(k)}(\mathbf{q},\omega)=\frac{4\pi\sigma_{ik}^4\eta_k}{1+m_k/m_i}\tau_{k\eta}^{*}(\mathbf{q},\omega)\left\{\mathbf{F}_{05}^{(ik)}(\mathbf{q})\odot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}-\frac{1}{3}\mathbf{F}_{03}^{(ik)}(\mathbf{q})\circ\left[\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\cdot\hat{\mathbf{1}}_4\right]\right.$$
$$+\frac{3}{8\sqrt{2}[1+m_k/m_i]^{1/2}}\left(\frac{1}{2}\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q}):\circ\left[\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})\cdot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\right]\cdot\hat{\mathbf{1}}_4+\frac{1}{2}\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q})\cdot\odot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})\right.$$
$$\left.\left.-\frac{1}{3}\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q})\cdot\circ[\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q}):\mathbf{I}]\left[\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\cdot\hat{\mathbf{1}}_4\right]\right)\right\},\tag{E1}$$

$$\mathbf{G}_T^{(k)}(\mathbf{q},\omega)=\frac{4\pi\sigma_{ik}^4\eta_k}{1+m_k/m_i}\tau_{k\eta}^{*}(\mathbf{q},\omega)\left\{\mathbf{F}_{05}^{(ik)}(\mathbf{q})\odot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}+\frac{1}{3}\mathbf{F}_{03}^{(ik)}(\mathbf{q})\circ\left[\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\cdot\hat{\mathbf{1}}_4\right]+\frac{3}{8\sqrt{2}[1+m_k/m_i]^{1/2}}\tau_{k\lambda}^{*}(\mathbf{q},\omega)\right.$$
$$\times\left(\frac{1}{2}\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q}):\circ\left[\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})\cdot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\right]\cdot\hat{\mathbf{1}}_4-\frac{1}{2}\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q})\cdot\odot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})\right.$$
$$\left.\left.+\frac{1}{3}\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q})\cdot\circ[\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q}):\mathbf{I}]\left[\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\cdot\hat{\mathbf{1}}_4\right]\right)\right\},\tag{E2}$$

$$\mathbf{G}_B^{(k)}(\mathbf{q},\omega)=\frac{8\pi\sigma_{ik}^4\eta_k}{1+m_k/m_i}\tau_{k\eta}^{*}(\mathbf{q},\omega)\left\{\mathbf{F}_{03}^{(ik)}(\mathbf{q})\odot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}+\frac{3\tau_{k\lambda}^{*}(\mathbf{q},\omega)}{32\sqrt{2}[1+m_k/m_i]^{1/2}}\left[\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q}):\hat{\boldsymbol{\mathcal{C}}}_P^{(k)}(\mathbf{q})\odot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\right.\right.$$
$$\left.\left.+\frac{1}{3}\left[\boldsymbol{\Xi}_0^{(ik)}(\mathbf{q})\odot\frac{\partial n_k(\mathbf{q})}{\partial\mathbf{q}}\right][\boldsymbol{\mathcal{C}}_P^{(k)}(\mathbf{q}):\mathbf{I}]\right]\right\},\tag{E3}$$

where $\circ$ denotes convolution with respect to the closest index of the tensor $\hat{\mathbf{1}}_4$.

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