Transport theory of dense, strongly inhomogeneous fluids

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The generalized Enskog-like kinetic equation (GEKE) derived recently for inhomogeneous fluids [L. A. Pozhar and K. E. Gubbins, J. Chem. Phys. **94**, 1367 (1991)] has been solved using the thirteen-moments approximation method to obtain linearized Navier–Stokes equations and the associated zero-frequency transport coefficients. Simplified transport coefficient expressions have been obtained for several special cases (simplified geometries, homogeneous fluid). For these cases it is shown that the main contributions to the transport coefficients can be related to those for dense homogeneous fluids calculated at "smoothed" number densities and pair correlation functions. The smoothing procedure has been derived rigorously and shown to be an intrinsic feature of the GEKE approach. These results have been established for an arbitrary dense inhomogeneous fluid with intermolecular interactions represented by a sum of hard-core repulsive and soft attractive potentials in an arbitrary external potential field and/or near structured solid surfaces of arbitrary geometries.

I. INTRODUCTION

In recent years it has become clear that the properties of fluids at interfaces and in micropores (pore widths less than 20 Å) differ markedly from those of bulk fluids. Such strongly inhomogeneous, dense fluids play a crucial role in a number of natural and industrial processes, including adsorption and transport in adsorbents and clays, dispersion of environmental pollutants, metabolism of living cells, etc. For equilibrium properties of strongly inhomogeneous fluids, considerable progress has been made over the last few years. Classical equations such as that due to Kelvin are now known to fail badly for highly inhomogeneous fluids (e.g., for confined fluids in pores with widths below 80 Å); however, statistical mechanical approaches such as density functional theory and some forms of integral equation theory can describe a wide range of equilibrium phenomena (phase transitions, adsorption, isosteric heat, solvation forces, etc.). Much less attention has been paid to transport properties of such highly inhomogeneous systems. However, from our experience with equilibrium properties we can anticipate that approaches based on continuum mechanics or on bulk-phase kinetic equations plus boundary conditions are likely to break down when the scales of spatial inhomogeneity and intermolecular spacing are comparable.

The most successful approach to transport properties of inhomogeneous fluids so far was proposed by Davis,[1,2] and is based on an intuitively reasonable extension of the revised Enskog theory.[3–5] Although Davis' theory advanced our understanding of the transport behavior of inhomogeneous fluids, explicit expressions for the transport coefficients were found only for the cases of a local equilibrium velocity distribution for weakly inhomogeneous fluids, with inhomogeneity in one direction. These results included an additional *ad hoc* assumption, according to which the *nonequilibrium inhomogeneous* fluid pair correlation function contact values were equated to those of the corresponding *homogeneous equilibrium* fluid calculated at the Fischer–Methfessel[6] smoothed density for the equilibrium inhomogeneous fluid.

In our previous work[7] we developed a rigorous microscopic theory describing nonequilibrium behavior of dense, strongly inhomogeneous fluid mixtures. Introducing the generalized Mori projection operator method[7] we have derived a functional perturbation theory (FPT) to describe the evolution of the many-body dynamic system, and have shown rigorously that generalized Langevin equations (GLE's) should be regarded as the first order form of FPT. Subsequently, we used the GLE's to obtain Enskog-like close-to-equilibrium linearized kinetic equations for the singlet distribution functions of dense inhomogeneous fluid mixtures. These equations proved to be a generalization of a linearized form of those[3] derived for mixtures of hard spheres to a case of inhomogeneous fluid mixtures in which the intermolecular interaction potentials could be represented as a sum of hard-core repulsive and soft attractive contributions. The number densities and structure factors (pair and direct correlation functions) occurring in these equations were those specific to the corresponding *equilibrium inhomogeneous* fluid mixtures; quite accurate theories now exist for these equilibrium correlation functions.[8]

In this paper we solve the kinetic equations derived previously[7] to obtain linearized Navier–Stokes equations and the associated transport coefficients. In carrying out this procedure we have defined the continuum variables (number density, macroscopic velocity, etc.) as corresponding velocity moments of the nonequilibrium singlet distribution function,[9,10] and have used the 13-moments approximation method, as modernized by Sung and Dahler.[11] The expressions for the transport coefficients are obtained without any additional *ad hoc* assumptions, and provide a rigorous generalization of Davis' smoothed density postulate. The theory does not involve any restrictions on the equilibrium inhomogeneous fluid densities or their spatial gradients.

We focus our main attention on the shear and bulk viscosities and the thermal conductivity. These transport coefficients have a tensorial nature; thus, shear viscosity is a fourth rank, while bulk viscosity and thermal conductivity are second rank tensors. The scalar quantities can be recovered by convoluting the tensorial ones with the corresponding contributions to flux tensors composed of the second partial derivatives of macroscopic velocity and temperature. The final expressions for the transport coefficients can be regarded as providing a rigorous density smoothing procedure that relates the various terms in the coefficients for the inhomogeneous fluid to corresponding quantities for a homogeneous fluid. The rigorous smoothing procedure derived here gives different prescriptions for the various transport coefficients, and does not relate them simply to the corresponding coefficients for the homogeneous fluid, but rather to various spatial integrals over the equilibrium inhomogeneous fluid number density and pair correlation function.

A particular interest of ours is the transport behavior of inhomogeneous fluids near solid walls and in narrow pores, and the theory explicitly includes the effects of such structured walls. Thus, we expect the theory to be able to account for the presence of a neighboring wall, or of confinement in a pore; such effects are known to be large.[12–16] In what follows we first consider the general case of arbitrary geometry and degree of inhomogeneity. We then consider several special cases. In the homogeneous fluid limit $[n(\mathbf{q})=\text{const}$, where $n(\mathbf{q})$ is the number density at $\mathbf{q}$, and walls are absent] the general expressions for the transport coefficients reduce to those of Sung and Dahler.[11] The second, and more interesting, special case is that of inhomogeneous fluids confined by solid surfaces of some simple geometry. Examples are fluids confined to a narrow slit, cylindrical or spherical capillary pore, in the absence of any spatially directed external potential field other than that due to the fluid-wall potential. We consider in detail the case of a fluid confined to a slit with structured, parallel walls. For such cases it is possible to derive scalar transport coefficients explicitly; the various contributions to these coefficients can be related to the corresponding terms in the coefficients for the homogeneous fluid, through the smoothing procedure derived. Finally, the special case of Davis' theory results[1] can be recovered by neglecting terms of order $[bn(\mathbf{q})]^2$, where $b=2\pi\sigma^3/3$ (σ is a hard-core diameter), and introducing his approximate smoothing procedure.

II. THE THIRTEEN-MOMENTS APPROXIMATION EQUATIONS

We consider an inhomogeneous fluid of nonreactive, structureless molecules in which the intermolecular interactions are assumed to be pairwise additive, central and decomposable into the sum

$$\varphi_I(q_{ij})=\varphi_H(q_{ij})+\varphi_S(q_{ij}), \tag{2.1}$$

where $\varphi_H(q_{ij})$ is a hard-core repulsive contribution,

$$\varphi_H(q_{ij})=\begin{cases}+\infty, & q_{ij}<\sigma,\\ 0, & q_{ij}>\sigma,\end{cases}$$

and $\varphi_S(q_{ij})$ represents an attractive soft interaction which is assumed to be continuous, and $\mathbf{q}_{ij}=q_{ij}\hat{\mathbf{q}}_{ij}=\mathbf{q}_i-\mathbf{q}_j$, where $\mathbf{q}_i$, $\mathbf{q}_j$ denote coordinate vectors assigned to centers of masses of interacting molecules i and j (of the same species), respectively. The inhomogeneity of the fluid is caused, in general, by both an external field of a continuous potential and fluid-wall molecule intermolecular interactions of the same kind as Eq. (2.1),

$$\varphi_{1w}(q_{1w})=\varphi_H^{1w}(q_{1w})+\varphi_S^{1w}(q_{1w}) \tag{2.2}$$

with the hard-core contribution,

$$\varphi_H^{1w}(q_{1w})=\begin{cases}+\infty, & q_{1w}<\sigma_{1w}\\ 0, & q_{1w}>\sigma_{1w}\end{cases},$$

and a continuous attractive part $\varphi_S^{1w}(q_{1w})$. Here $\mathbf{q}_{1w}=q_{1w}\hat{\mathbf{q}}_{1w}=\mathbf{q}_1-\mathbf{q}_w$, and $\mathbf{q}_1$, $\mathbf{q}_w$ are coordinate vectors of centers of masses of a fluid molecule and a wall molecule, respectively. The walls are considered impenetratable for fluid molecules and thermostated at temperature T, and wall molecules are unmovable from their average positions $\mathbf{q}_w$ (molecules of an infinitely large mass), and belong to the same species. Since the model assumes fixed wall atoms, there will be a net momentum production between the fluid and the wall, but no kinetic energy production. This neglect of kinetic energy flow between the fluid and wall should not affect the transport coefficient expressions, except very close to the wall. These are the primary goal of our work here. We also assume that there is no chemical reaction between any of the molecules in the system.

Neglecting delayed response of the system, and in close vicinity of the equilibrium state of the system, one can use kinetic equation (4.36) of Ref. 7 to describe the kinetic stage of the system evolution. [We note here that the multiplier $n_w(\mathbf{q})g_{1w}(\mathbf{q},\mathbf{q}^1)$ is to be inserted into the kernel of the last integral in the right hand side of Eq. (4.36) of Ref. 7. Also, the last terms in the left hand sides of Eqs. (4.41), (4.45) of Ref. 7 should be omitted.] This equation can be easily transformed to the form

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{q}}\right)\delta F(\mathbf{q},\mathbf{v};t)$$

$$=\int d\mathbf{q}'\,d\mathbf{v}'\,\Gamma(\mathbf{q},\mathbf{v};\mathbf{q}',\mathbf{v}')\,\delta F(\mathbf{q}',\mathbf{v}';t), \tag{2.3}$$

where t is time variable, $\mathbf{q}$, $\mathbf{v}$ and $\mathbf{q}'$, $\mathbf{v}'$ are coordinate vectors and velocities of fluid molecules, $\delta F(\mathbf{q},\mathbf{v};t)$ denotes the deviation of the nonequilibrium inhomogeneous fluid singlet distribution function $F(\mathbf{q},\mathbf{v};t)$ from its equilibrium form, and the dot $\cdot$ denotes the inner product. The quantity $\Gamma(\mathbf{q},\mathbf{v};\mathbf{q}',\mathbf{v}')$ is

$$\Gamma(\mathbf{q},\mathbf{v};\mathbf{q}',\mathbf{v}')=\sigma^2\int d\mathbf{v}_1 d\mathbf{v}_2\int d\hat{\sigma}\Phi(v_2)(\mathbf{v}_{21}\cdot\hat{\sigma})\theta(\mathbf{v}_{21}\cdot\hat{\sigma})[n(\mathbf{q}+\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma})\delta(\mathbf{v}-\mathbf{v}_1^*)-n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$

$$\times\delta(\mathbf{v}-\mathbf{v}_1)]\delta(\mathbf{q}-\mathbf{q}')\delta(\mathbf{v}'-\mathbf{v}_1)+\sigma^2\int d\mathbf{v}_1 d\mathbf{v}_2\int d\hat{\sigma}\Phi(v_1)(\mathbf{v}_{21}\cdot\hat{\sigma})\theta(\mathbf{v}_{21}\cdot\hat{\sigma})[n(\mathbf{q}'-\sigma\hat{\sigma})g(\mathbf{q}'-\sigma\hat{\sigma},\mathbf{q}')$$

$$\times\delta(\mathbf{q}-\mathbf{q}'+\sigma\hat{\sigma})\delta(\mathbf{v}-\mathbf{v}_1^*)-n(\mathbf{q}'+\sigma\hat{\sigma})g(\mathbf{q}'+\sigma\hat{\sigma},\mathbf{q}')\delta(\mathbf{q}-\mathbf{q}'-\sigma\hat{\sigma}')\delta(\mathbf{v}-\mathbf{v}_1)]\delta(\mathbf{v}'-\mathbf{v}_2)$$

$$+\sigma_{1w}^2\int d\mathbf{v}_1\int d\hat{\sigma}(-\mathbf{v}_1\cdot\hat{\sigma})\theta(-\mathbf{v}_1\cdot\hat{\sigma})[n_w(\mathbf{q}+\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}+\sigma_{1w}\hat{\sigma})\delta(\mathbf{v}-\mathbf{v}_1^*)-n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})$$

$$\times g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\delta(\mathbf{v}-\mathbf{v}_1)]\delta(\mathbf{v}'-\mathbf{v}_1)\delta(\mathbf{q}-\mathbf{q}')+n(\mathbf{q})\Phi(v)\mathbf{v}$$

$$\cdot\left(\frac{\partial C(\mathbf{q},\mathbf{q}')}{\partial\mathbf{q}}-g(\mathbf{q},\mathbf{q}')\frac{\partial f^H(\mathbf{q},\mathbf{q}')}{\partial\mathbf{q}}\right)+\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\cdot\mathbf{v}\Phi(v)\left(1+C(\mathbf{q},\mathbf{q}')-\int d\mathbf{q}''n(\mathbf{q}'')C(\mathbf{q}'',\mathbf{q}')\right). \tag{2.4}$$

In expression (2.4), $\Phi(v)=(\beta m/2\pi)^{3/2}\exp(-\beta mv^2/2)$ is the Maxwell–Boltzmann velocity distribution function, where $\beta=1/k_BT$, and k_B, T, and m denote the Boltzmann constant, temperature, and mass of a fluid molecule, respectively; $\mathbf{v}_1,\mathbf{v}_2,\mathbf{v}',\mathbf{v}$ are molecular velocities, $\mathbf{q},\mathbf{q}',\mathbf{q}''$ are coordinate vectors of molecules, $\hat{\sigma}=\sigma_x\mathbf{i}+\sigma_y\mathbf{j}+\sigma_z\mathbf{k}$ is the unit vector of direction cosines ($\mathbf{i},\mathbf{j},\mathbf{k}$ are the unit vectors of corresponding directions), $|\hat{\sigma}|=1$; $\delta(\mathbf{q}-\mathbf{q}')$, $\delta(\mathbf{v}'-\mathbf{v}_1)$, $\delta(\mathbf{q}-\mathbf{q}'+\sigma\hat{\sigma})$, $\delta(\mathbf{v}-\mathbf{v}_1)$, $\delta(\mathbf{q}-\mathbf{q}'-\sigma\hat{\sigma})$, $\delta(\mathbf{v}'-\mathbf{v}_2)$, etc., are Dirac δ functions, $\mathbf{v}_1^*$ is the post-collisional velocity corresponding to the precollisional velocities $\mathbf{v}_1$ and $\mathbf{v}_2$, $\mathbf{v}_1^*=\mathbf{v}_1-(\mathbf{v}_{21}\cdot\hat{\mathbf{q}}_{21})\hat{\mathbf{q}}_{21}$, $\mathbf{v}_{21}=\mathbf{v}_2-\mathbf{v}_1$, and $\theta(\mathbf{v}_{21}\cdot\hat{\sigma})$, $\theta(-\mathbf{v}_1\cdot\hat{\sigma})$ are the step functions. Quantities $n(\mathbf{q})$, $g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma})$, $C(\mathbf{q},\mathbf{q}')$ are the *equilibrium* inhomogeneous fluid number density, pair correlation function contact value and the direct correlation function, respectively. Similarly, $n_w(\mathbf{q})$, $g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})$ are the equilibrium wall molecule number density and the pair correlation function contact value specific to fluid-wall molecule interactions. Finally, $f^H(\mathbf{q},\mathbf{q}')=\exp[-\beta\varphi_H(\mathbf{q},\mathbf{q}')]-1=\theta(|\mathbf{q}-\mathbf{q}'|-\sigma)-1$ is the Mayer function specific to the fluid–fluid molecule hard-core interaction and the dots $\cdot$ mean inner products of tensors A and B, $\Sigma_m A_{i,\ldots,m}B_{m,\ldots,j}$. Integration $\int d\hat{\sigma}$ everywhere in this work means an integration over the surface of the sphere of radius $|\hat{\sigma}|=1$.

We note that the third term in the right-hand side of Eq. (2.4) explicitly contains the effects of any walls present in the system. All other terms in the right-hand side of Eq. (2.4) include the effects implicitly, through $n(\mathbf{q}'\pm\sigma\hat{\sigma})$, $g(\mathbf{q}'\pm\sigma\hat{\sigma},\mathbf{q}')$, $C(\mathbf{q},\mathbf{q}')$, and $f(\mathbf{q},\mathbf{q}')$.

The next logical step is to replace the kinetic equation (2.3) for $\delta F(\mathbf{q},\mathbf{v};t)$ with an equivalent set of equations for its velocity moments. For this purpose we will use the generalized Hermite polynomials[17] defined as

$$\psi_l(\mathbf{v})=\Psi_l(\xi)=\Phi^{-1}(\xi)(l_1!l_2!l_3!)^{-1/2}\left(-\frac{\partial}{\partial\xi_1}\right)^{l_1}\times\left(-\frac{\partial}{\partial\xi_2}\right)^{l_2}\left(-\frac{\partial}{\partial\xi_3}\right)^{l_3}\Phi(\xi), \tag{2.5}$$

where $\xi=(m\beta)^{1/2}\mathbf{v}$ denotes the dimensionless velocity and $\Phi(\xi)=(2\pi)^{-3/2}\exp(-\xi^2/2)$, $\xi=\xi_1\mathbf{i}+\xi_2\mathbf{j}+\xi_3\mathbf{k}$, and $l_1,l_2,l_3=0,1,2,\ldots$.

These polynomials form a basis vector set satisfying the orthogonality and completeness conditions,

$$\int d\xi\Phi(\xi)\Psi_l(\xi)\Psi_k(\xi)=\delta_{lk},\qquad \sum_i\Phi(\xi)\Psi_i(\xi)\Psi_i(\xi')=\delta(\xi-\xi'). \tag{2.6}$$

The polynomials from Eq. (2.5), can be considered as the ξ representatives of some abstract bra $\langle l|$ and ket $|l\rangle$ vectors,

$$\Psi_l(\xi)=\langle l|\xi\rangle=\langle l_1l_2l_3|\xi\rangle, \tag{2.7}$$

$$\Phi(\xi)\Psi_l(\xi)=\langle\xi|l\rangle=\langle\xi|l_1l_2l_3\rangle, \tag{2.8}$$

and the conditions (2.6) take the form $\langle l|k\rangle=\delta_{lk}$ and $\Sigma_i|i\rangle\langle i|=1$.

Then Eq. (2.3) can be "spanned" by the vectors of $\langle l|$ basis set above,

$$\frac{\partial}{\partial t}\langle l|\delta F\rangle+\left\langle l\left|\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{q}}\delta F\right.\right\rangle=\int d\mathbf{q}'\sum_i\langle l|\Gamma|i\rangle\langle i|\delta F\rangle, \tag{2.9}$$

where "projections" $\langle l|\delta F\rangle$ of $\delta F(\mathbf{q},\mathbf{v};t)$ on this basis set are velocity moments of $\delta F(\mathbf{q},\mathbf{v};t)$,

$$\langle m|\delta F\rangle=\int d\mathbf{v}\psi_m(\mathbf{v})\delta F(\mathbf{q},\mathbf{v};t), \tag{2.10}$$

and

$$\left\langle l\left|\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{q}}\delta F\right.\right\rangle=\int d\mathbf{v}\psi_l(\mathbf{v})\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{q}}\delta F(\mathbf{q},\mathbf{v};t), \tag{2.11}$$

$$\langle l|\Gamma|i\rangle=\int d\mathbf{v}\, d\mathbf{v}'\Phi(v')\psi_l(\mathbf{v})\Gamma(\mathbf{q},\mathbf{v};\mathbf{q}',\mathbf{v}')\psi_i(\mathbf{v}'). \tag{2.12}$$

The $\langle l|$ basis set consists of infinitely many vectors generating infinitely many moments of the singlet distribution function. Since we cannot solve the entire set of equations (2.9) for the singlet distribution function velocity moments, we should restrict ourselves to some reasonable number of the moments which could provide a macroscopically complete description of the hydrodynamic and thermal processes involved. The simplest approximation of this kind would be the 13-moments representation, for which the basis set of $\langle l|$ vectors is limited to elements $\{\langle i|\mathbf{v}\rangle; i\in G\}$,

$$\langle \hat{n}|\mathbf{v}\rangle\equiv\psi_n(\mathbf{v})\equiv 1, \tag{2.13}$$

$$\langle \hat{\mathbf{u}}|\mathbf{v}\rangle\equiv(m\beta)^{1/2}\psi_u(\mathbf{v})\equiv(m\beta)^{1/2}\mathbf{v}, \tag{2.14}$$

$$\langle \hat{T}|\mathbf{v}\rangle\equiv\left(\frac{2}{3}\right)^{1/2}\beta\psi_T(\mathbf{v})$$
$$\equiv\left(\frac{2}{3}\right)^{1/2}\left(\frac{\beta m v^2}{2}-\frac{3}{2}\right),\quad v^2\equiv|\mathbf{v}|^2, \tag{2.15}$$

$$\langle \hat{\mathbf{P}}^0|\mathbf{v}\rangle\equiv 2^{-1/2}\beta\psi_P(\mathbf{v})\equiv 2^{-1/2}\beta m(\mathbf{v}\mathbf{v}-\tfrac{1}{3}v^2\mathbf{I}), \tag{2.16}$$

$$\langle \hat{\mathbf{Q}}|\mathbf{v}\rangle\equiv(\tfrac{2}{5})^{1/2}(m\beta^3)^{1/2}\psi_Q(\mathbf{v})$$
$$\equiv\left(\frac{2}{5}\right)^{1/2}(m\beta)^{1/2}\left(\frac{\beta m v^2}{2}-\frac{5}{2}\right)\mathbf{v}, \tag{2.17}$$

labeled with the continuum variables corresponding to their ensemble averages, $\delta n(\mathbf{q},\mathrm{t})$, $\mathbf{u}(\mathbf{q},t)$, $\delta T(\mathbf{q},\mathrm{t})$, $\mathbf{P}^0(\mathbf{q},t)$, and $\mathbf{Q}(\mathbf{q},t)$ standing for particle density, velocity, and temperature deviations from their equilibrium values, and for "kinetic" contributions to the pressure tensor and energy flux, respectively, and $\mathbf{I}$ means the unit matrix. We define the continuum (macroscopic) variables above as corresponding velocity moments of the distribution function $\delta F(\mathbf{q},\mathbf{v};t)$, similar to those defined for homogeneous fluids,[9–11]

$$\delta n(\mathbf{q},t)=\int d\mathbf{v}\psi_n(\mathbf{v})\delta F(\mathbf{q},\mathbf{v};t)\equiv m^{-1}\delta\rho(\mathbf{q},t), \tag{2.18}$$

$$\rho(\mathbf{q})\mathbf{u}(\mathbf{q},t)=m\int d\mathbf{v}\psi_u(\mathbf{v})\delta F(\mathbf{q},\mathbf{v};t), \tag{2.19}$$

$$\tfrac{3}{2}n(\mathbf{q})k_B\delta T(\mathbf{q},t)=\int d\mathbf{v}\psi_T(\mathbf{v})\delta F(\mathbf{q},\mathbf{v};t), \tag{2.20}$$

$$\mathbf{P}^0(\mathbf{q},t)=\int d\mathbf{v}\psi_P(\mathbf{v})\delta F(\mathbf{q},\mathbf{v};t), \tag{2.21}$$

$$\mathbf{Q}(\mathbf{q},t)=\int d\mathbf{v}\psi_Q(\mathbf{v})\delta F(\mathbf{q},\mathbf{v};t). \tag{2.22}$$

In the definition, Eq. (2.19), $\rho(\mathbf{q})=mn(\mathbf{q})$ corresponds to equilibrium mass density. According to Eq. (2.8) the adjoint basis set $\{\langle\mathbf{v}|i\rangle, i\in G\}$ can be formed of the right-hand sides of Eqs. (2.13)–(2.17) multiplied by $\Phi(\mathbf{v})$.

In the 13-moments approximation the deviation $\delta F(\mathbf{q},\mathbf{v};t)$ of the nonequilibrium inhomogeneous fluid singlet distribution function from its equilibrium form is

$$\begin{aligned}\delta F(\mathbf{q},\mathbf{v};t)&=\sum_{i\in G}\langle\mathbf{v}|i\rangle\langle i|\delta F\rangle\\&=\Phi(v)[\psi_n(\mathbf{v})\delta n(\mathbf{q},t)+\psi_\mathbf{u}(\mathbf{v})\cdot\beta\rho(\mathbf{q})\mathbf{u}(\mathbf{q},t)\\&\quad+\psi_T(\mathbf{v})\beta^2k_Bn(\mathbf{q})\delta T(\mathbf{q},t)\\&\quad+\psi_P(\mathbf{v}):\tfrac{1}{2}\beta^2\mathbf{P}^0(\mathbf{q},t)+\psi_Q(\mathbf{v})\cdot\tfrac{2}{5}m\beta^3\mathbf{Q}(\mathbf{q},t)].\end{aligned} \tag{2.23}$$

The associated moment equations can be recovered from Eq. (2.9) after calculations of integrals Eqs. (2.10)–(2.12), in which Eq. (2.23) should be used to approximate $\delta F(\mathbf{q},\mathbf{v};t)$. These integrodifferential equations are given in Appendix A.

To be solved Eqs. (A1)–(A5) should be simplified, namely, the continuum variables there should be expanded in a Taylor series,

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

We note that the continuum variables $A(\mathbf{q},t)$, which are defined in Eqs. (2.18)–(2.22), are the differences between the dynamic variables in the nonequilibrium inhomogeneous system and the corresponding equilibrium inhomogeneous one. For example, the variables $A(\mathbf{q},t)$ considered do not include the number density $n(\mathbf{q},t)$ or the temperature $T(\mathbf{q},t)$, nor the differences in these quantities between the real system and a homogeneous one; instead, they include the differences $\delta n(\mathbf{q},t)$ and $\delta T(\mathbf{q},t)$ in these quantities between the nonequilibrium and equilibrium systems, both of which are inhomogeneous. We do not expect the differences due to nonequilibrium to be large even near walls, because the departure from equilibrium is assumed to be small. This assumption is supported by molecular simulation results (see, for example, Ref. 14). Since our main objective is to obtain expressions for the linear transport coefficients for inhomogeneous systems, it is only necessary to consider small departures.

Moreover, the direct correlation function in Eq. (A2) can be expressed in terms of the pressure tensor $\mathbf{P}(\mathbf{q})$ specific to an equilibrium inhomogeneous fluid by using the corresponding compressibility equation,[18]

$$C(\mathbf{q},\mathbf{q}')=\frac{\delta(\mathbf{q}-\mathbf{q}')}{n(\mathbf{q})}-\frac{\beta}{n(\mathbf{q})}\frac{\delta p(\mathbf{q})}{\delta n(\mathbf{q}')}+\tfrac{1}{3}\,\mathrm{Tr}\,\wp(\mathbf{q},\mathbf{q}'). \tag{2.24}$$

where $\delta p(\mathbf{q})/\delta n(\mathbf{q}')$ is the functional derivative of the equilibrium pressure $p(\mathbf{q})=\frac{1}{3}\,\mathrm{Tr}\,\mathbf{P}(\mathbf{q})$ with respect to the equilibrium number density $n(\mathbf{q}')$ taken at β=const, and $\mathrm{Tr}\,\wp(\mathbf{q},\mathbf{q}')$ denotes the trace of the tensor $\wp(\mathbf{q},\mathbf{q}')$. Thus, inserting the expression (2.24) for $C(\mathbf{q},\mathbf{q}')$ into Eq. (A2), and taking time Fourier transforms of Eqs. (A1)–(A5), one can find expressions, correct to the second order in spatial gradients of the continuum variables (2.18)–(2.22),

$$-i\omega\delta n(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot[n(\mathbf{q})\mathbf{u}(\mathbf{q},\omega)]=-\sigma^3 n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I}):\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}+\frac{\sigma^4}{2}n(\mathbf{q})$$
$$\times\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}I)\hat{\sigma}:\frac{\partial^2\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}+\sigma_{1w}^2 n(\mathbf{q})$$
$$\times\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}\cdot\mathbf{u}(\mathbf{q},\omega), \tag{2.25}$$

$$-i\omega\rho(\mathbf{q})\mathbf{u}(\mathbf{q},t)+\frac{\partial}{\partial\mathbf{q}}\cdot\Bigg[\Bigg(\int d\mathbf{q}'\frac{\delta p(\mathbf{q})}{\delta n(\mathbf{q}')}\delta n(\mathbf{q}',\omega)-n(\mathbf{q})\int d\mathbf{q}'d\mathbf{q}''\frac{\delta p(\mathbf{q}'')}{\delta n(\mathbf{q}')}\delta n(\mathbf{q}',\omega)-\frac{1}{3\beta}n(\mathbf{q})\int d\mathbf{q}'\,\mathrm{Tr}\,\wp(\mathbf{q},\mathbf{q}')\delta n(\mathbf{q}',\omega)$$
$$+\frac{1}{3\beta}n(\mathbf{q})\int d\mathbf{q}'d\mathbf{q}''n(\mathbf{q}'')\mathrm{Tr}\,\wp(\mathbf{q}'',\mathbf{q}')\delta n(\mathbf{q}',\omega)\Bigg)\mathbf{I}+k_B n(\mathbf{q})\delta T(\mathbf{q},\omega)\mathbf{I}+\mathbf{P}^0(\mathbf{q},\omega)\Bigg]$$
$$=\frac{36}{5\pi^2}b^2\eta n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:\frac{\partial^2\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-\frac{72}{5\pi^2}\frac{b^2}{\sigma}\eta n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$
$$\times(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}:\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}-(48\sqrt{2}/5\pi)\left(\frac{\sigma_{1w}}{\sigma}\right)^2 b\sigma\eta n(\mathbf{q})\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot\mathbf{u}(\mathbf{q},\omega)$$
$$+\frac{k_B\sigma^4}{4}n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:\frac{\partial^2\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-\frac{3k_B b}{4\pi}n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}$$
$$-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}$$
$$+\frac{\sigma^4}{4}n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}::\frac{\partial^2\mathbf{P}^0(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-\frac{3b}{4\pi}n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}:\frac{\partial\mathbf{P}^0(\mathbf{q},\omega)}{\partial\mathbf{q}}$$
$$+\frac{\sigma^2}{2}\left[\int d\hat{\sigma}n(\mathbf{q})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}+\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}\right]:\mathbf{P}^0(\mathbf{q},\omega)$$
$$+\frac{18}{25\pi^2}\beta b^2\eta n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:\frac{\partial^2\mathbf{Q}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-\frac{36}{25\pi^2}\frac{\beta}{\sigma}b^2\eta n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$
$$\times(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}:\frac{\partial\,\mathbf{Q}(\mathbf{q},\omega)}{\partial\mathbf{q}}+\frac{24}{25\pi}\beta b\eta\sigma\left[\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})-2\sqrt{2}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\right.$$
$$\left.\times\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\right]\cdot\mathbf{Q}(\mathbf{q},\omega), \tag{2.26}$$

$$-i\omega \tfrac{3}{2} k_B n(\mathbf{q}) \delta T(\mathbf{q},\omega) + \frac{\partial}{\partial \mathbf{q}} \cdot \mathbf{Q}(\mathbf{q},\omega) + k_B T \frac{\partial}{\partial \mathbf{q}} \cdot [n(\mathbf{q})\mathbf{u}(\mathbf{q},\omega)]$$

$$= \frac{3b\sigma}{8\pi} k_B T n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma} \vdots \frac{\partial^2 \mathbf{u}(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}} - \frac{3b}{4\pi} k_B T n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma}\hat{\sigma} : \frac{\partial \mathbf{u}(\mathbf{q},\omega)}{\partial \mathbf{q}}$$

$$+ \sigma_{1w}^2 k_B T n(\mathbf{q}) \int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma}) \hat{\sigma} \cdot \mathbf{u}(\mathbf{q},\omega) + \frac{24}{25\pi^2} b^2 \lambda n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$

$$\times \hat{\sigma}\hat{\sigma} : \frac{\partial^2 \delta T(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}} - \frac{32 b\sigma^2}{25\pi} \lambda n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma} \cdot \frac{\partial \delta T(\mathbf{q},\omega)}{\partial \mathbf{q}} + [\sigma^4/(2\sqrt{\pi\beta m})] n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$

$$\times \hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma} :: \frac{\partial^2 \mathbf{P}^0(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}} - (\sigma^3/\sqrt{\pi\beta m}) n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma}\hat{\sigma}\hat{\sigma} \vdots \frac{\partial \mathbf{P}^0(\mathbf{q},\omega)}{\partial \mathbf{q}} + (\sigma^2/\sqrt{\pi\beta m}) \int d\hat{\sigma} [n(\mathbf{q}) - n(\mathbf{q}-\sigma\hat{\sigma})]$$

$$\times g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma}\hat{\sigma} : \mathbf{P}^0(\mathbf{q},\omega) - \frac{9b\sigma}{40\pi} n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma}\hat{\sigma}\hat{\sigma} \vdots \frac{\partial^2 \mathbf{Q}(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}} - \frac{9b}{20\pi} n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma}\hat{\sigma} : \frac{\partial \mathbf{Q}(\mathbf{q},\omega)}{\partial \mathbf{q}}$$

$$+ \frac{3\sigma^2}{10} \left[\int d\hat{\sigma} [n(\mathbf{q}) + \tfrac{1}{3} n(\mathbf{q}-\sigma\hat{\sigma})] g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \hat{\sigma} + \frac{10}{3} \left(\frac{\sigma_{1w}}{\sigma}\right)^2 \int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma}) \hat{\sigma} \right] \cdot \mathbf{Q}(\mathbf{q},\omega), \tag{2.27}$$

$$-i\beta\omega \mathbf{P}^0(\mathbf{q},\omega) + 2\mathbf{S}_{un}(\mathbf{q},\omega) + \frac{4\beta}{5} \mathbf{S}_Q(\mathbf{q},\omega)$$

$$= \frac{\sigma^4}{2} n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma}\hat{\sigma} \vdots \frac{\partial^2 \mathbf{u}(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}} - \sigma^3 n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma} :$$

$$\times \frac{\partial \mathbf{u}(\mathbf{q},\omega)}{\partial \mathbf{q}} + 2\sigma_{1w}^2 n(\mathbf{q}) \int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma} \cdot \mathbf{u}(\mathbf{q},\omega) + k_B \left(\frac{\beta}{\pi m}\right)^{1/2} \sigma^4 n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})$$

$$\times g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma} : \frac{\partial^2 \delta T(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}} - 2k_B \left(\frac{\beta}{\pi m}\right)^{1/2} \sigma^3 n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma} \cdot \frac{\partial \delta T(\mathbf{q},\omega)}{\partial \mathbf{q}}$$

$$+ \left(\frac{\beta}{\pi m}\right)^{1/2} \sigma^4 n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma} :: \frac{\partial^2 \mathbf{P}^0(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}} - 2\left(\frac{\beta}{\pi m}\right)^{1/2} \sigma^3 n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I})$$

$$\times \hat{\sigma}\hat{\sigma}\hat{\sigma} \vdots \frac{\partial \mathbf{P}^0(\mathbf{q},\omega)}{\partial \mathbf{q}} + 2\sigma^2 \left(\frac{\beta}{\pi m}\right)^{1/2} \left[\int d\hat{\sigma} [n(\mathbf{q}) - 4n(\mathbf{q}-\sigma\hat{\sigma})] g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma} - 3\sqrt{2} \left(\frac{\sigma_{1w}}{\sigma}\right)^2 \right.$$

$$\left. \times \int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma} \right] : \mathbf{P}^0(\mathbf{q},\omega) + \frac{\sigma^4}{5} \beta n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma}\hat{\sigma} \vdots \frac{\partial^2 \mathbf{Q}(\mathbf{q},\omega)}{\partial \mathbf{q}\partial \mathbf{q}}$$

$$- \frac{2}{5} \sigma^3 \beta n(\mathbf{q}) \int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma}\hat{\sigma} : \frac{\partial \mathbf{Q}(\mathbf{q},\omega)}{\partial \mathbf{q}} + \frac{1}{5} \sigma^2 \beta \left[\int d\hat{\sigma} [2n(\mathbf{q}) - n(\mathbf{q}-\sigma\hat{\sigma})] g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma} \right.$$

$$\left. + 4\left(\frac{\sigma_{1w}}{\sigma}\right)^2 \int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma}) (\hat{\sigma}\hat{\sigma} - \tfrac{1}{3}\mathbf{I}) \hat{\sigma} \right] \cdot \mathbf{Q}(\mathbf{q},\omega), \tag{2.28}$$

$$-i\omega\mathbf{Q}(\mathbf{q},\omega)+\frac{5}{2}\frac{k_B}{\beta m}\frac{\partial}{\partial\mathbf{q}}[n(\mathbf{q})\delta T(\mathbf{q},\omega)]+\frac{1}{\beta m}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{P}^0(\mathbf{q},\omega)$$

$$=[\sigma^4/(4\beta\sqrt{\pi\beta m})]n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:\frac{\partial^2\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-[\sigma^3/(2\beta\sqrt{\pi\beta m})]n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})$$
$$\times g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}:\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}-[\sqrt{2}\sigma_{1w}^2/(\beta\sqrt{\pi\beta m})]n(\mathbf{q})\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}$$
$$-\tfrac{2}{3}\mathbf{I})\cdot\mathbf{u}(\mathbf{q},\omega)$$
$$+\frac{3}{8}\frac{k_B\sigma^4}{\beta m}n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:\frac{\partial^2\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-\frac{3}{4}\frac{k_B\sigma^3}{\beta m}n(\mathbf{q})\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}$$
$$\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}+\frac{3}{8}\frac{\sigma^4}{\beta m}n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}::\frac{\partial^2\mathbf{P}^0(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-\frac{3}{4}\frac{\sigma^3}{\beta m}n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}\vdots\frac{\partial\mathbf{P}^0(\mathbf{q},\omega)}{\partial\mathbf{q}}$$
$$+\frac{1}{4}\frac{\sigma^2}{\beta m}\int d\hat{\sigma}[3n(\mathbf{q})-2n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:\mathbf{P}^0(\mathbf{q},\omega)+\frac{27}{40}(\sigma^4/\sqrt{\pi\beta m})n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:$$
$$\times\frac{\partial^2\mathbf{Q}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}-\frac{27}{20}(\sigma^3/\sqrt{\pi\beta m})n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}:\frac{\partial\mathbf{Q}(\mathbf{q},\omega)}{\partial\mathbf{q}}+\frac{27}{20}(\sigma^2/\sqrt{\pi\beta m})$$
$$\times\Bigg[\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})-(52\sqrt{2}/27)\left(\frac{\sigma_{1w}}{\sigma}\right)^2$$
$$\times\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})-\frac{8}{27}\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}+\mathbf{I})\Bigg]\cdot\mathbf{Q}(\mathbf{q},\omega). \tag{2.29}$$

In convolutions denoted by $\cdot$, :, $\vdots$, and :: on the right-hand sides of Eqs. (2.25)–(2.29) the right index of $\mathbf{I}$ in tensors $\mathbf{I}$, $\mathbf{I}\hat{\sigma}$, $\mathbf{I}\hat{\sigma}\hat{\sigma}$, etc., are to be convoluted with the left index of the corresponding continuum variables, and indices $\hat{\sigma}$,$\hat{\sigma}\hat{\sigma}$, etc., are to be convoluted with indices of $\partial/\partial\mathbf{q}$, $\partial^2/\partial\mathbf{q}\partial\mathbf{q}$. In addition, quantities $\eta=(5/16\sigma^2)\ (m/\pi\beta)^{1/2}$ and $\lambda=75k_B/[64\sigma^2(\pi\beta m)^{1/2}]$ correspond to viscosity and thermal conductivity of a dilute gas. All other notations adopted in Eqs. (2.25)–(2.29) correspond to those introduced in Appendix A. Notations $\delta n(\mathbf{q},\omega)$, $u(\mathbf{q},\omega)$, $\delta T(\mathbf{q},\omega)$, $\mathbf{P}^0(\mathbf{q},\omega)$, and $\mathbf{Q}(\mathbf{q},\omega)$ denote time Fourier transforms of corresponding continuum variables.

III. THE LINEARIZED NAVIER–STOKES EQUATIONS

To obtain the linearized Navier–Stokes equation one should solve Eqs. (2.28) and (2.29), and insert the resulting expressions for $\mathbf{P}^0(\mathbf{q},\omega)$ and $\mathbf{Q}(\mathbf{q},\omega)$ into Eqs. (2.26) and (2.27). For this purpose Eqs. (2.28), (2.29) should be simplified. First, there are coupling terms of two kinds in Eqs. (2.28) and (2.29). The terms of the first kind are proportional to spatial derivatives $S_Q(\mathbf{q},\omega)$, $\partial\mathbf{Q}(\mathbf{q},\omega)/\partial\mathbf{q}$, and $(\partial^2/\partial\mathbf{q}\partial\mathbf{q})\mathbf{Q}(\mathbf{q},\omega)$ in Eq. (2.28) and $(\partial/\partial\mathbf{q})\cdot\mathbf{P}^0(\mathbf{q},\omega)$, $\partial\mathbf{P}^0(\mathbf{q},\omega)/\partial\mathbf{q}$, and $(\partial^2/\partial\mathbf{q}\partial\mathbf{q})\mathbf{P}^0(\mathbf{q},\omega)$ in Eq. (2.29). If the temperature and velocity of the fluid do not vary appreciably in a mean free path ($\sim\sigma$) [which is valid in the case considered here, because continuum variables $\mathbf{P}^0(\mathbf{q},\omega)$ and $\mathbf{Q}(\mathbf{q},\omega)$ are averaged quantities specific to a close-to-equilibrium fluid] the third order terms with the second derivatives of $\mathbf{P}^0(\mathbf{q},\omega)$, $\mathbf{Q}(\mathbf{q},\omega)$, and terms with $S_Q(\mathbf{q},\omega)$, and $(\partial/\partial\mathbf{q})\cdot\mathbf{P}^0(\mathbf{q},\omega)$ in Eqs. (2.28) and (2.29) should be neglected.[9,10] Moreover, since $|\sigma_x|$, $|\sigma_y|$, and $|\sigma_z|\leqslant 1$, the following conditions hold:

$$\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\underbrace{\sigma_1\cdots\sigma_k}_{m}=\frac{1}{2}\int d\hat{\sigma}[f(\mathbf{q}-\sigma\hat{\sigma})-f(\mathbf{q}+\sigma\hat{\sigma})]\underbrace{\sigma_i\cdots\sigma_k}_{m}\ll\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\underbrace{\sigma_i\cdots\sigma_j}_{m-1},\quad m=1,3,\ldots,\ i,j,k=x,y,z \tag{3.1}$$

$$\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\sigma_1^2>\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\sigma_i^2\sigma_j^2>\cdots>\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\underbrace{\sigma_i^2\cdots\sigma_l^2}_{m},\quad i,j,l=x,y,z,\ m=3,4,\ldots \tag{3.2}$$

for any integrable, positively defined function $f(\mathbf{q})$, and m signifies that there are m σ-components $\sigma_i,\ldots,\sigma_j$. Taking these relations into account one can prove that all terms with second derivatives of continuum variables in Eqs. (2.28) and (2.29) can be neglected. Finally, the derivatives $(\partial/\partial\mathbf{q})\mathbf{P}^0(\mathbf{q},\omega)$ in Eq. (2.28) and $(\partial/\partial\mathbf{q})\mathbf{Q}(\mathbf{q},\omega)$ in Eq. (2.29), being small themselves, come with multipliers which are proportional to the integrals of odd sets of $\hat{\sigma}$'s over $\hat{\sigma}$. Then the correlation Eq. (3.1) and the simplest approximation

$$\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\ldots\hat{\sigma}\cong\frac{1}{4\pi}\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\int d\hat{\sigma}\hat{\sigma}\cdots\hat{\sigma} \tag{3.3}$$

for the multipliers corresponding to these terms suggest neglect of these terms.

The coupling terms of the second kind are proportional to $\mathbf{Q}(\mathbf{q},\omega)$ [in Eq. (2.28)] and $\mathbf{P}^0(\mathbf{q},\omega)$ [Eq. (2.29)], and cannot be neglected. To evaluate such terms the approximation, Eq. (3.3), has been used.

This consideration leads to Eqs. (2.28) and (2.29) taking the forms of Eqs. (B1) and (B2) of Appendix B. Expressing $\mathbf{Q}(\mathbf{q},\omega)$ in terms of $\mathbf{P}^0(\mathbf{q},\omega)$ from Eq. (B1), inserting the expression obtained into Eq. (B2), and using the approximation, Eq. (3.3), for those terms on the right-hand side of Eq. (B2) which are proportional to $\mathbf{P}^0(\mathbf{q},\omega)$ and $(\partial/\partial\mathbf{q})\mathbf{u}(\mathbf{q},\omega)$, one can find the time Fourier transform $\mathbf{P}^0(q,\omega)$,

$$\mathbf{P}^0(\mathbf{q},\omega)=-2\eta_I^{(2)}(\mathbf{q},\omega):\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}+8\pi\eta\sigma_{1w}^2\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)\cdot\mathbf{u}(\mathbf{q},\omega)-8\pi\eta\tau_\eta^*(\mathbf{q},\omega)\mathbf{S}_{u\nabla n}(\mathbf{q},\omega)$$
$$-\frac{32}{15}\sqrt{\pi\beta m}\lambda\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}-\pi\sqrt{\pi\beta m}\lambda\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\widetilde{\mathbf{P}}_T(\mathbf{q})\delta T(\mathbf{q},\omega), \quad (3.4)$$

where the following notations have been introduced,

$$\eta_I^{(2)}(\mathbf{q},\omega)=4\pi\eta\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\left(\tfrac{1}{2}(2\mathbf{I}_4+\mathbf{I}_\delta-\tfrac{5}{3}\mathbf{II})+\frac{3b}{4\pi}\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}\right), \quad (3.5)$$

$$\tau_\eta^{-1}(\mathbf{q})=\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})+\frac{1}{3}\int d\hat{\sigma}[n(\mathbf{q}-\sigma\hat{\sigma})-n(\mathbf{q})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})+\sqrt{2}\left(\frac{\sigma_{1w}}{\sigma}\right)^2$$
$$\times\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma}), \quad (3.6)$$

$$\bar{\tau}_\eta(\mathbf{q})=(5\sqrt{\pi\beta m}/4\sigma^2)\tau_\eta(\mathbf{q}), \quad (3.7)$$

$$\tau_\eta^*(\mathbf{q},\omega)=\tau_\eta(\mathbf{q})/[1-i\omega\bar{\tau}_\eta(\mathbf{q})], \quad (3.8)$$

$$\tau_\lambda^{-1}(\mathbf{q})=\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})+\frac{27}{32}\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})-\frac{13\sqrt{2}}{8}\left(\frac{\sigma_{1w}}{\sigma}\right)^2$$
$$\times\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma}), \quad (3.9)$$

$$\bar{\tau}_\lambda(\mathbf{q})=(15\sqrt{\pi\beta m}/8\sigma^2)\tau_\lambda(\mathbf{q}), \quad (3.10)$$

$$\tau_\lambda^*(\mathbf{q},\omega)=\tau_\lambda(\mathbf{q})/[1-i\omega\bar{\tau}_\lambda(\mathbf{q})], \quad (3.11)$$

$$\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)=\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}-(3\sqrt{2}/16)\tau_\lambda^*(\mathbf{q},\omega)C_Q(\mathbf{q})$$
$$\cdot\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I}), \quad (3.12)$$

$$\mathbf{S}_{\mathbf{u}\nabla\mathbf{n}}(\mathbf{q},\omega)=\frac{1}{2}\left[\left(\mathbf{u}(\mathbf{q},\omega)\frac{\partial}{\partial\mathbf{q}}\right)+\left(\mathbf{u}(\mathbf{q},\omega)\frac{\partial}{\partial\mathbf{q}}\right)^T-\frac{2}{3}\mathbf{I}\left(\mathbf{u}(\mathbf{q},\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\right)\right]n(\mathbf{q}), \quad (3.13)$$

$$\widetilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)=\frac{3b}{2\pi}\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}+\frac{15}{128\lambda n(\mathbf{q})}C_Q(\mathbf{q})\cdot\lambda_I^{(2)}(\mathbf{q},\omega), \quad (3.14)$$

$$\lambda_I^{(2)}(\mathbf{q},\omega)=4\pi\lambda\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\left(\mathbf{I}+\frac{9b}{20\pi}\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\right), \quad (3.15)$$

$$\widetilde{\mathbf{P}}_T(\mathbf{q})=\mathbf{C}_\mathbf{Q}(\mathbf{q})\cdot\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}, \quad (3.16)$$

$$\mathbf{C}_\mathbf{Q}(\mathbf{q})=\int d\hat{\sigma}\left[[2n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})+4\left(\frac{\sigma_{1w}}{\sigma}\right)^2n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\right](\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}. \quad (3.17)$$

The fourth rank Cartesian tensor $\mathbf{I}_4$ above consists of three nonzero components $(\mathbf{I}_4)_{llll}=1$, $l=i,j,k$, and $\mathbf{I}_\delta=\mathbf{II}+\mathbf{I}_\delta^0$, where $\mathbf{II}$ is the tensorial product of the unit matrices and $\mathbf{I}_\delta^0$ is the fourth rank Cartesian tensor composed of components $(\mathbf{I}_\delta^0)_{lmps}=\delta_{lm}\delta_{ps}$ or $\delta_{ls}\delta_{mp}$, $l,m,p,s=i,j,k$. Inserting Eq. (3.4) for $\mathbf{P}^0(\mathbf{q},\omega)$ into Eq. (B1) and using the approximation, Eq. (3.3), for those terms on the right-hand side of Eq. (B1) which are proportional to $\mathbf{Q}(\mathbf{q},\omega)$, one can find the time Fourier transform $\mathbf{Q}(\mathbf{q},\omega)$,

$$\mathbf{Q}(\mathbf{q},\omega)=-\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}-4\pi\lambda\tau_\lambda^*(\mathbf{q},\omega)\tilde{\mathbf{Q}}_T(\mathbf{q},\omega)\delta T(\mathbf{q},\omega)-3\left(\frac{\pi}{\beta m}\right)^{1/2}\eta\tau_\lambda^*(\mathbf{q},\omega)\tilde{\mathbf{Q}}_{\nabla_\mathbf{u}}(\mathbf{q},\omega):\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}$$
$$-6\left(\frac{2\pi}{\beta m}\right)^{1/2}\sigma_{1w}^2\eta\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\tilde{\mathbf{Q}}_\mathbf{u}(\mathbf{q},\omega)\cdot\mathbf{u}(\mathbf{q},\omega)-\frac{15\pi}{4}\left(\frac{\pi}{\beta m}\right)^{1/2}\eta\tau_\lambda^*(\mathbf{q},\omega)\tau_\eta^*(\mathbf{q},\omega)\mathbf{C}_\mathbf{P}(\mathbf{q}):\mathbf{S}_{\mathbf{u}\nabla\mathbf{n}}(\mathbf{q},\omega),\quad(3.18)$$

where

$$\tilde{\mathbf{Q}}_T(\mathbf{q},\omega)=\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}+\frac{15}{128}\pi\tau_\lambda^*(\mathbf{q},\omega)\tau_\eta^*(\mathbf{q},\omega)\mathbf{C}_\mathbf{P}(\mathbf{q}):\tilde{\mathbf{P}}_\mathbf{T}(\mathbf{q}),\quad(3.19)$$

$$\tilde{\mathbf{Q}}_{\nabla_\mathbf{u}}(\mathbf{q},\omega)=\frac{3b}{2\pi}n(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})(\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I})\hat{\boldsymbol{\sigma}}+\frac{5}{16\eta}\mathbf{C}_\mathbf{P}(\mathbf{q}):\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega),\quad(3.20)$$

$$\tilde{\mathbf{Q}}_\mathbf{u}(\mathbf{q},\omega)=\int d\hat{\boldsymbol{\sigma}}\,n_w(\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})(\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I})-(5\sqrt{2}\pi/16)\tau_\eta^*(\mathbf{q},\omega)\mathbf{C}_\mathbf{P}(\mathbf{q}):\tilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega),\quad(3.21)$$

$$\mathbf{C}_\mathbf{P}(\mathbf{q})=\int d\hat{\boldsymbol{\sigma}}\{3[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})]+n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})\}g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}.\quad(3.22)$$

Inserting the time Fourier transforms $\mathbf{P}^0(\mathbf{q},\omega)$ and $\mathbf{Q}(\mathbf{q},\omega)$ given by Eqs. (3.4) and (3.18) into Eqs. (2.26) and (2.27), one can obtain the linearized Navier–Stokes equations,

$$-i\omega\rho(\mathbf{q})\mathbf{u}(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\boldsymbol{\Pi}(\mathbf{q},\omega)=\mathbf{R}_\mathbf{u}(\mathbf{q},\omega),\quad(3.23)$$

$$-\frac{3}{2}k_Bi\omega n(\mathbf{q})\delta T(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{J}(\mathbf{q},\omega)=R_T(\mathbf{q},\omega),\quad(3.24)$$

where

$$\boldsymbol{\Pi}(\mathbf{q},\omega)=\sum_{i=1}^{9}\boldsymbol{\Pi}_i(\mathbf{q},\omega)\quad\text{and}\quad\mathbf{J}(\mathbf{q},\omega)=\sum_{k=1}^{8}\mathbf{J}_k(\mathbf{q},\omega)$$

can be identified with the time Fourier transforms of the momentum and energy fluxes, respectively, and $\mathbf{R}_\mathbf{u}(q,\omega)$ and $R_T(\mathbf{q},\omega)$ are "thermodynamic sources." The explicit expressions for the second rank Cartesian tensors $\boldsymbol{\Pi}_i(\mathbf{q},\omega)$, $i=1,...,6$, vectors $\mathbf{J}_k(\mathbf{q},\omega)$, $k=1,...,6$, the vector $\mathbf{R}_\mathbf{u}(\mathbf{q},\omega)$ and the scalar $R_T(\mathbf{q},\omega)$ are given in Appendix C. The tensors $\boldsymbol{\Pi}_i(\mathbf{q},\omega)$, $i=7$, 8, 9, and vectors $\mathbf{J}_i(\mathbf{q},\omega)$, $k=7$, 8 give rise to viscosities and thermal conductivity, which are our main concern here:

$$\boldsymbol{\Pi}_7(\mathbf{q},\omega)=\left(\frac{3b\sigma}{4\pi}\mathbf{F}_{05}(\mathbf{q})\underset{\rightarrow}{\overset{\vdots}{\odot}}\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega):\hat{\mathbf{1}}_6+\frac{9}{20\pi}b\sigma\eta\tau_\lambda^*(\mathbf{q},\omega)\Xi_0(\mathbf{q})\underset{\rightarrow}{\odot}\tilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega):\hat{\mathbf{1}}_6\right)\vdots\frac{\partial^2\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}\equiv\boldsymbol{\Pi}_7^c(\mathbf{q},\omega)\vdots\frac{\partial^2\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}},\quad(3.25)$$

$$\boldsymbol{\Pi}_8(\mathbf{q},\omega)=-\left[2\left(\hat{\mathbf{1}}_4+\frac{3b}{4\pi}\mathbf{F}_4(\mathbf{q})\right):\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega)+\frac{36}{5\pi^2}b^2\eta\Psi_0(\mathbf{q})-\frac{3b\sigma}{4\pi}\mathbf{F}_{05}(\mathbf{q})\overset{\vdots}{\odot}\frac{\partial}{\partial\mathbf{q}}\frac{\partial\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega)}{\partial\mathbf{q}}\right.$$
$$+\frac{9b^2}{2\pi}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\eta\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_{05}(\mathbf{q})\underset{\rightarrow}{\overset{\vdots}{\odot}}\tilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4+\frac{9}{10\pi}b\eta\tau_\lambda^*(\mathbf{q},\omega)\Xi(\mathbf{q})\cdot\tilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega)$$
$$-\frac{9}{20\pi}b\sigma\eta\Xi_0(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\lambda^*(\mathbf{q},\omega)\tilde{\mathbf{Q}}_{\nabla_\mathbf{u}}(\mathbf{q},\omega)]-(27\sqrt{2}/20\pi^2)$$
$$\left.\times\left(\frac{\sigma_{1w}}{\sigma}\right)^2b^2\eta\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\Xi_0(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\tilde{\mathbf{Q}}_\mathbf{u}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4\right]:\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}=-\boldsymbol{\Pi}_8^c(\mathbf{q},\omega):\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}},\quad(3.26)$$

$$\boldsymbol{\Pi}_9(\mathbf{q},\omega)=3b\sigma\eta\tau_\eta^*(\mathbf{q},\omega)\left(\mathbf{F}_{05}(\mathbf{q})+\frac{3}{16}\tau_\lambda^*(\mathbf{q},\omega)\Xi_0(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\mathbf{C}_\mathbf{P}(\mathbf{q}):\hat{\mathbf{1}}_6\right)\vdots\left.\frac{\partial}{\partial\mathbf{q}}\right|_{\nabla_\mathbf{n}}[\mathbf{S}_{\mathbf{u}\nabla\mathbf{n}}(\mathbf{q},\omega)],\quad(3.27)$$

$$\mathbf{J}_7(\mathbf{q},\omega)=-\Bigg[\left(\left(\mathbf{I}+\frac{9b}{20\pi}\mathbf{F}_2(\mathbf{q})\right)\cdot\lambda_I^{(2)}(\mathbf{q},\omega)+\frac{24b^2}{25\pi^2}\lambda\mathbf{\Phi}_{02}(\mathbf{q})-\frac{9b\sigma}{40\pi}\mathbf{F}_{03}(\mathbf{q})\dot{\odot}\frac{\partial\lambda_I^{(2)}(\mathbf{q},\omega)}{\partial\mathbf{q}}\right.$$
$$-\frac{9}{10}b\sigma\lambda\tau_\lambda^*(\mathbf{q},\omega)\mathbf{F}_{03}(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\widetilde{\mathbf{Q}}_T(\mathbf{q},\omega)\mathbf{I}+\frac{16}{5\pi}b\lambda\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_3(\mathbf{q}):\widetilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)$$
$$\left.-\frac{8}{5\pi}b\sigma\lambda\mathbf{F}_{04}(\mathbf{q})\underset{\rightarrow}{\vdots\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)]-\frac{3}{4}b\sigma\lambda\tau_\lambda^*(\mathbf{q},\omega)\tau_\eta^*(\mathbf{q},\omega)F_{04}(\mathbf{q})\underset{\rightarrow}{\vdots\odot}\widetilde{\mathbf{P}}_T(\mathbf{q})\cdot\mathbf{I}\right]\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}$$
$$=-\mathbf{J}_7^c(\mathbf{q},\omega)\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}},\tag{3.28}$$

$$\mathbf{J}_8(\mathbf{q},\omega)=\frac{b\sigma}{5\pi}\left(\frac{9}{8}\mathbf{F}_{03}(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\lambda_I^{(2)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4+8\lambda\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_{04}(\mathbf{q})\underset{\rightarrow}{\vdots\odot}\widetilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4\right):\frac{\partial^2\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}=-\mathbf{J}_8^c(\mathbf{q},\omega):\frac{\partial^2\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}.\tag{3.29}$$

All new notations in Eqs. (3.25)–(3.29) have been defined in Appendixes C and D. The continuity equation is considered in Appendix E.

A. Transport coefficients

We now introduce the vorticity tensor $\mathbf{W}(\mathbf{q},\omega)$,

$$\mathbf{W}(\mathbf{q},\omega)=\frac{1}{2}\left[\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}-\left(\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}\right)^T\right].\tag{3.30}$$

Then

$$\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}=\mathbf{S}(\mathbf{q},\omega)+\mathbf{W}(\mathbf{q},\omega)+\frac{1}{3}\mathbf{I}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega)\tag{3.31}$$

and

$$\left.\frac{\partial}{\partial\mathbf{q}}\right|_{\nabla n}[\mathbf{S}_{u\nabla n}(\mathbf{q},\omega)]=\frac{1}{2}\mathbf{S}(\mathbf{q},\omega)\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}+\frac{1}{2}\left(\mathbf{S}(\mathbf{q},\omega)\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)^T-\frac{1}{2}\mathbf{W}(\mathbf{q},\omega)\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}-\frac{1}{2}\left(\mathbf{W}(\mathbf{q},\omega)\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)^T$$
$$-\frac{1}{3}\left(\mathbf{S}(\mathbf{q},\omega)\cdot\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)\mathbf{I}+\frac{1}{3}\left(\mathbf{W}(\mathbf{q},\omega)\cdot\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)\mathbf{I}+\frac{1}{6}\left(\mathbf{I}\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}+\frac{1}{3}\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\mathbf{I}\right)\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega),\tag{3.32}$$

where the transpose $[\mathbf{A}]^T$ of the kth rank tensor $\mathbf{A}$ is defined as $\{\mathbf{A}\}^T_{ij\ldots m}\equiv A_{m\ldots ji}$. Using expressions (3.30)–(3.32) and (3.25)–(3.27) one can represent contributions $\mathbf{\Pi}''(\mathbf{q},\omega)$ of the terms which are proportional to $(\partial^2/\partial\mathbf{q}\partial\mathbf{q})\mathbf{u}(\mathbf{q},\omega)$ into $(\partial/\partial\mathbf{q})\cdot\mathbf{\Pi}(\mathbf{q},\omega)$ in the form,

$$\mathbf{\Pi}''(\mathbf{q},\omega)=-2\hat{\eta}(\mathbf{q},\omega)\vdots\frac{\partial}{\partial\mathbf{q}}\mathbf{S}(\mathbf{q},\omega)-\hat{\mathbf{W}}(\mathbf{q},\omega)\vdots\frac{\partial}{\partial\mathbf{q}}\mathbf{W}(\mathbf{q},\omega)-\hat{\mathbf{K}}(\mathbf{q},\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega)\right),\tag{3.33}$$

where the fourth rank shear viscosity tensor $\hat{\eta}(\mathbf{q},\omega)$ is

$$\hat{\eta}(\mathbf{q},\omega)=\frac{1}{2}\left(\mathbf{\Pi}_8^c(\mathbf{q},\omega)\underset{1}{\vdots\odot}\hat{\mathbf{1}}_6-\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_7^c(\mathbf{q},\omega)-\mathbf{G}_1(\mathbf{q},\omega)\underset{1}{\vdots\odot}\hat{\mathbf{1}}_6\right),\tag{3.34}$$

the fourth rank turbulent viscosity tensor $\hat{\mathbf{W}}(\mathbf{q},\omega)$ has the form

$$\hat{\mathbf{W}}(\mathbf{q},\omega)=\mathbf{\Pi}_8^c(\mathbf{q},\omega)\underset{1}{\vdots\odot}\hat{\mathbf{1}}_6-\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_7^c(\mathbf{q},\omega)+\mathbf{G}_2(\mathbf{q},\omega)\underset{1}{\vdots\odot}\hat{\mathbf{1}}_6,\tag{3.35}$$

and the second rank bulk viscosity tensor is defined as

$$\hat{\mathbf{K}}(\mathbf{q},\omega)=\frac{1}{3}\left\{(\mathbf{\Pi}_8^c(\mathbf{q},\omega):\mathbf{I})\underset{1}{\odot}\mathbf{I}-\left[\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_7^c(\mathbf{q},\omega)\right):\mathbf{I}\right]\cdot\mathbf{I}-\mathbf{G}_3(\mathbf{q},\omega)\underset{1}{\odot}\mathbf{I}\right\}.\tag{3.36}$$

In expressions (3.34)–(3.36), $\odot_1$ denotes a convolution over the first left index of a tensor to the left of $\odot_1$ and the index of $\partial/\partial\mathbf{q}$ from the expression (3.33), which should be performed after inserting expressions (3.34)–(3.36) into Eq. (3.33), and dots over the symbol $\odot_1$ mean inner products. Moreover, convolutions in the large parentheses brackets in Eq. (3.36) and everywhere below should be performed first, and tensors $\mathbf{G}_1(\mathbf{q},\omega)$, $\mathbf{G}_2(\mathbf{q},\omega)$, and $\mathbf{G}_3(\mathbf{q},\omega)$ are defined as

$$\mathbf{G}_1(\mathbf{q},\omega)=3b\sigma\eta\tau_\eta^*(\mathbf{q},\omega)\left[\left(\mathbf{F}_{05}(\mathbf{q})\cdot\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)-\frac{1}{3}\mathbf{G}_A(\mathbf{q})+\frac{3}{16}\tau_\lambda^*(\mathbf{q},\omega)\left(\mathbf{G}_B(\mathbf{q})-\frac{1}{3}\mathbf{G}_C(\mathbf{q})\right)\right], \tag{3.37}$$

$$\mathbf{G}_2(\mathbf{q},\omega)=3b\sigma\eta\tau_\eta^*(\mathbf{q},\omega)\left[\left(\mathbf{F}_{05}(\mathbf{q})\cdot\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)+\frac{1}{3}\mathbf{G}_A(\mathbf{q})+\frac{3}{16}\tau_\lambda^*(\mathbf{q},\omega)(\mathbf{G}_B(\mathbf{q})+\tfrac{1}{3}\mathbf{G}_C(\mathbf{q})\right], \tag{3.38}$$

$$\mathbf{G}_3(\mathbf{q},\omega)=2b\sigma\eta\tau_\eta^*(\mathbf{q},\omega)\left\{\mathbf{F}_{03}(\mathbf{q})\cdot\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}+\frac{9}{32}\tau_\lambda^*(\mathbf{q},\omega)\left[\Xi_0(\mathbf{q})\underset{I}{\dot{\odot}}\mathbf{C}_\mathbf{P}(\mathbf{q}):\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\mathbf{I}-\frac{1}{3}\left(\Xi_0(\mathbf{q})\underset{1}{\odot}\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)\cdot[\mathbf{C}_\mathbf{P}(\mathbf{q}):\mathbf{I}]\right]\right\}, \tag{3.39}$$

$$\mathbf{G}_A(\mathbf{q})=\mathbf{F}_{03}(\mathbf{q})\underset{1_4}{\odot}\left(\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\cdot\hat{\mathbf{1}}_4\right), \tag{3.40}$$

$$\mathbf{G}_B(\mathbf{q})=\Xi_0(\mathbf{q})\underset{1_4}{\dot{\odot}}\left(\mathbf{C}_P(\mathbf{q})\cdot\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\right)\cdot\hat{\mathbf{1}}_4, \tag{3.41}$$

$$\mathbf{G}_C(\mathbf{q})=\Xi_0(\mathbf{q})\underset{1_4}{\dot{\odot}}[\mathbf{C}_P(\mathbf{q}):\mathbf{I}]\left(\frac{\partial n(\mathbf{q})}{\partial\mathbf{q}}\cdot\hat{\mathbf{1}}_4\right), \tag{3.42}$$

where the symbols $\odot_I$ and $\odot_{1_4}$ denote convolutions over an index of the tensor to the left of $\odot_I$ or $\odot_{1_4}$ with an index of $\mathbf{I}$ or $\hat{\mathbf{1}}_4$, respectively. Although the turbulent viscosity tensor $\hat{\mathbf{W}}(\mathbf{q},\omega)$ from Eq. (3.35) is nonzero itself, the convolution $\hat{\mathbf{W}}(\mathbf{q},\omega)\vdots(\partial/\partial\mathbf{q})\mathbf{W}(\mathbf{q},\omega)$ is of the third order and should be neglected. Similarly, from expressions (3.28) and (3.29) one can obtain contributions $\mathbf{J}''(\mathbf{q},\omega)$ to $(\partial/\partial\mathbf{q})\cdot\mathbf{J}(\mathbf{q},\omega)$ from the terms which are proportional to $(\partial^2/\partial\mathbf{q}\partial\mathbf{q})\delta T(\mathbf{q},\omega)$,

$$\mathbf{J}''(\mathbf{q},\omega)=-\hat{\lambda}(\mathbf{q},\omega):\frac{\partial^2\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}, \tag{3.43}$$

where the second rank thermal conductivity tensor $\hat{\lambda}(\mathbf{q},\omega)$ has the form

$$\hat{\lambda}(\mathbf{q},\omega)=\mathbf{J}_7^c(\mathbf{q},\omega)\underset{1}{\dot{\odot}}\hat{\mathbf{1}}_4+\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{J}_8^c(\mathbf{q},\omega). \tag{3.44}$$

Although expressions (3.34)–(3.36) and (3.44) for viscosity tensors and tensorial thermal conductivity, respectively, have a complicated structure, they can be reduced to reasonably simple forms which can be proved to generalize those for the corresponding homogeneous fluid transport coefficients. This is further discussed in Sec. IV.

IV. ANALYSIS OF RESULTS

With some additional and not very strong restrictions the linearized Navier–Stokes equations (3.23) and (3.24) and expressions for the transport coefficients (3.34), (3.36), and (3.44) obtained can be dramatically simplified.

We assume now that the fluid inhomogeneity is due to the fluid-wall potential, and that no other external fields are present. This case would include simple fluids confined in capillary pores whose walls are composed of simple atoms (for instance, carbon, silicon, zeolites, etc.). Then from correlations (3.1) and (3.2), it follows that in each set of terms in Eqs. (3.23) and (3.24) proportional to constants, $bn(\mathbf{q})$, and $b^2n^2(\mathbf{q})$, one can restrict consideration to terms of tensoriality $\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}$ in Eq. (3.23) and $\hat{\sigma}\hat{\sigma}$ in Eq. (3.24), and among those terms for any integrable, positively defined function $f(\mathbf{q})$ there would hold hierarchies of

$$\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\sigma_p^2\sigma_s^2\gg\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\sigma_p^2\sigma_s\sigma_l,\quad s\neq l,$$

and

$$\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\sigma_s^2\gg\int d\hat{\sigma}f(\mathbf{q}-\sigma\hat{\sigma})\sigma_s\sigma_l,\quad s\neq l,\quad p,s,l=i,j,k.$$

Thus, for small $\mathbf{u}(\mathbf{q},\omega)$ and $\delta T(\mathbf{q},\omega)$, Eqs. (3.23) and (3.24) take the forms

$$-i\omega\rho(\mathbf{q})\mathbf{u}(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\Pi^0(\mathbf{q},\omega)=\frac{48\sqrt{2}}{5\pi}b\sigma\eta n(\mathbf{q})\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\tfrac{2}{3}\mathbf{I}-\hat{\sigma}\hat{\sigma})\cdot\mathbf{u}(\mathbf{q},\omega), \tag{4.1}$$

$$-\tfrac{3}{2} i\omega k_B n(\mathbf{q})\delta T(\mathbf{q},\omega)+\frac{\partial}{\partial \mathbf{q}}\cdot \mathbf{J}^0(\mathbf{q},\omega)=0, \tag{4.2}$$

where

$$\begin{aligned}\mathbf{\Pi}^0(\mathbf{q},\omega)=&\mathbf{\Pi}_1(\mathbf{q},\omega)+\Bigg[k_B\left(n(\mathbf{q})\mathbf{I}+\frac{3b}{4\pi}\mathbf{\Phi}_2(\mathbf{q})\right)-\pi\sqrt{\pi\beta m}\lambda\tau_\lambda^*(\mathbf{q},\omega)\tau_\eta^*(\mathbf{q},\omega)\mathbf{C}_Q(\mathbf{q})\cdot\frac{\partial n(\mathbf{q})}{\partial \mathbf{q}}\\&-\frac{9}{2}(k_B\beta/\sqrt{\pi\beta m})b\eta\tau_\lambda^*(\mathbf{q},\omega)\Xi(\mathbf{q})\cdot\frac{\partial n(\mathbf{q})}{\partial \mathbf{q}}+\frac{72}{25\pi}\beta b^2\lambda\eta\Xi_0(\mathbf{q}):\left(\frac{\partial\tau_\lambda^*(\mathbf{q},\omega)}{\partial \mathbf{q}}\frac{\partial n(\mathbf{q})}{\partial \mathbf{q}}\right)\\&+\frac{24}{25\pi}\beta b\sigma\eta[B(\mathbf{q})\cdot\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)]^T\Bigg]\delta T(\mathbf{q},\omega)-\Bigg[\frac{3b\sigma}{8\pi}k_B\mathbf{\Phi}_{03}(\mathbf{q})+\frac{16}{5\pi}b\sqrt{\pi\beta m}\lambda\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}n(\mathbf{q}\\&-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})(\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I})\hat{\boldsymbol{\sigma}}-\frac{72}{25\pi}\beta b^2\eta\lambda\Xi_0(\mathbf{q})\cdot\frac{\partial}{\partial \mathbf{q}}[\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})]+\frac{96}{25}\beta b\sigma^2\eta\lambda\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\Xi(\mathbf{q})\\&+\frac{72}{25\pi}\beta b^2\lambda\eta\tau_\lambda^*(\mathbf{q},\omega)\Xi_0(\mathbf{q})\underset{I}{\dot{\odot}}\frac{\partial n(\mathbf{q})}{\partial \mathbf{q}}\mathbf{I}\Bigg]\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial \mathbf{q}}+\eta\Bigg\{\frac{48\sigma^2 b}{5\pi}\Psi(\mathbf{q})+8\pi\sigma_{1w}^2\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}n_w(\mathbf{q}\\&-\sigma_{1w}\hat{\boldsymbol{\sigma}})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})(\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{1}{3}\mathbf{I})\hat{\boldsymbol{\sigma}}+4\pi\sigma^2\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\left[\mathbf{A}(\mathbf{q})\vdots\frac{1}{2}(2\mathbf{I}_4+\mathbf{I}_\delta-\tfrac{5}{3}\mathbf{II})\right]^T\circ\mathbf{I}\Bigg\}\cdot\mathbf{u}(\mathbf{q},\omega)\\&-8\pi\eta\tau_\eta^*(\mathbf{q},\omega)\left(\hat{\mathbf{I}}_4+\frac{3b}{4\pi}\mathbf{F}_{04}(\mathbf{q})\right):\mathbf{S}_{u\nabla n}(\mathbf{q},\omega)-2\hat{\boldsymbol{\eta}}^0(\mathbf{q},\omega):\mathbf{S}(\mathbf{q},\omega)-\hat{\mathbf{K}}^0(\mathbf{q},\omega)\frac{\partial}{\partial \mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega),\end{aligned} \tag{4.3}$$

and

$$\begin{aligned}\mathbf{J}^0(\mathbf{q},\omega)=&\frac{1}{\beta}\left[\left(n(\mathbf{q})\mathbf{I}+\frac{3b}{4\pi}\mathbf{\Phi}_2(\mathbf{q})\right)-\frac{15\sqrt{2}}{8}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}n_w(\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})(\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}-\tfrac{2}{3}\mathbf{I})\right]\cdot\mathbf{u}(\mathbf{q},\omega)\\&+\left[\frac{36}{25\pi}b\sigma^2\lambda\mathbf{\Phi}_1(\mathbf{q})-4\pi\lambda\tau_\lambda^*(\mathbf{q},\omega)\left(\mathbf{I}+\frac{9b}{20\pi}\mathbf{F}_2(\mathbf{q})\right)\cdot\frac{\partial n(\mathbf{q})}{\partial \mathbf{q}}+\frac{6\pi}{5}\sigma^2\lambda\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{M}(\mathbf{q})\right]\delta T(\mathbf{q},\omega)\\&-\hat{\boldsymbol{\lambda}}^0(\mathbf{q},\omega)\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial \mathbf{q}},\end{aligned} \tag{4.4}$$

and where the transport coefficients are given by

$$\begin{aligned}\hat{\boldsymbol{\eta}}^0(\mathbf{q},\omega)=&\eta n(\mathbf{q})\Bigg[4\pi\tau_\eta^*(\mathbf{q},\omega)\left(\hat{\mathbf{I}}_4+\frac{3b}{4\pi}\int d\hat{\boldsymbol{\sigma}}n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})\langle\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\rangle\right):\left(\hat{\mathbf{I}}_4+\frac{3b}{4\pi}\int d\hat{\boldsymbol{\sigma}}'n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}}')g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}}')\right.\\&\left.\times\langle(\hat{\boldsymbol{\sigma}}'\hat{\boldsymbol{\sigma}}'-\tfrac{1}{3}\mathbf{I})\hat{\boldsymbol{\sigma}}'\hat{\boldsymbol{\sigma}}'\rangle\right)+\frac{18}{5\pi^2}b^2\int d\hat{\boldsymbol{\sigma}}n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})\langle\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\rangle\Bigg],\end{aligned} \tag{4.5}$$

$$\begin{aligned}\hat{\mathbf{K}}^0(\mathbf{q},\omega)=&\eta n(\mathbf{q})\Bigg(2b\tau_\eta^*(\mathbf{q},\omega)\int d\hat{\boldsymbol{\sigma}}\,n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})(\langle\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\rangle-\tfrac{1}{3}\mathbf{I})+\frac{12}{5\pi^2}b^2\\&\times\int d\hat{\boldsymbol{\sigma}}n(q-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})[\langle\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\rangle-\tfrac{2}{3}(\hat{\boldsymbol{\sigma}}^2\cdot\mathbf{I}_3)]\Bigg),\end{aligned} \tag{4.6}$$

$$\begin{aligned}\hat{\boldsymbol{\lambda}}^0(\mathbf{q},\omega)=&\lambda n(\mathbf{q})\Bigg[4\pi\tau_\lambda^*(\mathbf{q},\omega)\left(\mathbf{I}+\frac{9b}{20\pi}\int d\hat{\boldsymbol{\sigma}}n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})\langle\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\rangle\right):\left(\mathbf{I}+\frac{9b}{20\pi}\int d\hat{\boldsymbol{\sigma}}'\,n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}}')\right.\\&\left.\times g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}}')\langle\hat{\boldsymbol{\sigma}}'\hat{\boldsymbol{\sigma}}'\rangle\right)+\frac{24}{25\pi^2}b^2\int d\hat{\boldsymbol{\sigma}}\,n(\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})g(\mathbf{q},\mathbf{q}-\sigma\hat{\boldsymbol{\sigma}})\langle\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\rangle\Bigg].\end{aligned} \tag{4.7}$$

In expressions (4.5)–(4.7) tensors $\langle\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}\rangle$ and $\langle\hat{\sigma}\hat{\sigma}\rangle$ are those $\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}$ and $\hat{\sigma}\hat{\sigma}$, respectively, in which components $\sigma_p\sigma_s\sigma_l\sigma_m$ and $\sigma_l\sigma_m$ with odd powers of indices $p,s,l,m=i,j,k$ (e.g., $\sigma_i^3\sigma_j$, $\sigma_j\sigma_k\sigma_i^2$, etc.) have been neglected, because of hierarchies established at the beginning of this section.

As can be easily seen from Eqs. (4.5)–(4.7), the ratios $\hat{\boldsymbol{\eta}}^0(\mathbf{q},\omega)/n(\mathbf{q})$, $\hat{\mathbf{K}}^0(\mathbf{q},\omega)/n(\mathbf{q})$, and $\hat{\boldsymbol{\lambda}}^0(\mathbf{q},\omega)/n(\mathbf{q})$ do not depend on local values of the number density $n(\mathbf{q})$. Similarly to the transport coefficients for the general case defined by Eqs. (3.34), (3.36), and (3.44), those from Eqs. (4.5)–(4.7) depend on position $\mathbf{q}$ and frequency ω. The zero-frequency (or long time) limits of expressions (3.34), (3.36), and (3.44), or Eqs. (4.5)–(4.7) provide tensorial transport coefficients for the general case of inhomogeneous fluids in time-independent external fields and/or in the presence of structured solid walls.

The general form of the relation between the number density and transport coefficients (or so called "smoothing procedure"[1,2]) is $\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}$. Moreover, as can be seen from Eqs. (3.34), (3.36), (3.44), or (4.5)–(4.7), there are two of its reductions involved:

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}$$

$$=\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}(\hat{\sigma}\cdot\hat{\sigma}),$$

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$

$$=\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\cdot\hat{\sigma})(\hat{\sigma}\cdot\hat{\sigma}).$$

Additional smoothing procedures appear in the general case of Eqs. (3.34)–(3.36) and (3.44), and are

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{k}$$

and

$$\int d\hat{\sigma}\, g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{k},\quad k=1,\ldots,5.$$

In the case of shear viscosity, bulk viscosity, and thermal conductivity defined by Eqs. (4.5)–(4.7), the reductions of the main smoothing procedure are

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\sigma_l^2\sigma_s^2$$

and

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\sigma_p^2,\quad l,s,p=i,j,k,$$

respectively. In the following subsections we consider several special cases of the further simplification of expressions (4.5)–(4.7) for the transport coefficients.

A. Transport coefficients in immediate vicinity of structured solid walls

Although, in general, there exists a variety of contributions to the transport coefficients, Eqs. (3.34), (3.36), and (3.44), caused by the presence of walls, the main contributions caused by hard-core fluid-wall intermolecular interactions are those which contribute to $\tau_\eta^*(\mathbf{q},\omega)$ and $\tau_\lambda^*(\mathbf{q},\omega)$ [Eqs. (3.8) and (3.11), respectively; at the zero frequency limit the τ^*'s are reduced to $\tau_\eta(\mathbf{q})$ and $\tau_\lambda(\mathbf{q})$ defined by Eqs. (3.6) and (3.9)]. This fact becomes even more obvious after natural reduction of the transport coefficients to those of Eqs. (4.5)–(4.7), which assume no external field other than that of the fluid-wall interactions (see the beginning of this section). Quantities $\tau_\eta(\mathbf{q})$ and $\tau_\lambda(\mathbf{q})$ are multipliers in the expressions for the main contributions to the shear viscosity and thermal conductivity tensors for all cases, including those for homogeneous fluids. As follows from expressions (3.6) and (3.9), the contributions to $\tau_\eta(\mathbf{q})$ and $\tau_\lambda(\mathbf{q})$ caused by hard-core fluid-wall intermolecular interactions are proportional to $\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})$, and are nonzero only for distances l from the walls which are about σ_{1w}.

However, for separations $l\approx\sigma_{1w}$ the values of $\tau_\eta(\mathbf{q})$ and $\tau_\lambda(\mathbf{q})$ can differ significantly from those for $l>\sigma_{1w}$. Since both functions $n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})$ and $g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})$ are positively defined, $\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\geqslant 0$, and values of $\tau_\eta(\mathbf{q})$ at $l\approx\sigma_{1w}$ could be smaller than those at $l>\sigma_{1w}$. This could lead to a decrease of shear (and bulk) viscosities at distances $l\approx\sigma_{1w}$ from the walls. Moreover, from Eq. (3.6) it can be seen that the larger the ratio $(\sigma_{1w}/\sigma)^2$ is, the larger is such a decrease. Macroscopically, for walls of simple geometries this could result in sliding of the fluid monolayer nearest to a wall along the wall. This phenomenon (known as a slip in velocity) has been discovered theoretically[19] and confirmed by different experimental investigations in fluid mechanics (for example, in the case of a flow of hard spherical colloid particles in cylindrical channels[16]), and by computer simulations of low density gas flows[20,21] and flows of simple liquids.[22] Here we have provided a possible microscopic justification for these observations.

For the thermal conductivity the situation is quite different. The hard-core, fluid-wall intermolecular interaction contribution to $\tau_\lambda(\mathbf{q})$ is negative [see Eq. (3.9)], which can lead to an increase in the thermal conductivity of a fluid at distances $l\approx\sigma_{1w}$ from the walls. Once again, the value of this increase is defined by the ratio $(\sigma_{1w}/\sigma)^2$, as well as by $\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})$. Quantities $\tau_\eta(\mathbf{q})$ and $\tau_\lambda(\mathbf{q})$ are related to characteristic times $\bar{\tau}_\eta(\mathbf{q})$ and $\bar{\tau}_\lambda(\mathbf{q})$ of the momentum and energy redistribution responses of a fluid by relations (3.7) and (3.10), respectively. Thus, the results obtained show that in the immediate vicinity of walls the hard-core, fluid-wall intermolecular interactions accelerate the momentum redistribution into a direction normal to the walls, and do not effect significantly the tangential momentum redistributions. In addition, these interactions slow down the energy redistribution.

B. Dense homogeneous fluids

For homogeneous fluids the equilibrium number densities do not depend on molecular positions, $n(\mathbf{q})=n$, and $g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})=g(\sigma)$. Subsequently, in the absence of solid walls, $n_w(\mathbf{q})=0$, and the corresponding Navier–Stokes equations, which can be obtained from Eqs. (3.23) and (3.24) or (4.1) and (4.2), take the forms

$$-i\omega\rho\mathbf{u}(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Pi}_H(\mathbf{q},\omega)=0, \quad (4.8)$$

$$-\tfrac{3}{2}ik_B\omega n\delta T(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{J}_H(\mathbf{q},\omega)=0, \quad (4.9)$$

where

$$\mathbf{\Pi}_H(\mathbf{q},\omega)=I\left[\left(\frac{\partial p}{\partial\rho}\right)_\beta\delta\rho(\mathbf{q},\omega)+nk_B[1+nbg(\sigma)]\delta T(\mathbf{q},\omega)\right]-2\hat{\boldsymbol{\eta}}_H^0(\omega):\mathbf{S}(\mathbf{q},\omega)-\hat{\mathbf{K}}_H^0\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega), \quad (4.10)$$

and

$$\mathbf{J}_H(\mathbf{q},\omega)=nk_BT[1+nbg(\sigma)]\mathbf{u}(\mathbf{q},\omega)-\hat{\lambda}_H^0(\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\delta T(\mathbf{q},\omega), \quad (4.11)$$

and where tensorial viscosities $\hat{\boldsymbol{\eta}}_H^0(\omega)$, $\hat{\mathbf{K}}_H^0(\omega)$ and thermal conductivity $\hat{\lambda}_H^0(\omega)$ do not depend on position $\mathbf{q}$ in the fluid, and are reductions of those of Eqs. (3.34), (3.36), and (3.44), or those defined by Eqs. (4.5)–(4.7):

$$\hat{\boldsymbol{\eta}}_H^0(\omega)=\eta\left\{(1-i\omega\bar{\tau}_\eta)^{-1}\frac{1}{g(\sigma)}\left(\hat{\mathbf{1}}_4+\frac{3}{4\pi}nbg(\sigma)\mathbf{T}_\eta\right):\left[\hat{\mathbf{1}}_4+\frac{3}{4\pi}nbg(\sigma)(\mathbf{T}_\eta-\tfrac{4}{9}\pi\mathbf{II})\right]+\frac{18}{5\pi^2}n^2b^2g(\sigma)\mathbf{T}_\eta\right\}, \quad (4.12)$$

$$\hat{\mathbf{K}}_H^0(\omega)=\frac{16}{15\pi}n^2b^2g(\sigma)\eta\mathbf{I}, \quad (4.13)$$

$$\hat{\lambda}_H^0(\omega)=\lambda\left((1-i\omega\bar{\tau}_\lambda)^{-1}\frac{1}{g(\sigma)}[1+\tfrac{3}{5}nbg(\sigma)]^2+\frac{32}{25\pi}n^2b^2g(\sigma)\right)\mathbf{I}. \quad (4.14)$$

In Eqs. (4.12)–(4.14) the quantities $\bar{\tau}_\eta$, $\bar{\tau}_\lambda$ are reductions of those defined by Eqs. (3.7) and (3.10), respectively,

$$\bar{\tau}_\eta=\frac{5}{16}\left(\frac{m\beta}{\pi}\right)^{1/2}[n\sigma^2g(\sigma)]^{-1}, \quad (4.15)$$

$$\bar{\tau}_\lambda=\frac{15}{32}\left(\frac{m\beta}{\pi}\right)^{1/2}[n\sigma^2g(\sigma)]^{-1}, \quad (4.16)$$

and the fourth rank symmetrical Cartesian tensor T_η has nonzero components as follows

$$(\mathbf{T}_\eta)_{llll}=\frac{4}{5}\pi,\quad l=i,j,k,$$
$$(\mathbf{T}_\eta)_{pqrs}=\frac{4}{15}\pi\begin{cases}\delta_{pr}\delta_{qs}\\ \delta_{ps}\delta_{qr}\\ \delta_{pq}\delta_{rs}\end{cases}\quad p,q,r,s=i,j,k. \quad (4.17)$$

Scalar shear viscosity $\eta_{Hsc}^0(\omega)$ and thermal conductivity $\lambda_{Hsc}^0(\omega)$ coefficients can be obtained by calculating the convolutions $\hat{\boldsymbol{\eta}}_H^0(\omega):\mathbf{S}(\mathbf{q},\omega)$ and $\hat{\lambda}_H^0(\omega)\cdot(\partial/\partial\mathbf{q})\delta T(\mathbf{q},\omega)$, in Eqs. (4.10) and (4.11), respectively,

$$\hat{\boldsymbol{\eta}}_H^0(\omega):\mathbf{S}(\mathbf{q},\omega)=\eta_{Hsc}^0(\omega)\mathbf{S}(\mathbf{q},\omega), \quad (4.18)$$

$$\hat{\lambda}_H^0(\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\delta T(\mathbf{q},\omega)=\lambda_{Hsc}^0(\omega)\frac{\partial}{\partial\mathbf{q}}\delta T(\mathbf{q},\omega), \quad (4.19)$$

where

$$\eta_{Hsc}^0(\omega)=\eta\left((1-i\omega\bar{\tau}_\eta)^{-1}\frac{1}{g(\sigma)}[1+\tfrac{2}{5}nbg(\sigma)]^2+\frac{48}{25\pi}n^2b^2g(\sigma)\right), \quad (4.20)$$

and

$$\lambda_{Hsc}^0(\omega)=\lambda\left((1-i\omega\bar{\tau}_\eta)^{-1}\frac{1}{g(\sigma)}[1+\tfrac{3}{5}nbg(\sigma)]^2+\frac{32}{25\pi}n^2b^2g(\sigma)\right). \quad (4.21)$$

The scalar bulk viscosity $K_{Hsc}^0(\omega)$ follows directly from Eq. (4.13),

$$K_{Hsc}^0(\omega)=\frac{16}{15\pi}n^2b^2g(\sigma)\eta. \quad (4.22)$$

Expressions (4.20)–(4.22) are identical to those obtained for dense homogeneous fluids in Ref. 11, and at the zero frequency limit lead to the familiar transport coefficients of dense homogeneous fluids. Similarly, substituting Eqs. (4.18) and (4.19) into Eqs. (4.10) and (4.11), one can recover Eqs. (3.14a) and (3.14b) of Ref. 11 for the Fourier time transforms of the momentum and energy fluxes, respectively, and the Navier–Stokes equations (3.13a) and (3.13b) of Ref. 11.

C. Fluids inhomogeneous in only one direction

We assume that the fluid is inhomogeneous only in the z direction. Assigning the origin of a spherical coordinate system (r,θ,ϕ) to position $\mathbf{q}=q_x\mathbf{i}+q_y\mathbf{j}+q_z\mathbf{k}\equiv x\mathbf{i}+y\mathbf{j}+z\mathbf{k}$, so that θ is an angle between the z direction and spherical radius r, and, thus $\sigma_x=\sin\theta\cos\phi$, $\sigma_y=\sin\theta\sin\phi$, and $\sigma_z=\cos\theta$, we can calculate the transport coefficient tensors (4.5)–(4.7) and derive explicit expressions for the terms $-2\hat{\boldsymbol{\eta}}^0(\mathbf{q},\omega):\mathbf{S}(\mathbf{q},\omega)$, $-\hat{\mathbf{K}}^0(\mathbf{q},\omega)(\partial/\partial\mathbf{q})\cdot\mathbf{u}(\mathbf{q},\omega)$, and $\hat{\lambda}^0(\mathbf{q},\omega)\cdot(\partial/\partial\mathbf{q})\delta T(\mathbf{q},\omega)$ on the right-hand sides of Eqs. (4.3) and (4.4), respectively,

$$2\hat{\eta}^0(\mathbf{q},\omega):\mathbf{S}(\mathbf{q},\omega)=2\hat{\eta}^0(z,\omega):\mathbf{S}(\mathbf{q},\omega)$$

$$=2\eta n(z)[C_1(z,\omega)\mathbf{S}(\mathbf{q},\omega)+C_2(z,\omega)\mathbf{S}^d(\mathbf{q},\omega)+C_3(z,\omega)S_{zz}(\mathbf{q},\omega)\mathbf{I}+C_4(z,\omega)S_{zz}(\mathbf{q},\omega)\hat{\mathbf{1}}_{kk}], \quad (4.23)$$

$$\hat{\mathbf{K}}^0(\mathbf{q},\omega)\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega)=\hat{\mathbf{K}}^0(z,\omega)\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega)=\eta n(z)[K_1(z,\omega)\mathbf{I}+K_2(z,\omega)\hat{\mathbf{1}}_{kk}]\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega), \quad (4.24)$$

$$\hat{\lambda}^0(\mathbf{q},\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\delta T(\mathbf{q},\omega)=\hat{\lambda}^0(z,\omega)\cdot\frac{\partial}{\partial\mathbf{q}}\delta T(\mathbf{q},\omega)=\lambda n(z)\{\tilde{L}_1(z,\omega)\mathbf{I}+\tilde{L}_2(z,\omega)\hat{\mathbf{1}}_{kk}\}\cdot\frac{\partial}{\partial\mathbf{q}}\delta T(\mathbf{q},\omega), \quad (4.25)$$

where $S_{zz}(\mathbf{q},\omega)$ is the zz (or kk) component of the shear rate tensor $S(\mathbf{q},\omega)$, the second rank tensor $\hat{\mathbf{1}}_{kk}$ has all components equal to zero but for the kk component which is equal to 1, and the second rank tensor $\mathbf{S}^d(\mathbf{q},\omega)$ is equal to the shear rate tensor $\mathbf{S}(\mathbf{q},\omega)$ in which components $S_{ik}(\mathbf{q},\omega)$, $S_{ki}(\mathbf{q},\omega)$, $S_{jk}(\mathbf{q},\omega)$, and $S_{kj}(\mathbf{q},\omega)$ [or $S_{xz}(\mathbf{q},\omega)$, $S_{zx}(\mathbf{q},\omega)$, $S_{yz}(\mathbf{q},\omega)$, and $S_{zy}(\mathbf{q},\omega)$, respectively] are set equal to zero. All other new notations in expressions (4.23)–(4.25) correspond to scalar quantities and are defined as

$$C_1(z,\omega)=4\pi\tau_\eta^*(z,\omega)\left(1+\frac{3b}{2}\beta^0(z)\right)^2+\frac{36}{5\pi}b^2\beta^0(z), \quad (4.26)$$

$$C_2(z,\omega)=6b[\tfrac{1}{4}\alpha(z)-\beta^0(z)]\left[\pi\tau_\eta^*(z,\omega)\left(2+\frac{3b}{2}\beta^0(z)+\frac{3b}{8}\alpha(z)\right)+\frac{6}{5\pi}b\right], \quad (4.27)$$

$$C_3(z,\omega)=3b[\beta^0(z)-\tfrac{1}{4}\alpha(z)]\left[\pi\tau_\eta^*(z,\omega)\left(2+\frac{3b}{4}\chi(z)+\frac{3b}{8}\alpha(z)-\frac{1}{3}\xi(z)\frac{[1+(3b/4)\chi(z)]}{[\beta^0(z)-\frac{1}{4}\alpha(z)]}\right.\right.$$

$$\left.\left.+\frac{3b}{2}\beta^0(z)\frac{[\gamma(z)-\beta^0(z)-\frac{1}{8}\alpha(z)]}{[\beta^0(z)-\frac{1}{4}\alpha(z)]}\right)+\frac{6}{5\pi}b\right], \quad (4.28)$$

$$C_4(z,\omega)=6b[\gamma(z)-\beta^0(z)-\tfrac{1}{8}\alpha(z)]\left[\pi\tau_\eta^*(z,\omega)\left(2+\frac{3b}{8}\alpha(z)+\frac{3b}{2}\gamma(z)-\frac{3b}{4}\beta^0(z)\right)+\frac{6}{5\pi}b\right], \quad (4.29)$$

$$K_1(z,\omega)=2b\left\{\pi\tau_\eta^*(z,\omega)[\chi(z)-\tfrac{2}{3}\nu(z)]+\frac{2}{5\pi}b\chi(z)\right\}, \quad (4.30)$$

$$K_2(z,\omega)=2b\xi(z)\left(\pi\tau_\eta^*(z,\omega)+\frac{2}{5\pi}b\right), \quad (4.31)$$

$$\tilde{L}_1(z,\omega)=4\pi\tau_\lambda^*(z,\omega)\left(1+\frac{9b}{20}\chi(z)\right)^2+\frac{24}{25\pi}b^2\chi(z), \quad (4.32)$$

$$\tilde{L}_2(z,\omega)=\frac{3b}{5}\xi(z)\left[3\pi\tau_\lambda^*(z,\omega)\left(2+\frac{9b}{10}\chi(z)+\frac{9b}{20}\xi(z)\right)+\frac{8}{5\pi}b\right], \quad (4.33)$$

where the quantities $\tau_\eta^*(z,\omega)=\tau_\eta(z)/[1-i\omega\bar{\tau}_\eta(z,\omega)]$ and $\tau_\lambda^*(z,\omega)=\tau_\lambda(z)/[1-i\omega\bar{\tau}_\lambda(z,\omega)]$ [see Eqs. (3.8) and (3.11), respectively] are reduced to $\tau_\eta^*(z)=\tau_\eta(z)$ and $\tau_\lambda^*(z)=\tau_\lambda(z)$ at the zero-frequency limit,

$$\tau_\eta^{-1}(z)=2\pi\left[\nu(z)+\tfrac{1}{3}\nu_1(z)+\sqrt{2}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\nu_2(z)\right], \quad (4.34)$$

$$\tau_\lambda^{-1}(z)=2\pi\left[\nu(z)-\frac{27}{32}\nu_1(z)-\frac{13\sqrt{2}}{8}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\nu_2(z)\right], \quad (4.35)$$

$$\nu_1(z)\equiv\int_0^\pi d\theta\sin\theta[n(z-\sigma\cos\theta)-n(z)]g(z,z-\sigma\cos\theta), \quad (4.36)$$

$$\nu_2(z)\equiv\int_0^\pi d\theta\sin\theta n_w(z-\sigma_{1w}\cos\theta)g_{1w}(z,z-\sigma_{1w}\cos\theta), \quad (4.37)$$

and

$$\alpha(z)\equiv\int_0^\pi d\theta\sin^5\theta N(z,z-\sigma\cos\theta), \quad (4.38)$$

$$\beta^0(z) \equiv \int_0^\pi d\theta \sin^3\theta \cos^2\theta N(z,z-\sigma\cos\theta), \tag{4.39}$$

$$\gamma(z) \equiv \int_0^\pi d\theta \sin\theta \cos^4\theta N(z,z-\sigma\cos\theta), \tag{4.40}$$

$$\xi(z) \equiv \int_0^\pi d\theta (2\sin\theta\cos^2\theta - \sin^3\theta) N(z,z-\sigma\cos\theta), \tag{4.41}$$

$$\chi(z) \equiv \int_0^\pi d\theta \sin^3\theta N(z,z-\sigma\cos\theta), \tag{4.42}$$

$$\nu(z) \equiv \int_0^\pi d\theta \sin\theta N(z,z-\sigma\cos\theta), \tag{4.43}$$

and where

$$N(z,z-\sigma\cos\theta) \equiv n(z-\sigma\cos\theta) g(z,z-\sigma\cos\theta). \tag{4.44}$$

In coordinate representation the Navier–Stokes equations (4.1) and (4.2) take the forms

$$-i\omega\rho(z)u_l(\mathbf{q},\omega) + \left(\frac{\partial}{\partial\mathbf{q}}\cdot\Pi^0(\mathbf{q},\omega)\right)_l^- = 2\eta_l^{(1)}(z,\omega)\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{S}(\mathbf{q},\omega)\right)_l + 2\eta_l^{(2)}(z,\omega)\frac{\partial}{\partial q_l}S_{zz}(\mathbf{q},\omega) - 2\eta_l^{(3)}(z,\omega)\frac{\partial}{\partial z}S_{zl}(\mathbf{q},\omega)$$
$$+K_l(z,\omega)\frac{\partial}{\partial q_l}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega)\right) + \frac{48\sqrt{2}}{5}\eta b\sigma\left(\frac{\sigma_{1w}}{\sigma}\right)^2 n(z)[\tfrac{4}{3}\nu_2(z) - \chi_w(z)$$
$$-\xi_w(z)\delta_{lk}]u_l(\mathbf{q},\omega), \quad l=i,j,k, \text{ (corresponding to } x,y,z, \text{ respectively)}, \tag{4.45}$$

$$-\tfrac{3}{2}i\omega k_B n(z)\delta T(\mathbf{q},\omega) + \left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{J}^0(\mathbf{q},\omega)\right)^- = \lambda n(z)\tilde{L}_1(z,\omega)\nabla^2\delta T(\mathbf{q},\omega) + \lambda n(z)\tilde{L}_2(z,\omega)\frac{\partial^2}{\partial z^2}\delta T(\mathbf{q},\omega), \tag{4.46}$$

where

$$\left(\frac{\partial}{\partial\mathbf{q}}\cdot\Pi^0(\mathbf{q},\omega)\right)^- \quad \text{and} \quad \left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{J}^0(\mathbf{q},\omega)\right)^-$$

are divergences of the fluxes Eqs. (4.3) and (4.4), from which terms

$$-2\hat{\eta}^0(\mathbf{q},\omega)\overset{:}{\odot}\frac{\partial}{\partial\mathbf{q}}\mathbf{S}(\mathbf{q},\omega),$$

$$-\mathbf{K}^0(\mathbf{q},\omega)\underset{1}{\odot}\frac{\partial}{\partial\mathbf{q}}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{u}(\mathbf{q},\omega)\right),$$

and

$$-\hat{\lambda}^0(\mathbf{q},\omega):\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}\delta T(\mathbf{q},\omega),$$

respectively, have been extracted; $u_l(\mathbf{q},\omega)$ is the l component of the velocity, δ_{lk} is Kronecker's delta, $S_{zl}(\mathbf{q},\omega)$ is the zl (or kl) component of the shear rate tensor, and $\xi_w(z)$ and $\chi_w(z)$ are defined by Eqs. (4.41) and (4.42), respectively, where $N(z,z-\sigma\cos\theta)$ has been changed to $n_w(z-\sigma_{1w}\cos\theta)g_{1w}(z,z-\sigma_{1w}\cos\theta)$.

In Eq. (4.45) the scalar shear viscosities, η_l's, and bulk viscosities $K_l(z,\omega)$'s are

$$\eta_l^{(1)}(z,\omega) = \eta n(z)[C_1(z,\omega) + (1-\delta_{lk})C_2(z,\omega)], \tag{4.47}$$

$$\eta_l^{(2)}(z,\omega) = \eta n(z)\{C_3(z,\omega) + [C_2(z,\omega) + C_4(z,\omega)]\delta_{lk}\}, \tag{4.48}$$

$$\eta_l^{(3)}(z,\omega) = \eta n(z)C_2(z,\omega)(\delta_{lk}-1), \tag{4.49}$$

$$K_l(z,\omega) = \eta n(z)[K_1(z,\omega) + \delta_{lk}K_2(z,\omega)], \quad l=i,j,k. \tag{4.50}$$

The thermal conductivities in Eq. (4.46) are

$$\lambda_1(z,\omega) = \lambda n(z)\tilde{L}_1(z,\omega) \tag{4.51}$$

and

$$\lambda_2(z,\omega) = \lambda n(z)\tilde{L}_2(z,\omega). \tag{4.52}$$

The transport coefficients (4.47)–(4.52) can be calculated immediately provided the equilibrium number density $n(z)$ and pair correlation function contact values $g(z,z-\sigma\cos\theta)$ are known for the composite potential φ_I.

Once again the transport coefficients for homogeneous fluids can be easily recovered from Eqs. (4.47)–(4.52). Indeed, for such fluids

$$\beta^0(z) - \tfrac{1}{4}\alpha(z) = 0, \quad \xi(z) = 0, \quad \gamma(z) - \beta^0(z) - \tfrac{1}{8}\alpha(z) = 0,$$

$$\chi(z) - \tfrac{2}{3}\nu(z) = 0, \quad \nu_1(z) = 0,$$

and $\nu_2(z) = \chi_w(z) = \xi_w(z) = 0$

[since $n_w(z)=0$], and one can derive

$$\eta_l^{(2)}(\omega) = \eta_l^{(3)}(\omega) = K_2(\omega) = \tilde{L}_2(\omega) = 0,$$

$$\eta_l^{(1)}(\omega) = \eta_{Hsc}^0(\omega), \quad \lambda_1(\omega) = \lambda_{Hsc}^0(\omega),$$

and

$$K_l(\omega)=K^0_{Hsc}(\omega),$$

where $\eta^0_{Hsc}(\omega)$, $\lambda^0_{Hsc}(\omega)$, and $K^0_{Hsc}(\omega)$ are defined by Eqs. (4.20)–(4.22), respectively, for all $l=i,\ j,\ k$.

In the particular case of a fluid in a narrow slit pore the results Eqs. (4.47)–(4.52), can be simplified further. We choose the z direction to be orthogonal to the pore walls, which are parallel to each other. Then the shear rate tensor will have just four nonzero components $S_{xz}=S_{zx}$, $S_{yz}=S_{zy}$, because in a narrow pore of several molecular diameters width, $u_z(\mathbf{q},\omega)=0$. As a result, $\mathbf{S}^d(\mathbf{q},\omega)=0$. Subsequently, the right-hand side of the momentum conservation equation (4.45) takes the form

$$2\eta n(z)C_1(z,\omega)\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{S}(\mathbf{q},\omega)\right)_l+(48\sqrt{2}/5)\eta b\sigma\left(\frac{\sigma_{1w}}{\sigma}\right)^2$$

$$\times n(z)[\tfrac{4}{3}\nu_2(z)-\chi_w(z)]u_l(\mathbf{q},\omega),$$

where $l=i,j$, and one finds a unique scalar shear viscosity coefficient

$$\eta_{\text{slit}}(z,\omega)=\eta n(z)C_1(z,\omega). \tag{4.53}$$

At the zero frequency limit it follows from Eqs. (4.53) and (4.26) that

$$\eta_{\text{slit}}(z)=\eta n(z)\left[4\pi\tau_\eta(z)\left(1+\frac{3b}{2}\beta^0(z)\right)^2+\frac{36}{5\pi}b^2\beta^0(z)\right]. \tag{4.54}$$

Similarly, the right-hand side of the energy conservation equation (4.46) is reduced to

$$\lambda n(z)[\widetilde{L}_1(z,\omega)+\widetilde{L}_2(z,\omega)]\frac{\partial^2}{\partial z^2}\delta T(\mathbf{q},\omega), \tag{4.55}$$

so that the scalar thermal conductivity $\lambda_{\text{slit}}(z)$ in the zero frequency limit is

$$\lambda_{\text{slit}}(z)=\lambda n(z)[\widetilde{L}_1(z)+\widetilde{L}_2(z)], \tag{4.56}$$

where $\widetilde{L}_1(z)$ and $\widetilde{L}_2(z)$ are defined by Eqs. (4.32) and (4.33) and calculated at $\tau^*_\lambda(z,\omega)=\tau_\lambda(z)$.

Other examples of fluid inhomogeneous in only one direction include fluids confined in narrow capillary pores of spherical and cylindrical geometries. The corresponding linearized Navier–Stokes equations and transport coefficients can be found for these cases after rewriting Eqs. (4.45) and (4.46) in proper coordinate system representations. We postpone investigation of such systems to our future work.

D. Inhomogeneity and the ratios (transport coefficient)/$n(q)$

As follows from the results obtained earlier, the transport coefficients, both in the general case [Eqs. (3.34), (3.36), and (3.44)] and in the case of external fields caused by the fluid-wall interactions only [Eqs. (4.5)–(4.7)], are functionally dependent on the position $\mathbf{q}$ in the fluid. Although the ratios (transport coefficient)/$n(\mathbf{q})$ have been proved to be independent of local values of $n(\mathbf{q})$, and consequently their dependence on $\mathbf{q}$ is not dramatic, it can still be significant. From a practical point of view it would be helpful to know for which specific inhomogeneous fluid systems, if any, the spatial dependence of the transport coefficients is negligibly small.

For this reason, we first consider the transport coefficients in the case of external fields generated by fluid-wall intermolecular interactions only, Eqs. (4.5)–(4.7). It's clear that the ratios (transport coefficient)/$n(\mathbf{q})$ would be independent of $\mathbf{q}$ if the quantities

$$\tau^*_\eta(\mathbf{q},\omega),\quad \tau^*_\lambda(\mathbf{q},\omega),$$

$$\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma},$$

$$\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma},$$

and

$$\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$

are independent of $\mathbf{q}$. In this case, since the spatial gradient of the number density of the equilibrium, inhomogeneous fluid is large, and, also, $\sigma_i,\sigma_j,\sigma_k\leqslant 1$, one can expect that

$$\frac{\partial}{\partial\mathbf{q}}\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\sigma_m\sigma_l\sigma_p\sigma_s\ll\frac{\partial}{\partial\mathbf{q}}n(\mathbf{q}),$$

$$m,l,p,s=i,j,k$$

and, consequently,

$$\frac{\partial}{\partial\mathbf{q}}\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\sigma_m\sigma_s\ll\frac{\partial}{\partial\mathbf{q}}n(\mathbf{q}),$$

$$\frac{\partial}{\partial\mathbf{q}}\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\ll\frac{\partial}{\partial\mathbf{q}}n(\mathbf{q}).$$

Moreover, from the definitions of the quantities $\tau^*_\eta(\mathbf{q},\omega)$ and $\tau^*_\lambda(\mathbf{q},\omega)$, Eqs. (3.8) and (3.11), respectively, it follows from the condition

$$\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\sigma_m\sigma_l\sigma_p\sigma_s\cong\text{const},$$

that for distances larger than σ_{1w} from the walls one can derive

$$\frac{\partial}{\partial\mathbf{q}}[\tau^*_\eta(\mathbf{q},\omega)]^{-1}\cong\frac{\partial}{\partial\mathbf{q}}[\tau^*_\lambda(\mathbf{q},\omega)]^{-1}\ll\frac{\partial}{\partial\mathbf{q}}n(\mathbf{q}).$$

Indeed, these quantities depend on $\mathbf{q}$ through $\tau_\eta(\mathbf{q})$ and $\tau_\lambda(\mathbf{q})$, respectively. Then from Eqs. (3.6) and (3.9) one can show that for separations $|\mathbf{q}|>\sigma_{1w}$ from walls the dependence of τ^*_η and τ^*_λ on $\mathbf{q}$ is defined by $\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$, because of the inequality

$$\int d\hat{\sigma}[n(\mathbf{q}-\sigma\hat{\sigma})-n(\mathbf{q})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$

$$\ll\int d\hat{\sigma}n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}).$$

Consequently, we conclude that for inhomogeneous fluids for which $\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$ is almost independent of $\mathbf{q}$, i.e.,

$$\frac{\partial}{\partial \mathbf{q}} \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) \ll \frac{\partial n(\mathbf{q})}{\partial \mathbf{q}},$$

the ratios (transport coefficient)/$n(\mathbf{q})$ will be almost independent of $\mathbf{q}$ as well. It can also be shown that this inequality is the necessary condition to have such ratios independent of $\mathbf{q}$ for the general case, Eqs. (3.34), (3.36), and (3.44). Noticing that

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma}) = \int d\hat{\sigma} n(\mathbf{q}+\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma}),$$

and recollecting that even for inhomogeneous fluids confined in narrow capillary pores of several molecular diameters width, the condition

$$\left|\frac{\partial^2}{\partial q_m \partial q_s} n(\mathbf{q})\right| \ll \frac{1}{\sigma}\left|\frac{\partial}{\partial q_p} n(\mathbf{q})\right|, \quad m,s,p=i,j,k$$

holds, one can expand $n(\mathbf{q}+\sigma\hat{\sigma})$ in the kernel of the integral $\int d\hat{\sigma}\, n(\mathbf{q}+\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma})$ in a Taylor series in σ in the neighborhood of $\mathbf{q}$. Restricting the series to the first three terms gives

$$a_2 n(\mathbf{q}) + \sigma \sum_{l=i,j,k} a_l^{(1)} \frac{\partial n(\mathbf{q})}{\partial q_l} + \frac{\sigma^2}{2} \sum_{l=i,j,k} a_{ll}^{(0)} \frac{\partial^2 n(\mathbf{q})}{\partial q_l^2} = b_0, \tag{4.57}$$

where

$$a_2 = \int d\hat{\sigma}\, g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma}), \tag{4.58}$$

$$\mathbf{a}^{(1)} = \int d\hat{\sigma}\hat{\sigma} g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma}), \tag{4.59}$$

$$\mathbf{a}^{(0)} = \int d\hat{\sigma} \langle\hat{\sigma}\hat{\sigma}\rangle g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma}), \tag{4.60}$$

$$b_0 = \int d\hat{\sigma}\, n(\mathbf{q}+\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}+\sigma\hat{\sigma}). \tag{4.61}$$

In expression (4.57) we have neglected the contributions of $\sigma_l\sigma_n$ terms with $l \neq n$ into $a^{(0)}$, and assumed a_2, $\mathbf{a}^{(1)}$, $\mathbf{a}^{(0)}$ to be independent of $\mathbf{q}$. Although this additional restriction is not obvious in the particular case of external potentials generated by the fluid-wall interactions only, more detailed analysis shows that this condition is required to assure that the ratios (transport coefficient)/$n(\mathbf{q})$ are independent of $\mathbf{q}$ in the general case [see Eqs. (3.34), (3.36), and (3.44)].

For a fluid inhomogeneous in only one direction (e.g., the z direction), Eq. (4.57) is reduced to

$$a_2 n(z) + \sigma a_z^{(1)} \frac{dn(z)}{dz} + \frac{\sigma^2}{2} a_{zz}^{(0)} \frac{d^2 n(z)}{dz^2} = b_0, \tag{4.62}$$

where explicit expressions for a_2, $a_z^{(1)}$, and $a_{zz}^{(0)}$,

$$a_2 = 2\pi \int_0^\pi d\theta \sin\theta g(z,z+\sigma\cos\theta), \tag{4.63}$$

$$a_z^{(1)} = 2\pi \int_0^\pi d\theta \sin\theta \cos\theta g(z,z+\sigma\cos\theta), \tag{4.64}$$

$$a_{zz}^{(0)} = 2\pi \int_0^\pi d\theta \sin\theta \cos^2\theta g(z,z+\sigma\cos\theta), \tag{4.65}$$

can be derived from Eqs. (4.58)–(4.61) using a consideration similar to that in Sec. IV C, $b_0 = \nu(z)$ [see Eq. (4.43)], and all notation correspond to those introduced in Sec. IV C.

If we choose the origin of the Cartesian coordinate system to lie somewhere inside a wall, than Eq. (4.62), as noted earlier, would hold for $z - z_w \geqslant \sigma_{1w}/2$ (the positive direction of the z axis corresponds to the direction from the wall into the fluid). Equation (4.62) is an inhomogeneous, linear, second-order differential equation, and at $z \geqslant \sigma_{1w}/2 + z_w$ has the solution

$$n(z) = \tilde{n}(z) + \frac{b_0}{a_2}, \tag{4.66}$$

where $\tilde{n}(z)$ is a general solution of the corresponding homogeneous equation, which, since quantities a_2, $a_z^{(1)}$, $a_{zz}^{(0)}$, and $b_0 \neq 0$ are real and positive, describes the damped harmonic space oscillator;[23] for $(a_z^{(1)})^2 - 2a_{zz}^{(0)} a_2 \neq 0$ it takes the form

$$\tilde{n}(z) = \begin{cases} 0, & z < z_w + \sigma_{1w}/2 \\ C_1 \exp[S_1(z - z_w - \sigma_{1w}/2)] + C_2 \exp[S_2(z - z_w - \sigma_{1w}/2)], & z \geqslant z_w + \sigma_{1w}/2 \end{cases} \tag{4.67}$$

where C_1, C_2 denote constants, $S_{1,2}$ are

$$S_{1,2} = -\mu \pm (\mu^2 - \omega_0^2)^{1/2}, \tag{4.68}$$

and where the damping constant μ and the undamped natural circular frequency ω_0 are

$$\mu = -\frac{a_z^{(1)}}{\sigma a_{zz}^{(0)}}, \tag{4.69}$$

$$\omega_0^2 = \frac{2a_2}{\sigma^2 a_{zz}^{(0)}}. \tag{4.70}$$

At $(a_z^{(1)})^2-2a_{zz}^{(0)}a_2=0$ the critically damped solution is

$$\tilde{n}(z)=\begin{cases}[C_1+C_2(z-z_w-\sigma_{1w}/2)]\exp[-\mu(z-z_w-\sigma_{1w}/2)], & z\geqslant z_w+\sigma_{1w}/2\\ 0, & z<z_w+\sigma_{1w}/2.\end{cases} \tag{4.71}$$

Since the relation (3.1) still holds, it is likely that for inhomogeneous fluids $(a_z^{(1)})^2-2a_{zz}^{(0)}a_2<0$ [see Eqs. (3.1) and (4.58)–(4.60)], and the solution (4.67) can be written as

$$\tilde{n}(z)=\begin{cases}0, & z<z_w+\sigma_{1w}/2\\ C_3\exp[-\mu(z-z_w-\sigma_{1w}/2)]\sin[\omega_N(z-z_w-\sigma_{1w}/2)+\alpha], & z\geqslant z_w+\sigma_{1w}/2\end{cases} \tag{4.72}$$

where the characteristic circular frequency ω_N is

$$\omega_N=(\omega_0^2-\mu^2)^{1/2}. \tag{4.73}$$

The constants C_1, C_2, or C_3 and α in Eqs. (4.67), (4.71), and (4.72) should be chosen so that the solution $\tilde{n}(z)$ defined by Eqs. (4.67), (4.71), or (4.72) would satisfy the boundary conditions for the particular inhomogeneous fluid-wall system of interest.

The main conclusion of the discussion above is that for inhomogeneous fluids in which the equilibrium number densities $n(\mathbf{q})$ behave qualitatively like damped spatial oscillators one should expect the ratios (transport coefficient)/$n(\mathbf{q})$ to be only weakly dependent on $\mathbf{q}$. Simulation data (for instance, Ref. 24) for the equilibrium number densities of fluids confined in narrow slit pores of width greater than 3σ exhibit such damped oscillatory behavior for $n(\mathbf{q})$.

The qualitative consideration above can be extended to inhomogeneous fluids in narrow capillary pores of cylindrical and spherical geometries, which we will consider in the near future and, hopefully, to other systems of relatively simple geometries. Thus, we conclude that for inhomogeneous fluids confined in pores of some simple geometries the ratios (transport coefficient)/$n(\mathbf{q})$ should be only weakly dependent on $\mathbf{q}$ at separations from the walls $|\mathbf{q}|>\sigma_{1w}/2$. This conclusion is in a good agreement with that obtained by Davis and co-workers[12,13,24] from simulation data for velocity profiles of Couette flow in narrow slit pores of several molecular diameters in width. Though such fluids are strongly inhomogeneous, for strictly geometrical reasons the ratios (transport coefficient)/$n(\mathbf{q})$ behave as if the fluids are weakly inhomogeneous, and the corresponding Navier–Stokes equations are rather simple generalizations of those for homogeneous fluids.

V. CLOSING REMARKS

The transport theory derived above is a rigorous generalization to inhomogeneous fluids of the Enskog-like approach suggested by Sung and Dahler[11] for homogeneous fluids. Although rigorous this theory remains tractable, an advantage that derives from dividing the potential into hard-core and soft contributions. The transport coefficients thus derived have a simple and tractable structure, and can be easily investigated and evaluated. The theory incorporates some approximations. The two basic ones are truncation of the set of moments equations and neglect of dynamic memory.

The shortcomings of the 13-moments approximation can be alleviated, in principle, by expanding the basis set beyond the first 13 velocity moments of the singlet dynamic distribution function. Although we do not have enough information on nonequilibrium inhomogeneous fluids to estimate the omission properly, it's well known that for homogeneous fluids more accurate estimates of the transport coefficients at zero frequency in the conventional Chapman–Enskog procedure lead to slight modifications of the numerical values of the contributions proportional to $n^2b^2g(\sigma)$; these correction factors are $(1.016)^{-1}$ for shear viscosity and $(1.025)^{-1}$ for thermal conductivity.[9,10] Thus, one does not expect the use of the 13-moments basis set truncation to lead to large errors. To correct this omission, one can use the Gross–Jackson kinetic modeling procedure,[25] which should be extended to inhomogeneous fluids.

The main contribution to dynamic memory effects is likely to come from repeated core collisions (not included in the theory presented here); there will also be smaller contributions due to the soft part of the potential. The neglect of these dynamic memory effects can be corrected for through analytic models, or by using molecular simulation data. Thus, one can make an approximate correction for these effects by adjusting the theoretical results to match simulation data for a fluid of hard spheres of the same hard sphere diameter, as has been done by Sung and Dahler,[11] who used Alder[26] and Dymond[27] correction factors. For inhomogeneous fluids the application of such ideas will be somewhat more complicated, since the density (and hence, the effective hard-core diameter, in the Weeks, Chandler, and Anderson (WCA) approximation discussed later) varies with position.

Calculations based on Eqs. (3.34), (3.36), (3.44), or (4.5)–(4.7) require determination of the local equilibrium number density $n(\mathbf{q})$, the hard-core diameter σ, and evaluation of contact values of the pair correlation function $g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$ for the intermolecular interaction potential φ_I of Eq. (2.1). The latter should be chosen so that it mimics some more realistic intermolecular potential, e.g., the Lennard-Jones model, φ_{LJ}. To do this, one can use the Weeks, Chandler, and Anderson[28] or Barker and Henderson[29] (BH) methods. Both methods have their pros and cons from the transport theory point of view. The WCA method supplies a hard-core diameter, σ_{WCA}, which depends on the equilibrium number density and temperature of the fluid, whereas the BH procedure yields a σ_{BH} that depends only on temperature. From a dynamical point of view there is scarcely any difference between collisional encounters described by potentials φ_I and φ_{LJ}, and it's reasonable to take into account the averaged effects of such small differences in the potentials by choosing the hard-core diameter σ to be a functional of density and temperature.[9,11]

In using the WCA choice of hard-core diameter, we note that the theory incorporates an assumption that the hard-core diameter σ corresponding to local densities $n(\mathbf{q})$ and $n(\mathbf{q}+\xi)$ is the same, provided $|\xi| \ll \sigma$. We believe this may be a good approximation for many situations, since the density dependence of σ is weak.[28] Nevertheless, the theory should be regarded as a zero-order theory with respect to the density dependence of σ, provided the WCA choice of hard-core diameter has been used. In order to avoid having to calculate σ for every local value of $n(\mathbf{q})$ it should be possible to introduce an averaged density n^*, and then calculate $\sigma_{WCA}(n^*)$.

The BH choice of hard-core diameter looks much more attractive for inhomogeneous fluids, because σ_{BH} does not depend on the density of the fluid. In this case the theory developed above should be regarded as an exact theory with respect to the density dependence of σ. However, alleviation for the neglect of the dynamic memory may become more complicated, because it is no longer clear that the main contribution to the memory can be equated to those caused by the repeated hard-core collisions only.

The contact values of the pair correlation function $g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$ can be obtained by direct computer simulations for a fluid with the intermolecular interaction potential φ_I of Eq. (2.1). Moreover, for homogeneous fluids Sung and Dahler[11] found that for the WCA choice of hard-core diameter the following correlation holds,

$$\frac{g(\sigma_{WCA})}{g_H(\sigma_{WCH})} \cong \frac{g(\sigma_{LJ})}{g_H(\sigma_{LJ})}, \tag{5.1}$$

where $g_H(\sigma_{LJ})$ and $g_H(\sigma_{WCH})$ are the contact values of the pair correlation functions specific to the hard sphere fluids with hard sphere diameters equated to σ_{LJ} (where σ_{LJ} is the Lennard-Jones parameter) and σ_{WCA}, respectively, and $g(\sigma_{LJ})$ and $g(\sigma_{WCA})$ are the contact values of the pair-correlation functions for the Lennard-Jones fluid. Similar correlation may hold for the corresponding local contact values of the pair correlation functions in the case of inhomogeneous fluids, and this could lead to a reasonable approximation of $g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$ specific to the composite potential φ_I.

Finally, we note that at the simplest level one can estimate the quantities

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\langle\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}\rangle$$

and

$$\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\langle\hat{\sigma}\hat{\sigma}\rangle$$

in Eqs. (4.5)–(4.7) heuristically, as was done in Ref. 1 for a fluid inhomogeneous in only one direction. While such an approach may give immediate results, it will be of uncertain validity and likely to break down in unforseen ways. We plan to test the theoretical expressions for the transport coefficients presented here via molecular simulations for fluids near walls and confined within pores, and these results will be presented in future papers.

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APPENDIX A: INTEGRODIFFERENTIAL FORM OF THE MOMENT EQUATIONS

The integrodifferential equations obtained by using the 13-moments approximation are

$$\frac{\partial}{\partial t}\delta n(\mathbf{q},t)+\frac{\partial}{\partial \mathbf{q}}\cdot[n(\mathbf{q})\mathbf{u}(\mathbf{q},t)]=\sigma^2 n(\mathbf{q})\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\cdot[\mathbf{u}(\mathbf{q}-\sigma\hat{\sigma},t)-\mathbf{u}(\mathbf{q},t)]+\sigma_{1w}^2 n(\mathbf{q})$$
$$\times\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}\cdot\mathbf{u}(\mathbf{q},t), \tag{A1}$$

$$\frac{\partial}{\partial t}[\rho(\mathbf{q})\mathbf{u}(\mathbf{q},t)]+\frac{\partial}{\partial \mathbf{q}}\cdot\mathbf{P}^0(\mathbf{q},t)+k_B\frac{\partial}{\partial \mathbf{q}}\cdot[n(\mathbf{q})\delta T(\mathbf{q},t)]\mathbf{I}+\frac{1}{\beta}\frac{\partial}{\partial \mathbf{q}}\delta n(\mathbf{q},t)$$
$$=\frac{1}{\beta}\int d\mathbf{q}'\left[n(\mathbf{q})\left(\frac{\partial C(\mathbf{q},\mathbf{q}')}{\partial \mathbf{q}}-g(\mathbf{q},\mathbf{q}')\frac{\partial f^H(\mathbf{q},\mathbf{q}')}{\partial \mathbf{q}}\right)+\frac{\partial n(\mathbf{q})}{\partial \mathbf{q}}\left(1+C(\mathbf{q},\mathbf{q}')-\int d\mathbf{q}'' n(\mathbf{q}'')C(\mathbf{q}'',\mathbf{q}')\right)\right]\delta n(\mathbf{q}',t)$$
$$+2\sigma^2\left(\frac{m}{\pi\beta}\right)^{1/2} n(\mathbf{q})\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot[\mathbf{u}(\mathbf{q}-\sigma\hat{\sigma},t)-\mathbf{u}(\mathbf{q},t)]-2\sqrt{2}\sigma_{1w}^2\left(\frac{m}{\pi\beta}\right)^{1/2} n(\mathbf{q})$$

$$\times \int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot\mathbf{u}(\mathbf{q},t)+\frac{\sigma^2 k_B}{2} n(\mathbf{q}) \int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})$$

$$\times \hat{\sigma}[\delta T(\mathbf{q}-\sigma\hat{\sigma},t)-\delta T(\mathbf{q},t)]+\frac{\sigma^2}{2}\int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:[n(\mathbf{q})\mathbf{P}^0(\mathbf{q}-\sigma\hat{\sigma},t)-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{P}^0(\mathbf{q},t)]$$

$$+\frac{\sigma^2}{2}\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:\mathbf{P}^0(\mathbf{q},t)+\frac{\sigma_{1w}^2}{2}\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:\mathbf{P}^0(\mathbf{q},t)$$

$$+\frac{\sigma^2}{5}\left(\frac{\beta m}{\pi}\right)^{1/2}\int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot[n(\mathbf{q})\mathbf{Q}(\mathbf{q}-\sigma\hat{\sigma},t)-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{Q}(\mathbf{q},t)]$$

$$-(2\sqrt{2}/5)\sigma_{1w}^2\left(\frac{\beta m}{\pi}\right)^{1/2}\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot\mathbf{Q}(\mathbf{q},t), \tag{A2}$$

$$\frac{3}{2}k_B n(\mathbf{q})\frac{\partial}{\partial t}\delta T(\mathbf{q},t)+\frac{\partial}{\partial \mathbf{q}}\cdot\mathbf{Q}(\mathbf{q},t)+k_B T\frac{\partial}{\partial \mathbf{q}}\cdot[n(\mathbf{q})\mathbf{u}(\mathbf{q},t)]$$

$$=\frac{\sigma^2}{2\beta}n(\mathbf{q})\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\cdot[\mathbf{u}(\mathbf{q}-\sigma\hat{\sigma},t)-\mathbf{u}(\mathbf{q},t)]+\frac{\sigma_{1w}^2}{\beta}n(\mathbf{q})\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}$$

$$\cdot\mathbf{u}(\mathbf{q},t)+(k_B/\sqrt{\pi\beta m})\sigma^2 n(\mathbf{q})\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})[\delta T(\mathbf{q}-\sigma\hat{\sigma},t)-\delta T(\mathbf{q},t)]+(\sigma^2/\sqrt{\pi\beta m})$$

$$\times\int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I}):[n(\mathbf{q})\mathbf{P}^0(\mathbf{q}-\sigma\hat{\sigma},t)-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{P}^0(\mathbf{q},t)]+\frac{3\sigma^2}{10}\int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}$$

$$\cdot[n(\mathbf{q})\mathbf{Q}(\mathbf{q}-\sigma\hat{\sigma},t)-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{Q}(\mathbf{q},t)]+\frac{2\sigma^2}{5}\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\cdot\mathbf{Q}(\mathbf{q},t)$$

$$+\sigma_{1w}^2\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}\cdot\mathbf{Q}(\mathbf{q},t), \tag{A3}$$

$$\beta\frac{\partial}{\partial t}\mathbf{P}^0(\mathbf{q},t)+2\mathbf{S}_{\mathrm{un}}(\mathbf{q},t)+\frac{4\beta}{5}\mathbf{S}_{\mathbf{Q}}(\mathbf{q},t)$$

$$=\sigma^2 n(\mathbf{q})\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\cdot[\mathbf{u}(\mathbf{q}-\sigma\hat{\sigma},t)-\mathbf{u}(\mathbf{q},t)]+2\sigma_{1w}^2 n(\mathbf{q})\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})$$

$$\times g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\cdot\mathbf{u}(\mathbf{q},t)+2k_B\sigma^2\left(\frac{\beta}{\pi m}\right)^{1/2}n(\mathbf{q})\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})$$

$$\times[\delta T(\mathbf{q}-\sigma\hat{\sigma},t)-\delta T(\mathbf{q},t)]+2\left(\frac{\beta}{\pi m}\right)^{1/2}\sigma^2\int d\hat{\sigma}\, g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:[n(\mathbf{q})\mathbf{P}^0(\mathbf{q}-\sigma\hat{\sigma},t)-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{P}^0(\mathbf{q},t)]$$

$$-6\left(\frac{\beta}{\pi m}\right)^{1/2}\sigma^2\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:\mathbf{P}^0(\mathbf{q},t)-6\sqrt{2}\left(\frac{\beta}{\pi m}\right)^{1/2}\sigma_{1w}^2\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})$$

$$\times g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:\mathbf{P}^0(\mathbf{q},t)+\frac{2}{5}\beta\sigma^2\int d\hat{\sigma}\, g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\cdot[n(\mathbf{q})\mathbf{Q}(\mathbf{q}-\sigma\hat{\sigma},t)$$

$$-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{Q}(\mathbf{q},t)]\quad+\frac{1}{5}\beta\sigma^2\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma}) g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\cdot\mathbf{Q}(\mathbf{q},t)$$

$$+\frac{4}{5}\beta\sigma_{1w}^2\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma}) g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\cdot\mathbf{Q}(\mathbf{q},t), \tag{A4}$$

$$\frac{\partial}{\partial t}\mathbf{Q}(\mathbf{q},t)+\frac{5}{2}\frac{k_B}{\beta m}\frac{\partial}{\partial \mathbf{q}}[n(\mathbf{q})\delta T(\mathbf{q},t)]+\frac{1}{\beta m}\frac{\partial}{\partial \mathbf{q}}\cdot\mathbf{P}^0(\mathbf{q},t)$$

$$=(\sigma^2/2\beta\sqrt{\pi\beta m})n(\mathbf{q})\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot[\mathbf{u}(\mathbf{q}-\sigma\hat{\sigma},t)-\mathbf{u}(\mathbf{q},t)]$$

$$-(\sqrt{2}\sigma_{1w}^2/\beta\sqrt{\pi\beta m})n(\mathbf{q})\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot\mathbf{u}(\mathbf{q},t)+\frac{3\sigma^2}{4}\frac{k_B}{\beta m}n(\mathbf{q})$$

$$\times\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}[\delta T(\mathbf{q}-\sigma\hat{\sigma},t)-\delta T(\mathbf{q},t)]+\frac{\sigma^2}{4\beta m}\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:\mathbf{P}^0(\mathbf{q},t)$$

$$+\frac{3\sigma^2}{4\beta m}\int d\hat{\sigma}\, g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:[n(\mathbf{q})\mathbf{P}^0(\mathbf{q}-\sigma\hat{\sigma},t)-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{P}^0(\mathbf{q},t)]-(2\sigma^2/5\sqrt{\pi\beta m})\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})$$

$$\times g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}+\mathbf{I})\cdot\mathbf{Q}(\mathbf{q},t)+(27\sigma^2/20\sqrt{\pi\beta m})\int d\hat{\sigma}\, g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot[n(\mathbf{q})\mathbf{Q}(\mathbf{q}-\sigma\hat{\sigma},t)$$

$$-n(\mathbf{q}-\sigma\hat{\sigma})\mathbf{Q}(\mathbf{q},t)]-(13\sqrt{2}\sigma_{1w}^2/5\sqrt{\pi\beta m})\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\cdot\mathbf{Q}(\mathbf{q},t). \tag{A5}$$

In Eqs. (A1)–(A5) $\mathbf{I}$ denotes the unit matrix, and quantities

$$\underbrace{\hat{\sigma}\ldots\hat{\sigma}}_{n},\quad n=2,3,\ldots$$

are the nth rank Cartesian tensorial products of the direction cosines vector $\hat{\sigma}$ with itself; thus, for instance, $\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}$ is the fourth rank Cartesian tensor composed of 81 components $(\sigma_i\sigma_l\sigma_m\sigma_s)$, $i,l,m,s=x,y,z$. Similarly, $[\hat{\sigma}\hat{\sigma}-(1/3)\mathbf{I}]\hat{\sigma}$, $[\hat{\sigma}\hat{\sigma}-(1/3)\mathbf{I}]\hat{\sigma}\hat{\sigma}$, etc. are tensorial products of the tensors $[\hat{\sigma}\hat{\sigma}-(1/3)\mathbf{I}]$ and $\hat{\sigma}$ or $\hat{\sigma}\hat{\sigma}$. The second rank Cartesian tensors $\mathbf{S}_{un}(\mathbf{q},t)$ and $\mathbf{S}_Q(\mathbf{q},t)$ are defined as

$$\mathbf{S}_{\mathbf{un}}(\mathbf{q},t)=\frac{1}{2}\left\{\frac{\partial}{\partial\mathbf{q}}[\mathbf{u}(\mathbf{q},t)n(\mathbf{q})]+\left(\frac{\partial}{\partial\mathbf{q}}[\mathbf{u}(\mathbf{q},t)n(\mathbf{q})]\right)^T-\frac{2}{3}\mathbf{I}\left(\frac{\partial}{\partial\mathbf{q}}\cdot[\mathbf{u}(\mathbf{q},t)n(\mathbf{q})]\right)\right\}, \tag{A6}$$

$$\mathbf{S}_Q(\mathbf{q},t)=\frac{1}{2}\left[\left(\frac{\partial}{\partial\mathbf{q}}\mathbf{Q}(\mathbf{q},t)\right)+\left(\frac{\partial}{\partial\mathbf{q}}\mathbf{Q}(\mathbf{q},t)\right)^T-\frac{2}{3}\mathbf{I}\left(\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{Q}(\mathbf{q},t)\right)\right], \tag{A7}$$

where $\{(\partial/\partial\mathbf{q})[\mathbf{u}(\mathbf{q},t)n(\mathbf{q})]\}^T$ and $\{(\partial/\partial\mathbf{q})[\mathbf{Q}(\mathbf{q},t)]\}^T$ denote the transposes of the tensors $(\partial/\partial\mathbf{q})[\mathbf{u}(\mathbf{q},t)n(\mathbf{q})]$ and $(\partial/\partial\mathbf{q})[\mathbf{Q}(\mathbf{q},t)]$, respectively.

APPENDIX B: REDUCED EQUATIONS FOR $\mathbf{P}^0(\mathbf{q},\omega)$ AND $\mathbf{Q}(\mathbf{q},\omega)$

Reduced equations for the time Fourier transforms of the "kinetic" contributions to the energy flux and the pressure tensor are

$$-i\omega\mathbf{Q}(\mathbf{q},\omega)+[8\sigma^2/15\sqrt{\pi\beta m}]\left[\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})+\frac{27}{32}\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})-(13\sqrt{2}/8)\right.$$

$$\left.\times\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\right]\mathbf{Q}(\mathbf{q},\omega)$$

$$=-\frac{5k_B}{2\beta m}\left(\frac{\partial}{\partial\mathbf{q}}[n(\mathbf{q})\delta T(\mathbf{q},\omega)]+\frac{9bn(\mathbf{q})}{20\pi}\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}\right)-[\sigma^3n(\mathbf{q})/2\beta\sqrt{\pi\beta m}]$$

$$\times\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}:\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}-\frac{\sqrt{2}\sigma_{1w}^2n(\mathbf{q})}{\beta\sqrt{\pi\beta m}}\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})$$

$$\times\cdot\mathbf{u}(\mathbf{q},\omega)+\frac{\sigma^2}{4\beta m}\int d\hat{\sigma}[3n(\mathbf{q})-2n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}:\mathbf{P}^0(\mathbf{q},\omega), \tag{B1}$$

$$-i\omega\mathbf{P}^0(\mathbf{q},\omega)+\frac{2}{\beta}\mathbf{S}_{un}(\mathbf{q},\omega)=-\frac{\sigma^3}{\beta}n(\mathbf{q})\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\hat{\sigma}:\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}+\frac{2\sigma_{1w}^2}{\beta}n(\mathbf{q})$$

$$\times\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\cdot\mathbf{u}(\mathbf{q},\omega)-(2k_B\sigma^3/\sqrt{\pi\beta m})n(\mathbf{q})$$

$$\times\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}-(4\sigma^2/5\sqrt{\pi\beta m})$$

$$\times\left(\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})+\frac{1}{3}\int d\hat{\sigma} g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})[n(\mathbf{q}-\sigma\hat{\sigma})-n(\mathbf{q})]+\sqrt{2}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\right.$$

$$\left.\times\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\right)\mathbf{P}^0(\mathbf{q},\omega)+\frac{\sigma^2}{5}\left[\int d\hat{\sigma}[2n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]\right.$$

$$\times g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}+4\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\sigma}\, n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})$$

$$\left.\times(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\hat{\sigma}\right]\cdot\mathbf{Q}(\mathbf{q},\omega). \tag{B2}$$

If one assumes $n(\mathbf{q})=\text{const.}$ $n_w(\mathbf{q})=0$, and $g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})=g(\sigma)$, then from Eqs. (2.25)–(2.27) and Eqs. (B1) and (B2), one can recover the 13-moments approximation equations for dense homogeneous (bulk) fluids.[11]

APPENDIX C: THE FIRST SIX CONTRIBUTIONS TO THE MOMENTUM AND ENERGY FLUXES, AND $\mathbf{R}_u(\mathbf{q},\omega)$, $R_T(\mathbf{q},\omega)$

The explicit expressions for the first six contributions to the momentum flux $\mathbf{\Pi}(\mathbf{q},\omega)$ are

$$\mathbf{\Pi}_1(\mathbf{q},\omega)=\left(\int d\mathbf{q}'\frac{\delta p(\mathbf{q})}{\delta n(\mathbf{q}')}\delta n(\mathbf{q}',\omega)-n(\mathbf{q})\int\int d\mathbf{q}'d\mathbf{q}''\frac{\delta p(\mathbf{q}'')}{\delta n(\mathbf{q}')}\delta n(\mathbf{q}',\omega)-\frac{1}{3\beta}n(\mathbf{q})\int d\mathbf{q}'\,\mathrm{Tr}\,\wp(\mathbf{q},\mathbf{q}')\delta n(\mathbf{q}',\omega)\right.$$

$$\left.+\frac{1}{3\beta}n(\mathbf{q})\int\int d\mathbf{q}'d\mathbf{q}''n(\mathbf{q}'')\mathrm{Tr}\,\wp(\mathbf{q}'',\mathbf{q}')\delta n(\mathbf{q}',\omega)\right)\mathbf{I}, \tag{C1}$$

$$\mathbf{\Pi}_2(\mathbf{q},\omega)=\left[k_B\left(n(\mathbf{q})\mathbf{I}+\frac{3b}{4\pi}\Phi_2(\mathbf{q})\right)-\pi\sqrt{\pi\beta m}\lambda\tau_\lambda^*(\mathbf{q},\omega)\tau_\eta^*(\mathbf{q},\omega)\left(\hat{\mathbf{1}}_4+\frac{3b}{4\pi}\mathbf{F}_4(\mathbf{q})\right):\tilde{\mathbf{P}}_T(\mathbf{q})+\frac{3b\sigma}{8}\sqrt{\pi\beta m}\lambda\mathbf{F}_{05}(\mathbf{q})\dot{\vdots}\!\odot\frac{\partial}{\partial\mathbf{q}}\right.$$

$$\times[\tau_\lambda^*(\mathbf{q},\omega)\tau_\eta^*(\mathbf{q},\omega)\tilde{\mathbf{P}}_T(\mathbf{q})]-\frac{96}{25}\beta b\sigma^2\lambda\eta\tau_\lambda^*(\mathbf{q},\omega)\Xi(\mathbf{q})\cdot\tilde{\mathbf{Q}}_T(\mathbf{q},\omega)+\frac{72}{25}\frac{\beta b^2}{\pi}\lambda\eta\Xi_0(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\lambda^*(\mathbf{q},\omega)\tilde{\mathbf{Q}}_T(\mathbf{q},\omega)]$$

$$\left.+\frac{16}{15}\sqrt{\pi\beta m}\sigma^2\lambda n(\mathbf{q})\tau_\eta^*(\mathbf{q},\omega)[\mathbf{A}(\mathbf{q}):\tilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)]^T+\frac{24}{25\pi}b\sigma\beta\eta[\mathbf{B}(\mathbf{q})\cdot\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)]^T\right]\delta T(\mathbf{q},\omega), \tag{C2}$$

$$\mathbf{\Pi}_3(\mathbf{q},\omega)=-\left[\frac{3b\sigma}{8\pi}k_B\Phi_{03}(\mathbf{q})+\frac{32}{15}\sqrt{\pi\beta m}\lambda\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\left(\hat{\mathbf{1}}_6+\frac{3b}{4\pi}\mathbf{F}_4(\mathbf{q}):\hat{\mathbf{1}}_6\right):\tilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)-\frac{4}{5\pi}\sqrt{\pi\beta m}b\sigma\lambda\mathbf{F}_{05}(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}\right.$$

$$\times[\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\tilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)]+\frac{24}{25\pi}\beta b\sigma^2\eta\Xi(\mathbf{q})\cdot\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)-\frac{18}{25\pi^2}\beta b^2\eta\Xi_0(\mathbf{q})\dot{\odot}\frac{\partial\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)}{\partial\mathbf{q}}$$

$$\left.+\frac{3}{8}\sqrt{\pi\beta m}b\sigma\lambda\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{F}_{05}(\mathbf{q})\dot{\vdots}\!\odot\tilde{\mathbf{P}}_T(\mathbf{q})\mathbf{I}+\frac{72}{25\pi}\beta b^2\lambda\eta\tau_\lambda^*(\mathbf{q},\omega)\Xi_0(\mathbf{q}):\tilde{\mathbf{Q}}_T(\mathbf{q},\omega)\mathbf{I}\right]\cdot\frac{\partial\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}}, \tag{C3}$$

$$\mathbf{\Pi}_4(\mathbf{q},\omega)=\left(\frac{4}{5\pi}\sqrt{\pi\beta m}b\sigma\lambda\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_{05}(\mathbf{q})\underset{\rightarrow}{\overset{\vdots}{\odot}}\widetilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4+\frac{18}{25\pi^2}\beta b^2\eta\Xi_0(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\lambda_I^{(2)}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4\right):\frac{\partial^2\delta T(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}, \quad (C4)$$

$$\mathbf{\Pi}_5(\mathbf{q},\omega)=\Bigg[\frac{48\sigma^2}{5\pi}b\eta\Psi(\mathbf{q})+8\pi\sigma_{1w}^2\eta\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)+6\sigma_{1w}^2b\eta\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_4(\mathbf{q}):\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)-3\sigma_{1w}^2\sigma b\eta\mathbf{F}_{05}(\mathbf{q})\overset{\vdots}{\odot}\frac{\partial}{\partial\mathbf{q}}$$

$$\times[\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)]-(9\sqrt{2}/5\pi)\sigma_{1w}^2b\eta\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\Xi(\mathbf{q})\cdot\widetilde{\mathbf{Q}}_\mathbf{u}(\mathbf{q},\omega)+(9\sqrt{2}/10\pi)\sigma_{1w}^2b\sigma\eta\Xi_0(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}$$

$$\times[\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{Q}}_\mathbf{u}(\mathbf{q},\omega)]+\sigma^2[\mathbf{A}(\mathbf{q}):\eta_I^{(2)}(\mathbf{q},\omega)]^T\circ\mathbf{I}+\frac{3}{5}\sigma^2\eta\tau_\lambda^*(\mathbf{q},\omega)[\mathbf{B}(\mathbf{q})\cdot\widetilde{\mathbf{Q}}_{\nabla u}(\mathbf{q},\omega)]\circ\mathbf{I}\Bigg]\cdot\mathbf{u}(\mathbf{q},\omega), \quad (C5)$$

$$\mathbf{\Pi}_6(\mathbf{q},\omega)=\Bigg[-8\pi\eta\tau_\eta^*(\mathbf{q},\omega)\left(\hat{\mathbf{1}}_4+\frac{3b}{4\pi}\mathbf{F}_4(\mathbf{q})\right)+3b\sigma\eta\tau_\eta^*(\mathbf{q},\omega)\mathbf{F}_{05}(\mathbf{q})\overset{\vdots}{\odot}\frac{\partial}{\partial\mathbf{q}}\bigg|_\mathbf{u}\hat{\mathbf{1}}_4+3b\sigma\eta\mathbf{F}_{05}(\mathbf{q})\odot\frac{\partial}{\partial\mathbf{q}}[\tau_\eta^*(\mathbf{q},\omega)]$$

$$-\frac{9}{8}b\eta\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\Xi(\mathbf{q})\cdot\mathbf{C}_p(\mathbf{q})+\frac{9}{16}b\sigma\eta\Xi_0(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{C}_p(\mathbf{q})]$$

$$+\frac{9}{16}b\sigma\eta\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\Xi_0(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\mathbf{C}_p(\mathbf{q}):\frac{\partial}{\partial\mathbf{q}}\bigg|_\mathbf{u}\hat{\mathbf{1}}_4\Bigg]:\mathbf{S}_{\mathbf{u}\nabla n}(\mathbf{q},\omega). \quad (C6)$$

In expressions (C1)–(C6) $[\mathbf{D}]^T$ means the transpose of the pth rank Cartesian tensor $\mathbf{D}$ defined by the expression $\{[\mathbf{D}]^T\}_{lm\ldots s}=D_{s\ldots ml}$, and an open dot ($\circ$) denotes a convolution over the second left index of a tensor to the left of $\circ$ and a regular index of the tensor to the right; notations $\odot$ and $\odot_\rightarrow$ denote convolutions over a $\hat{\sigma}$ index of a tensor to the left of the corresponding convolution sign and a $(\partial/\partial\mathbf{q})$ index of a tensor to the right; in the case of $\odot_\rightarrow$ the $(\partial/\partial\mathbf{q})$ index of a tensor to the right should be taken after executing convolutions of tensors $\hat{\mathbf{1}}_6$. $\hat{\mathbf{1}}_4$, or $\mathbf{I}$ with the corresponding continuum variable or its spatial gradient. The sixth- and fourth-rank Cartesian tensors $\hat{\mathbf{1}}_6$, $\hat{\mathbf{1}}_4$ are composed of components $(\hat{1}_6)_{lmnspq}=\delta_{lq}\delta_{mp}\delta_{ns}$, $(\hat{1}_4)_{lmns}=\delta_{ls}\delta_{mn}$, respectively ($\delta$-$s$ here are Kronecker symbols), and are considered in Appendix D. Gradients $(\partial/\partial\mathbf{q})|_\mathbf{u}$ in Eq. (C6) and $(\partial/\partial\mathbf{q})|_{\nabla n}$ in Eq. (3.27) are to be calculated at $\mathbf{u}(\mathbf{q},\omega)$ and $\nabla n(\mathbf{q})$ fixed, respectively, and $\nabla\equiv(\partial/\partial\mathbf{q})$. All other new notations in Eqs. (C1)–(C6) are as follows:

$$\mathbf{\Phi}_m(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}\,n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{m}+\frac{\sigma}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\int d\hat{\sigma}\,n(\mathbf{q})n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{m+1},\quad m=1,2,\ldots \quad (C7)$$

$$\mathbf{F}_m(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{m}+\frac{\sigma}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\int d\hat{\sigma}\,n(\mathbf{q})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{m+1},\quad m=1,2,\ldots \quad (C8)$$

$$\Xi(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})+\frac{\sigma}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\int d\hat{\sigma}n(\mathbf{q})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I}), \quad (C9)$$

$$\Psi(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}\,n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})+\frac{\sigma}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\int d\hat{\sigma}n(\mathbf{q})n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I}), \quad (C10)$$

$$\mathbf{F}_{0m}(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}\,g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{m},\quad m=1,2,\ldots \quad (C11)$$

$$\mathbf{\Phi}_{0m}(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}\,n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\underbrace{\hat{\sigma}\cdots\hat{\sigma}}_{m},\quad m=1,2,\ldots \quad (C12)$$

$$\Xi_0(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\hat{\sigma}\mathbf{I}\hat{\sigma}), \quad (C13)$$

$$\Psi_0(\mathbf{q})=n(\mathbf{q})\int d\hat{\sigma}\,n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\hat{\sigma}\mathbf{I}\hat{\sigma}), \quad (C14)$$

$$\mathbf{A}(\mathbf{q})=\sigma\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{F}_4(\mathbf{q})+\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\sigma}\,n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}+\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma}\hat{\sigma}, \quad (C15)$$

$$\mathbf{B}(\mathbf{q})=\sigma\frac{\partial}{\partial\mathbf{q}}\cdot\left(\int d\hat{\sigma}\,n(\mathbf{q})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}+\frac{\sigma}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\int d\hat{\sigma}n(\mathbf{q})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})\hat{\sigma}\right)$$
$$+\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I})-2\sqrt{2}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{2}{3}\mathbf{I}). \tag{C16}$$

The first six contributions to the energy flux $\mathbf{J}(\mathbf{q},\omega)$ are

$$\mathbf{J}_1(\mathbf{q},\omega)=\frac{1}{\beta}\Bigg[\left(n(\mathbf{q})\mathbf{I}+\frac{3b}{4\pi}\boldsymbol{\Phi}_2(\mathbf{q})\right)-(15\sqrt{2}/8)\left(\frac{\sigma_{1w}}{\sigma}\right)^2\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\left(\mathbf{I}+\frac{9b}{20\pi}\mathbf{F}_2(\mathbf{q})\right)\cdot\mathbf{Q}_\mathbf{u}(\mathbf{q})+(27\sqrt{2}/64\pi)$$
$$\times\left(\frac{\sigma_{1w}}{\sigma}\right)^2 b\sigma\mathbf{F}_{03}(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{Q}}_\mathbf{u}(\mathbf{q},\omega)]+\frac{15}{4\pi}\left(\frac{\sigma_{1w}}{\sigma}\right)^2 b\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_3(\mathbf{q}):\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)$$
$$-\frac{15}{8\pi}\left(\frac{\sigma_{1w}}{\sigma}\right)^2 b\sigma\mathbf{F}_{04}(\mathbf{q})\overset{\vdots}{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)]+\frac{5}{8\pi\eta}[\mathbf{L}(\mathbf{q}):\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega)]^T+\frac{9}{32}\tau_\lambda^*(\mathbf{q},\omega)$$
$$\times[\mathbf{M}(\mathbf{q})\cdot\widetilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega)]^T\Bigg]\cdot\mathbf{u}(\mathbf{q},\omega), \tag{C17}$$

$$\mathbf{J}_2(\mathbf{q},\omega)=\frac{1}{\beta}\Bigg[\frac{5}{2}\sigma\tau_\eta^*(\mathbf{q},\omega)\mathbf{F}_3(\mathbf{q})+\frac{5}{4}\sigma^2\mathbf{F}_{04}(\mathbf{q})\odot\frac{\partial}{\partial\mathbf{q}}\tau_\eta^*(\mathbf{q},\omega)-\frac{625}{128}\frac{\pi^2\sigma}{b}\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\left(\mathbf{I}+\frac{9b}{20\pi}\mathbf{F}_2(\mathbf{q})\right)\cdot\mathbf{C}_p(\mathbf{q})$$
$$+\frac{1125}{1024}\pi\sigma^2\mathbf{F}_{03}(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{C}_p(\mathbf{q})]\Bigg]:\mathbf{S}_{\mathbf{u}\nabla n}(\mathbf{q},\omega), \tag{C18}$$

$$\mathbf{J}_3(\mathbf{q},\omega)=(3b\sigma/\sqrt{\pi\beta m})\eta\left(2\tau_\eta^*(\mathbf{q},\omega)\mathbf{F}_{04}(\mathbf{q})+\frac{225}{128}\pi\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{F}_{03}(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\mathbf{C}_p(\mathbf{q}):\hat{\mathbf{1}}_6\right)\vdots\frac{\partial}{\partial\mathbf{q}}[\mathbf{S}_{\mathbf{u}\nabla n}(\mathbf{q},\omega)], \tag{C19}$$

$$\mathbf{J}_4(\mathbf{q},\omega)=-(1/\sqrt{\pi\beta m})\Bigg[\frac{9b^2}{5\pi}\eta\boldsymbol{\Phi}_{03}(\mathbf{q})+\frac{3b}{\pi}\mathbf{F}_3(\mathbf{q}):\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega)-\frac{3b\sigma}{2\pi}\mathbf{F}_{04}(\mathbf{q})\overset{\vdots}{\odot}\frac{\partial}{\partial\mathbf{q}}\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega)$$
$$+\frac{9b^2}{\pi}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\eta\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_{04}(\mathbf{q})\overset{\vdots}{\odot}\widetilde{\mathbf{P}}_\mathbf{u}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4+3\pi\eta\tau_\lambda^*(\mathbf{q},\omega)\left(\mathbf{I}+\frac{9b}{20\pi}\mathbf{F}_2(\mathbf{q})\right)\cdot\widetilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega)$$
$$-\frac{27}{40}b\sigma\eta\mathbf{F}_{03}\dot{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\lambda^*(\mathbf{q},\omega)\widetilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega)]-\frac{81\sqrt{2}}{40\pi}\left(\frac{\sigma_{1w}}{\sigma}\right)^2 b^2\eta\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{F}_{03}(\mathbf{q})\underset{\rightarrow}{\dot{\odot}}\widetilde{\mathbf{Q}}_\mathbf{u}(\mathbf{q},\omega)\cdot\hat{\mathbf{1}}_4\Bigg]:\frac{\partial u(\mathbf{q},\omega)}{\partial\mathbf{q}}, \tag{C20}$$

$$\mathbf{J}_5(\mathbf{q},\omega)=(3b\sigma/2\sqrt{\pi\beta m})\left(\frac{1}{\pi}\mathbf{F}_{04}(\mathbf{q})\overset{\vdots}{\odot}\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega):\hat{\mathbf{1}}_6+\frac{9}{20}\eta\tau_\lambda^*(\mathbf{q},\omega)\mathbf{F}_{03}(\mathbf{q})\dot{\odot}\widetilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega):\hat{\mathbf{1}}_6\right)\vdots\frac{\partial^2\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}\partial\mathbf{q}}, \tag{C21}$$

$$\mathbf{J}_6(\mathbf{q},\omega)=\Bigg(\frac{36}{25\pi}b\sigma^2\lambda\boldsymbol{\Phi}_1(\mathbf{q})-\frac{15}{2}b\lambda\tau_\lambda^*(\mathbf{q},\omega)\tau_\eta^*(\mathbf{q},\omega)\mathbf{F}_3(\mathbf{q}):\widetilde{\mathbf{P}}_T(\mathbf{q})-4\pi\lambda\tau_\lambda^*(\mathbf{q},\omega)\left(\mathbf{I}+\frac{9b}{20\pi}\mathbf{F}_2(\mathbf{q})\right)\cdot\widetilde{\mathbf{Q}}_T(\mathbf{q},\omega)$$
$$+\frac{9}{10}b\sigma\lambda\mathbf{F}_{03}(\mathbf{q})\dot{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\lambda^*(\mathbf{q},\omega)\widetilde{\mathbf{Q}}_T(\mathbf{q},\omega)]+\frac{32}{15}\sigma^2\lambda\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{L}(\mathbf{q}):\widetilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)+\frac{3}{10}\sigma^2\mathbf{M}(\mathbf{q})\cdot\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)$$
$$+\frac{3}{4}b\sigma\lambda\mathbf{F}_{04}(\mathbf{q})\overset{\vdots}{\odot}\frac{\partial}{\partial\mathbf{q}}[\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\widetilde{\mathbf{P}}_T(\mathbf{q})]\Bigg)\delta T(\mathbf{q},\omega). \tag{C22}$$

Here

$$\mathbf{L}(\mathbf{q})=\sigma\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{F}_3(\mathbf{q})+\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}\hat{\sigma} \tag{C23}$$

and

$$\mathbf{M}(\mathbf{q})=\sigma\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{F}_2(\mathbf{q})+\int d\hat{\sigma}[n(\mathbf{q})-n(\mathbf{q}-\sigma\hat{\sigma})]g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}+\frac{4}{3}\int d\hat{\sigma}\,n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}$$
$$+\frac{10}{3}\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\sigma}n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}. \tag{C24}$$

The right-hand side of Eq. (3.23) takes the form

$$\mathbf{R}_{\mathbf{u}}(\mathbf{q},\omega)=\Bigg[\frac{48}{5\pi}b\sigma^2\eta\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Psi}(\mathbf{q})-(48\sqrt{2}/5\pi)b\sigma\eta n(\mathbf{q})\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\boldsymbol{\sigma}}n_w(\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}$$
$$+\sigma^2\left(\frac{\partial}{\partial\mathbf{q}}\cdot[\mathbf{A}(\mathbf{q}):\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega)]^T\right)^T+6\left(\frac{\sigma_{1w}}{\sigma}\right)^2 b\sigma\eta\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{A}(\mathbf{q}):\tilde{\mathbf{P}}_{\mathbf{u}}(\mathbf{q},\omega)-(9\sqrt{2}/5\pi)$$
$$\times\left(\frac{\sigma_{1w}}{\sigma}\right)^2 b\sigma\eta\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{B}(\mathbf{q})\cdot\tilde{\mathbf{Q}}_{\mathbf{u}}(\mathbf{q},\omega)+\frac{3}{5}\sigma^2\eta\left(\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_\lambda^*(\mathbf{q},\omega)\mathbf{B}(\mathbf{q})\cdot\tilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega)]^T\right)^T\Bigg]\cdot\mathbf{u}(\mathbf{q},\omega)$$
$$-\pi\sigma^2\eta\left[4\tau_\eta^*(\mathbf{q},\omega)\mathbf{A}(\mathbf{q})+\frac{3}{4}\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{B}(\mathbf{q})\cdot\mathbf{C}_{\mathbf{P}}(\mathbf{q})\right]:\mathbf{S}_{\mathbf{u}\nabla n}(\mathbf{q},\omega)+\sqrt{\pi\beta m}\lambda\Bigg[\frac{16}{25\pi}b\sigma^2\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Phi}_2(\mathbf{q})$$
$$+\frac{16}{15}\sigma^2\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{A}(\mathbf{q}):\tilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)]^T-\frac{\pi}{2}\sigma^2\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{A}(\mathbf{q}):\tilde{\mathbf{P}}_T(\mathbf{q})$$
$$+\frac{\sigma^2}{5\pi\lambda}\frac{\partial}{\partial\mathbf{q}}\cdot[\mathbf{B}(\mathbf{q})\cdot\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)]^T-\frac{4}{5}\sigma^2\tau_\lambda^*(\mathbf{q},\omega)\mathbf{B}(\mathbf{q})\cdot\tilde{\mathbf{Q}}_T(\mathbf{q},\omega)\Bigg]\delta T(\mathbf{q},\omega). \tag{C25}$$

For the right-hand side of Eq. (3.24) one can derive

$$R_T(\mathbf{q},\omega)=\frac{1}{\beta}\Bigg(\frac{3}{4\pi}b\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Phi}_2(\mathbf{q})+\sigma_{1w}^2n(\mathbf{q})\int d\hat{\boldsymbol{\sigma}}n_w(\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}+\frac{5}{8\pi\eta}\frac{\partial}{\partial\mathbf{q}}\cdot[\mathbf{L}(\mathbf{q}):\boldsymbol{\eta}_I^{(2)}(\mathbf{q},\omega)]^T+\frac{9}{32}\frac{\partial}{\partial\mathbf{q}}$$
$$\cdot[\tau_\lambda^*(\mathbf{q},\omega)\mathbf{M}(\mathbf{q})\cdot\tilde{\mathbf{Q}}_{\nabla\mathbf{u}}(\mathbf{q},\omega)]^T+\frac{5}{2}\sigma_{1w}^2\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{L}(\mathbf{q}):\tilde{\mathbf{P}}_{\mathbf{u}}(\mathbf{q},\omega)-(9\sqrt{2}/16)\sigma_{1w}^2\tau_\lambda^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{M}(\mathbf{q})$$
$$\cdot\tilde{\mathbf{Q}}_{\mathbf{u}}(\mathbf{q},\omega)\Bigg)\cdot\mathbf{u}(\mathbf{q},\omega)-\frac{5}{2}\frac{1}{\beta}\left(\tau_\eta^*(\mathbf{q},\omega)\mathbf{L}(\mathbf{q})+\frac{225\pi}{256}\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{M}(\mathbf{q})\cdot\mathbf{C}_{\mathbf{P}}(\mathbf{q})\right):\mathbf{S}_{\mathbf{u}\nabla n}(\mathbf{q},\omega)$$
$$+\lambda\Bigg(\frac{32b\sigma^2}{25\pi}\frac{\partial}{\partial\mathbf{q}}\cdot\mathbf{\Phi}_1(\mathbf{q})-\pi\sigma^2\tau_\eta^*(\mathbf{q},\omega)\tau_\lambda^*(\mathbf{q},\omega)\mathbf{L}(\mathbf{q}):\tilde{\mathbf{P}}_T(\mathbf{q})-\frac{6}{5}\pi\sigma^2\tau_\lambda^*(\mathbf{q},\omega)\mathbf{M}(\mathbf{q})\cdot\tilde{\mathbf{Q}}_T(\mathbf{q},\omega)$$
$$+\frac{32}{15}\sigma^2\frac{\partial}{\partial\mathbf{q}}\cdot[\tau_\eta^*(\mathbf{q},\omega)n(\mathbf{q})\mathbf{L}(\mathbf{q}):\tilde{\mathbf{P}}_{\nabla T}(\mathbf{q},\omega)]+\frac{3\sigma^2}{10\lambda}\frac{\partial}{\partial\mathbf{q}}\cdot[\mathbf{M}(\mathbf{q})\cdot\boldsymbol{\lambda}_I^{(2)}(\mathbf{q},\omega)]\Bigg)\delta T(\mathbf{q},\omega). \tag{C26}$$

If $\mathbf{u}(\mathbf{q},\omega)$ and $\delta T(\mathbf{q},\omega)$ are sufficiently small (i.e., the system is close to an equilibrium state, as assumed) $\mathbf{R}_{\mathbf{u}}(\mathbf{q},\omega)$ and $R_T(\mathbf{q},\omega)$ are negligibly small, although $\partial n(\mathbf{q})/\partial\mathbf{q}$ may be large, even of the order $n(\mathbf{q})/\sigma$. In the immediate vicinity of walls the main contribution to $\mathbf{R}_{\mathbf{u}}(\mathbf{q},\omega)$ would be that from the second term on the right-hand side of Eq. (C25); thus, for $\mathbf{R}_{\mathbf{u}}(\mathbf{q},\omega)$ and $R_T(\mathbf{q},\omega)$ one will have

$$\mathbf{R}_{\mathbf{u}}(\mathbf{q},\omega)=-\frac{48\sqrt{2}}{5\pi}b\sigma\eta n(\mathbf{q})\left(\frac{\sigma_{1w}}{\sigma}\right)^2\int d\hat{\boldsymbol{\sigma}}\,n_w(\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\hat{\boldsymbol{\sigma}}\cdot\mathbf{u}(\mathbf{q},\omega) \tag{C27}$$

and

$$R_T(\mathbf{q},\omega)=0. \tag{C28}$$

Thus, although due to the assumed immobility of the wall molecules there is momentum production in the system, this production is only noticeable in the immediate neighborhood of walls.

APPENDIX D: TENSORS $\hat{\mathbf{1}}_{2m}$

We define the $2m$th rank tensors $\hat{\mathbf{1}}_{2m}$ so that

$$(\hat{\mathbf{1}}_{2m})_{\underbrace{l_1s_1p_1,\ldots,p_2s_2l_2}_{2m}}=\underbrace{\delta_{l_1l_2}\delta_{s_1s_2}\delta_{p_1p_2}\cdots}_{m},\quad m=1,2,\ldots \tag{D1}$$

where the δ_{ls}'s are Kronecker symbols and $l_1,s_1,p_1,\ldots,p_2,s_2,l_2=1,2,3,\ldots,n$. Then for any mth rank tensor A one can prove

$$\hat{\mathbf{1}}_{2m}\,\textcircled{m}\,\mathbf{A}=\mathbf{A}, \tag{D2}$$

$$\mathbf{A}\,\textcircled{m}\,\hat{\mathbf{1}}_{2m}=\mathbf{A}, \tag{D3}$$

$$\hat{\mathbf{1}}_{2m}\,\textcircled{m}\,\hat{\mathbf{1}}_{2m}=\hat{\mathbf{1}}_{2m}, \tag{D4}$$

where $\textcircled{m}$ denotes m-multiple convolution,

$$\sum_{\alpha,\ldots,\beta=1}^{n} \mathbf{B}_{i\ldots k\alpha\ldots\beta}\mathbf{A}_{\beta\ldots\alpha l\ldots p}. \tag{D5}$$

Thus, with respect to the mth rank tensors **A** the tensor $\hat{\mathbf{1}}_{2m}$ plays the same role as the unit matrix **I** with respect to vectors (i.e., first rank tensors), and at $m=1$, $\hat{\mathbf{1}}_2=\mathbf{I}$. Although the tensors $\hat{\mathbf{1}}_{2m}$ have some other interesting algebraic properties, for our purposes here we use just Eqs. (D1)–(D4), where $m=2,3$ for convenient tensorial representation of the formulas derived.

APPENDIX E: THE CONTINUITY EQUATION

From Eq. (2.25) one can obtain the time Fourier transformed form of the continuity equation,

$$-i\omega\delta n(\mathbf{q},\omega)+\frac{\partial}{\partial\mathbf{q}}\cdot\left[\left(n(\mathbf{q})\mathbf{I}+\sigma^3 n(\mathbf{q})\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})+\frac{\sigma^4}{2}\frac{\partial}{\partial\mathbf{q}}\cdot\left[n(\mathbf{q})\int d\hat{\sigma} n(\mathbf{q}-\sigma\hat{\sigma})\right.\right.\right.$$
$$\left.\left.\left.\times g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\right]\right)\cdot\mathbf{u}(\mathbf{q},\omega)-\frac{\sigma^4}{2}n(\mathbf{q})\int d\hat{\sigma}\, n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I}):\frac{\partial\mathbf{u}(\mathbf{q},\omega)}{\partial\mathbf{q}}\right]$$
$$=\sigma^2\left\{\sigma\frac{\partial}{\partial\mathbf{q}}\cdot\int d\hat{\sigma}\, n(\mathbf{q})n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})+\frac{\sigma^2}{2}\frac{\partial^2}{\partial\mathbf{q}\partial\mathbf{q}}:\int d\hat{\sigma}\, n(\mathbf{q})n(\mathbf{q}-\sigma\hat{\sigma})g(\mathbf{q},\mathbf{q}-\sigma\hat{\sigma})\hat{\sigma}(\hat{\sigma}\hat{\sigma}-\tfrac{1}{3}\mathbf{I})\right.$$
$$\left.+\left(\frac{\sigma_{1w}}{\sigma}\right)^2 n(\mathbf{q})\int d\hat{\sigma} n_w(\mathbf{q}-\sigma_{1w}\hat{\sigma})g_{1w}(\mathbf{q},\mathbf{q}-\sigma_{1w}\hat{\sigma})\hat{\sigma}\right\}\cdot\mathbf{u}(\mathbf{q},\omega).$$

At small $\mathbf{u}(\mathbf{q},\omega)$ the right-hand side of Eq. (E1) tends to zero.

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