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Statistical dynamics of a classical particle in the continuous potential of randomly fixed scatterers

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The statistical dynamics of a Lorentz system produced by freezing in a dynamical bath in thermal equilibrium with a tagged particle which continues to move in the static environment after the quench is described in terms of canonical ensemble averages over the phase-space variables of the system: scatterer positions and coordinates of the particle. A generalized hydrodynamics theory for the fluctuation spectra of the densities of particle number and energy, of their currents, and of their velocities is developed in terms of dispersion-relation representations for the above correlation functions. The coupling between number and energy-density fluctuations showing up via off-diagonal elements of the generalized diffusivity matrix is elucidated. The transition to the localized state and the accompanying slowing down of the zero-frequency relaxation rate of velocity fluctuations is investigated. Simple approximations based upon Lorentzian or Gaussian relaxation kernels are presented and the dependence of spectra and diffusivities on the ratio of mean potential fluctuations and mean kinetic energy is discussed. In the second part a kinetic equation is derived for the 2×2 correlation-function matrix of the two phase-space densities of the two constants of the motion, particle number, and energy. For its collision kernel a novel, systematic operator expansion is presented which is manifestly preserving both particle number and energy for arbitrary scatterer densities and interaction potentials. The correlation functions of the currents resulting from the leading order in the expansion are given explicitly in terms of incomplete gamma functions. They yield, in the long-wavelength limit, the proper dispersion-relation representation of the velocity-correlation matrix.

I. INTRODUCTION

The statistical dynamics of a classical particle moving in the potential of randomly fixed scatterers has received increasing attention recently. This model system was originally devised by Lorentz to describe gas mixtures of large mass ratio. Its popularity and usefulness,[1] however, is mostly due to other reasons two of which are: (i) It serves as a model for the statistical behavior of a tagged particle in the dynamical environment of a many-body bath. (ii) It allows us to study a classical analog of the quantum-mechanical problem of electron localization[2] by impurity disorder.[3]

The Lorentz model has also been investigated[4] from the viewpoint of mathematical physics to elucidate various approximation schemes used in statistical dynamics of many-body systems. In addition there have been studied many variants, e.g., with special scatterer shapes, special arrangements of the scatterers or of the boundary conditions, or with other restrictions on the phase space of the system. Also the Hamiltonian dynamics of the original Lorentz model has been abandoned by introducing explicitly stochasticity,[5] e.g., by defining the final state after a collision with a scatterer in some statistical manner.

We are mostly interested in the two former aspects of the Lorentz model, one of which is that it retains many properties of the fully dynamical system for which it serves as a model although the dynamical degrees of freedom of the bath of scatterers are frozen in. For example, the velocity autocorrelation of the Lorentz model decays algebraically[1,6–10] at long times in a manner similar to that of a particle in a fluid. However the power law as well as the sign of the long-time tail is different. Furthermore, density expansions of the Lorentz model's self-diffusion constant display divergencies[11] similar to those found for transport coefficients of fluids. Also their renormalization[1,12] is similar. The second aspect of the Lorentz model has been investigated by Götze *et al.*[10] in a theory for the localized and the diffusive phase and the transition between them in Lorentz systems with overlapping hard spheres.

Computer experiments simulating various realizations of the hard-sphere Lorentz systems have been performed to investigate mean-square displacements as functions of time and scatterer density, the velocity-autocorrelation function[7,8,13] and its long-time tail, the nonanalytic density dependence of the diffusivity,[14] the behavior near the boundary between localized and diffusive phases, and the position of the boundary.[7] Lagar'kov *et al.*[15] investigated the energy dependence of the particle's velocity fluctuations in a potential with an attractive part by making use of a microcanonical ensemble of the initial positions and momenta.

We will employ in this work canonical ensemble averages. They are appropriate for Lorentz systems produced by freezing in a dynamical bath of N_s particles in thermal equilibrium with a tagged particle which continues to move in the static environment after the quench. Averages of any quantity depending on the particle coordinates $\vec{r}_0, \vec{p}_0$ and the scatterer positions $\{\vec{r}_n;\ n=1,\ \ldots, N_s\}$ are then canonical emsemble averages over initial conditions and scatterer configurations with the correct statistical weight for the phase-space coordinates $\vec{r}_0, \vec{p}_0, \{\vec{r}_n\}$ of the system at the time of the quench. Such a Lorentz model is a simplified though still reasonably realistic model of the real dynamical system since the phase-space motion of the particle through different frozen replicas of the original bath is described with the proper statistical weight, and equal-time averages of any quantity $A(\vec{r}_0, \vec{p}_0, \{\vec{r}_n\})$ are identical to those in the dynamical bath.

The Lorentz model has only two constants of motion; particle number $N_0=1$ and particle energy H_0. The energy of the particle moving in a particular realization of the static-scatterer configuration is conserved since the collisions are elastic. However its value H_0 fluctuates in a canonical ensemble of initial conditions $\vec{r}_0, \vec{p}_0$ and scatterer positions. Consequently the statistical dynamics of the energy density of the moving particle $\epsilon(\vec{r},t)=H_0\delta(\vec{r}-\vec{r}_0(t))$ differs from the statistical dynamics of the particle number density $\rho(\vec{r},t)=\delta(\vec{r}-\vec{r}_0(t))$ despite their time evolution in a particular scatterer configuration being the same. What counts with respect to statistical dynamics is that ϵ and ρ differ by a fluctuating quantity on which any dynamical variable is statistically dependent—the trajectory $\vec{r}_0(t)$ in a potential landscape depends on the energy H_0. This holds true, to a lesser extent, even for hard-sphere Lorentz systems.[16] If however fluctuations of H_0 are eliminated by microcanonical-ensemble averages, energy-density fluctuations no longer constitute another "hydrodynamic" mode of the system besides number-density fluctuations. To overcome conceptual difficulties in accepting the energy density as a second relevant mode we consider first a system of many, mutually noninteracting particles in a random potential. Consider the number and energy density at a fixed $\vec{r},t$ in various realizations of the scatterer environment. One first observes that their fluctuations are not the same since, e.g., a higher than average particle-number concentration does not imply that the deviation of the energy density from its mean value will be positive as well. Furthermore it is plausible that a fluctuation of $\epsilon(\vec{r},t)$ caused by particles having, say, much more than average energy relaxes differently towards the mean than a number-density fluctuation of particles with, say, average energy since the paths through the potential landscape taken by these two kinds of particles are quite different.

Fluctuations of ρ and ϵ being densities of conserved quantities have infinite lifetimes in the limit $k\to 0$. In that limit they relax for long times diffusively since their currents are not conserved. However, the system's relative simplicity allows us to study fluctuations of number and energy density and of other dynamically relevant variables in greater detail and to test many-body theories. So in this work we investigate for a Lorentz system with continuous potentials the statistical dynamics of fluctuations of: (i) the space densities of the two conserved quantities N_0 and H_0, of their currents, and of their velocities and (ii) of the two phase-space densities of N_0 and H_0.

We prefer continuous interaction potentials between the particle and the scatterers for two reasons: Not only is such a Lorentz system closer to reality but its dynamics are also more interesting than that of a hard-sphere Lorentz model. In the latter the particle moves with constant speed through a scatterer configuration along a path which is independent of the initial kinetic energy. In the former system the path depends crucially on the initial relative size of the kinetic and potential energy. Furthermore, not only the direction but also the size of the particle's velocity fluctuates along its trajectory in a way which is quite similar to the motion through a dynamic environment. Similarly there is a dynamical exchange of kinetic and potential energy albeit restricted by conservation of H_0. Correlation functions and in particular transport coefficients like the self-diffusion constant depend not only on the scatterer density measuring the mean potential energy but also on the mean kinetic energy ("temperature"). Thus in contrast to the hard-sphere system the criterion[2] for localization does not reduce to the purely geometrical question that the scatterer density should be high enough. In a Lorentz system with continuous potentials, say of Lennard-Jones type, the mean-square displacement depends on the variance of the momentum distribution. Hence for determining the position of the boundary between localized and diffusive phase one also has to ask whether the particle's mean kinetic energy is sufficiently high to overcome a sufficiently large portion of those potential barriers which are present on the average at a given scatterer density.

In Sec. II we present the theoretical framework for describing the statistical dynamics of our Lorentz system in terms of correlation functions. A generalized "hydrodynamics" theory for the fluctuation spectra of the space densities of particle number and energy, of their currents, and of their velocities is developed in Sec. III. This theory is based upon dispersion-relation representations for the 2×2 matrices of correlation functions between all of the above pairs of variables. We elucidate the effect of the coupling between number density and energy density showing up in their low k, ω fluctuation spectra via nonzero off-diagonal elements of the 2×2 diffusivity matrix. We furthermore investigate dispersion-relation representations for the generalized diffusivities, their relaxation kernels, and of the other relaxation kernels. The transition to the localized state and the accompanying slowing down of the zero-frequency relaxation rate of velocity fluctuations together with the change of the low-frequency velocity fluctuation spectrum is discussed. Simple approximations based upon Lorentzian or Gaussian relaxation kernels are presented and the dependence of spectra and diffusivities on the ratio of mean potential fluctuations to mean kinetic energy is investigated.

In Sec. IV we introduce phase-space densities of the particle number and of the energy: $H_0\delta(\vec r-\vec r_0(t))\delta(\vec p-\vec p_0(t))$. Dynamically the latter is a one point quantity since only the phase-space point $(\vec r_0(t),\vec p_0(t))$ moves. Statistically, however, it is a two-point variable since the scatterer coordinates are included in H_0. Due to this simplification in comparison with a fully dynamical system we are able to develop a kinetic theory for fluctuations of the above phase-space densities, which explicitly and manifestly ensures particle number as well as energy conservation for arbitrary scatterer densities and arbitrarily strong interaction potentials. We derive the kinetic equation for the 2×2 matrix of correlation functions of the two phase-space densities. We present a novel, systematic operator expansion for the collision kernel which guarantees the conservation of particle number and energy without truncating the phase space and which has the correct operator structure at small times. The resulting correlation functions of the space densities of particle number, energy, their currents and of the velocities are given.

II. STATISTICAL DESCRIPTION OF THE SYSTEM

Our system may be defined by freezing in a dynamical bath, e.g., a fluid or a disordered solid, in thermal equilibrium with a tagged particle which continues to move in the static environment after the quench. So consider a classical particle of mass m in the potential

$$U_0(\vec r)=\sum_{n=1}^{N_s}u_0(|\vec r-\vec r_n|) \tag{2.1}$$

of N_s scatterers fixed in d dimensions at positions $\{\vec r_n; n=1,\ldots,N_s\}$. The particle interacts with the scatterers via a central symmetric pair potential $u_0(r)$ which could be of Lennard-Jones type or any other continuous potential occurring in nature. The particle moves through the static environment on that trajectory along which its energy

$$H_0=\frac{p_0^2}{2m}+\sum_{n=1}^{N_s}u_0(|\vec r_0-\vec r_n|) \tag{2.2}$$

is kept constant by continuously exchanging momentum with the scatterers. And so neither magnitude nor direction of the particle's momentum is a constant of the motion whereas the energy H_0 is one. It is the second dynamically relevant conserved quantity of the system, the particle number $N_0=1$ being the other one.

Any quantity A describing the system is a function of the particle's initial values $\vec r_0$, $\vec p_0$ and of the scatterer configuration $\{\vec r_n\}$. Both are considered to be fluctuating variables. Their statistical weight $e^{-\beta(H_0+U)}$ is taken to be that of a dynamical bath of potential energy $U(\{\vec r_n\})$ in thermal equilibrium with a marked particle. Hence the average of A

$$\langle A\rangle=\frac{\int d\{\vec r_n\}d\vec r_0 d\vec p_0 A e^{-\beta(H_0+U)}}{\int d\{\vec r_n\}d\vec r_0 d\vec p_0 e^{-\beta(H_0+U)}} \tag{2.3}$$

is defined by the canonical emsemble average over the phase space variables $\vec r_0$, $\vec p_0$, $\{\vec r_n\}$ of the system. The variance of the momentum distribution

$$\beta^{-1}=\frac{1}{d}\frac{\langle p_0^2\rangle}{m}=k_BT \tag{2.4a}$$

defines a "temperature," e.g., that of the fluid before the quench and we identify a "thermal" velocity v_{th} by

$$m v_{\text{th}}^2=k_BT\ . \tag{2.4b}$$

Note that (2.3) is *not* the configuration average of an initial-value average evaluated in a particular scatterer configuration. We do not discuss such "quenched" averages used for evaluating, e.g., the electrical resistance of metals due to randomly distributed impurities since we want the Lorentz gas to closely model the statistics of the original dynamical system. Only with the canonical definition (2.3) equal-time averages are identical to those of the original dynamical system at temperature T before the quench thus reflecting its static structure. This fact is easily seen by considering, e.g., the average energy $\langle H_0\rangle$ of the marked particle.

In the following we list some formulas[17,18] employed for describing the system in terms of corrrelation functions

$$\phi_{AB}(t)=\langle\delta A^*(t)\delta B\rangle=(A|e^{-i\mathcal{L}t}|B) \tag{2.5}$$

between the fluctuations $(\delta A=A-\langle A\rangle)$ of variables A,B which depend on $\vec r_0(t)$, $\vec p_0(t)$, and $\{\vec r_n\}$.

The function $\phi_{AB}(t)$ describes[18] the statistical dynamics of fluctuations *and* of the linear response of variable A to an external field coupling to variable B through its action on $\vec{r}_0, \vec{p}_0$. The underlying fluctuation dissipation theorem can be derived for our system along the standard lines[19] of linear response theory. The scalar product in (2.5) is defined in terms of equal-time correlations

$$(A|B) = \langle \delta A^* \delta B \rangle \ . \tag{2.6}$$

The time evolution $A(t) = e^{i\mathfrak{L}t}A$ is described by the unitary operator $e^{i\mathfrak{L}t}$, i.e., by the Liouville operator $\mathfrak{L}$.

We will mostly discuss the Laplace transform

$$\phi_{AB}(z) = \left(A \left| \frac{1}{\mathfrak{L} - z} \right| B \right) = \pm i \int_{-\infty}^{\infty} dt \Theta(\pm t) e^{izt} \phi_{AB}(t) \ , \quad \mathrm{Im} z \gtrless 0 \tag{2.7}$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\phi''_{AB}(\omega)}{\omega - z} \ , \tag{2.8}$$

[where $\Theta(\pm t)$ is the step function] of $\phi_{AB}(t)$ or the spectral function $\phi''_{AB}(\omega)$, i.e., the discontinuity of $\phi_{AB}(z)$ across the real axis $\phi_{AB}(\omega \pm i0) = \phi'_{AB}(\omega) \pm i\phi''_{AB}(\omega)$, given by the Fourier transform of $\phi_{AB}(t)$

$$\phi''_{AB}(\omega) = \pi(A|\delta(\omega - L)|B) = \frac{1}{2} \int_{-\infty}^{\infty} dt e^{i\omega t} \phi_{AB}(t) \ . \tag{2.9}$$

Approximations are best formulated for the inverse of (2.7) rather than the correlation function itself. To this end a dispersion-relation representation[17,18,20]

$$\phi_{AA}(z) = -[z - \omega_{AA} + \Sigma_{AA}(z)]^{-1} \phi_{AA}(t=0) \tag{2.10}$$

in terms of a characteristic frequency ω_{AA} and a complex self-energy $\Sigma_{AA}(z) = \sigma_{AA}(z)/(A|A)$ is used. Both can be generated within Mori's[21] projection-operator formalism which allows for an easy generalization[18] to a set of variables.

The complex functions $\sigma_{AA}(z)$ and $\phi_{AA}(z)$ have the same analytical properties. For Hermitian variables A with definite time inversion symmetry $\phi''_{AA}(\omega)$ as well as $\sigma''_{AA}(\omega)$ being the imaginary parts at $z = \omega + i0$ are real, even in ω, and non-negative. The corresponding matrices are positive semidefinite in the case of several variables.[18] The real parts $\phi'_{AA}(\omega)$, $\sigma'_{AA}(\omega)$ are odd in ω as a consequence of the Kramers Kronig relation connecting both via the Cauchy integral (2.8). This symmetry implies

$$\lim_{\omega \to 0} \sigma_{AA}(\omega \pm i0) = \pm i \sigma''_{AA}(\omega = 0) \tag{2.11}$$

for variables A for which the limit exists.

III. FLUCTUATIONS OF THE DENSITIES, THEIR CURRENTS, AND OF VELOCITIES

In this section we investigate within a "generalized hydrodynamics" theory the fluctuation spectra of the densities

$$a^1(\vec{k}) = \rho(\vec{k}) = e^{-i\vec{k}\cdot\vec{r}_0} \ , \tag{3.1a}$$

$$a^2(\vec{k}) = \tilde{\epsilon}(\vec{k}) = \delta H_0 e^{-i\vec{k}\cdot\vec{r}_0} \ , \tag{3.1b}$$

of particle number and energy, of their currents

$$\vec{j}^i(\vec{k}) = \frac{1}{m} \vec{p}_0 a^i(\vec{k}) \tag{3.2}$$

and of the associated generalized velocities

$$\vec{v}^i = \vec{j}^i(\vec{k}=0) \ . \tag{3.3}$$

Although $\tilde{\epsilon} = \epsilon - \rho(\epsilon|\rho)/(\rho|\rho)$ is only the part of the energy density $\epsilon(\vec{k}) = H_0 e^{-i\vec{k}\cdot\vec{r}_0}$ which is orthogonal to ρ we prefer not to introduce a new word for $\tilde{\epsilon}$. Its analog in fluids is related to the local temperature.[22] Note that in contrast to ordinary self-diffusion in fluids where the energy of the tagged particle is not conserved here one has to consider two velocities (3.3) and consequently a 2 × 2 correlation matrix of velocities.

A. Correlation functions of densities, currents, and velocities

Rotational invariance of (2.3) forbids correlations between densities and transverse currents and enforces the current correlation matrix

$$\left(j^i_\alpha(\vec{k}) \left| \frac{1}{\mathfrak{L} - z} \right| j^j_\beta(\vec{k}) \right) = C^{ij}_{\alpha\beta}(\vec{k},z)$$

$$= \frac{k_\alpha k_\beta}{k^2} C^{ij}_l(k,z) + \left(\delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2} \right) C^{ij}_t(k,z) \tag{3.4}$$

to be diagonal with respect to Cartesian components $\alpha, \beta = 1, \ldots, d$ in a coordinate system in which, e.g.

$$\vec{k} = k(1,0,\ldots,0) \ . \tag{3.5}$$

The 2 × 2 correlation matrices $C^{ij}_{l,t}(k,)$ of the longitudinal and transverse currents of particle number and energy are symmetric and thus we have to investigate only 3 longitudinal and 3 transverse current correlation functions. The velocity correlation matrix $\psi^{ij}(t) = d^{-1}\langle \vec{v}^i(t) \cdot \vec{v}^j \rangle$ is contained in the longitudinal or transverse current correlation matrix

$$\left(v^i_\alpha \left| \frac{1}{\mathfrak{L} - z} \right| v^j_\beta \right) = \lim_{k \to 0} C^{ij}_{\alpha\beta}(\vec{k},z) = \delta_{\alpha\beta} \psi^{ij}(z) \tag{3.6}$$

and dynamic correlation functions involving a density

$a^i(\vec{k})$ are related via the continuity equations

$$\mathcal{L}a^i(\vec{k}) = -\vec{k}\cdot\vec{j}^{\,i}(\vec{k}) = -kj_l^i(\vec{k}) \tag{3.7}$$

to the longitudinal current correlation matrix. For the density correlation matrix

$$S^{ij}(k,z) = \left(a^i(\vec{k}) \left| \frac{1}{\mathcal{L}-z} \right| a^j(\vec{k}) \right) , \tag{3.8}$$

e.g., one obtains

$$z^2 S^{ij}(k,z) + zS^{ij}(t=0) = k^2 C_l^{ij}(k,z) , \tag{3.9}$$

where

$$S^{ij}(t=0) = (a^i(\vec{k})\,|\,a^j(\vec{k})) = \begin{vmatrix} 1 & 0 \\ 0 & k_B T^2 \; c_v \end{vmatrix} \tag{3.10}$$

denotes the wave-number-independent equal-time density correlation matrix. The quantity

$$c_v = \frac{1}{k_B T^2}\langle (\delta H_0)^2 \rangle = \frac{d}{2}k_B + \frac{1}{k_B T^2}\langle (\delta U_0)^2 \rangle \tag{3.11}$$

is not the specific heat[22] per particle of the bath of scatterers before the quench. However, one can expect $\frac{1}{4}\langle (\delta U_0)^2 \rangle$ to be a fairly good approximation to the variance of the potential energy per particle in the bath if all interaction potentials are the same.

The conserved densities $a^1(\vec{k},t) = \rho(\vec{k},t)$ and $a^2(\vec{k},t) = \delta H_0 \rho(\vec{k},t)$ evolve similarly in time within a particular realization of the ensemble. Differing however by the statistical factor δH_0 which measures the particle's energy deviation from its mean their fluctuation dynamics are none the less different: The correlations

$$S(k,t) = \left\langle e^{i\vec{k}\cdot[\vec{r}_0(t)-\vec{r}_0]} \begin{vmatrix} 1 & \delta H_0 \\ \delta H_0 & (\delta H_0)^2 \end{vmatrix} \right\rangle \tag{3.12}$$

being averages of the phase factor $e^{i\vec{k}\cdot\Delta\vec{r}_0(t)}$ over the ensemble (2.3) of particle trajectories with weights 1, δH_0, or $(\delta H_0)^2$ decay differently since the time evolution of a dynamical quantity like the displacement depends on the energy of the particle. It is this statistical dependence of $\vec{r}_0(t)$ on H_0 existing even for a hard-sphere system[16] that leads to the different dynamics of the three correlation functions in (3.12).

A moment expansion shows that the weightings enforce different decay characteristics already for short times: Energy fluctuations, e.g., damp out initially by a factor $1+2k_B/c_v$ faster than the density fluctuations. In addition to this the diffusivities governing the long-time behavior of the fluctuations are quite different, and, what is more important, there are off-diagonal elements in the diffusivity matrix which thus couple number and energy density fluctuations. Hence fluctuations of $\bar{\epsilon}(k,t)$ should be incorporated *explicitly* in order to guarantee a correct description of the system's dynamics in particular for $\omega,k \to 0$. The influence of other modes of the form $f(H_0)e^{-i\vec{k}\cdot\vec{r}_0(t)}$ upon the low k, ω spectrum[16,23] is discussed in Sec. III B.

The form (3.12) suggests to evaluate first the average of the phase factor $\langle e^{-i\vec{k}\cdot\Delta\vec{r}_0(t)}\rangle_{E_0}$ or its self-energy in a representation (2.10) for a fixed particle energy $H_0 = E_0$ with the weight $\sim \delta(H_0-E_0)e^{-\beta U}$ and then integrate the microcanonical average with the probability density $\langle \delta(H_0-E_0) \rangle$ over all E_0. However the former strongly depends on E_0 and the latter requires knowledge of the density of states. Similarly one might define (2.10) with an average over positions $\vec{r}_0$, $\{\vec{r}_n\}$ and initial velocity directions $\vec{v}_0/v_0$ and then average the so obtained correlation function over v_0 with the Boltzmann weight. This can be done for a hard-sphere potential where, e.g., the generalized diffusivity depends almost trivially on v_0.[23] For motion in a continuous potential, however, the dependence of a generalized transport coefficient on the initial kinetic energy v_0^2 as well as on E_0 seems to be far from simple. Thus we stick throughout this work to canonical averages. That, of course, does not bear upon the question whether computer experimental results are easier obtained along the above described lines.

B. Density excitation spectra for small k, ω

Consider the dispersion-relation representation of the density correlation matrix

$$S(k,z) = -[z + k^2 D(k,z)]^{-1} S(t=0) \tag{3.13}$$

in terms of the complex two by two matrix of generalized diffusivities $D(k,z)$. Using (3.9) one can identify $D(k=0,z)S(t=0)$ with $C_l(k=0,z) = \psi(z)$ and thus the positive semidefinite matrix D of diffusion constants

$$D = \lim_{\omega\to 0}\lim_{k\to 0} D''(k,\omega) = \psi''(\omega=0) S^{-1}(t=0) \tag{3.14}$$

obtains in terms of Green-Kubo integrals

$$\psi''(\omega=0) = \frac{1}{d}\int_0^\infty dt \left\langle \vec{v}_0(t)\cdot\vec{v}_0 \begin{vmatrix} 1 & \delta H_0 \\ \delta H_0 & (\delta H_0)^2 \end{vmatrix} \right\rangle . \tag{3.15}$$

They depend on temperature and scatterer density. Also here the remarks made in connection with (3.12) apply. Note that the diffusivity matrix has nonzero off-diagonal elements.

Since only the densities $a^i(k=0)$ but none of their currents $\vec{j}^{\,i}(k=0)$ are constants of the motion both density fluctuations relax for finite small ω diffusively in the limit $k \to 0$. If other conserved densities coupling to $a^i(\vec{k})$ can be neglected one expects the matrix $D(k,z)$ to be well behaved at $k,z=0$, i.e., the limit $D(k\to 0, z\to 0+i0)=i\psi''(k=0,\omega=0)S^{-1}\times(t=0)$ exists. If, furthermore, $D(k,z)$ allows to be replaced for small k,z by the value $D(0,0+i0)$ at the origin one obtains in that frequency and wave number range the spectrum of number and energy density fluctuations to be superpositions of two centrally peaked Lorentzians

$$S^{jj}(k,z)=-\left(\frac{Z_j}{z+ik^2D_+}+\frac{1-Z_j}{z+ik^2D_-}\right)S^{jj}(t=0)\ ,\qquad \mathrm{Im}z>0 \quad (3.16)$$

with relaxation rates determined by the non-negative eigenvalues $D_\pm$ of D^{ij}. The residues

$$Z_1=1-Z_2=\tfrac{1}{2}\left(1+\frac{D^{11}-D^{22}}{D_+-D_-}\right) \quad (3.17)$$

add up to 1.

Hence the Kubo relation $\lim_{\omega\to 0}\lim_{k\to 0}\omega^2\times S^{ii''}(k,\omega)/k^2S^{ii}(t=0)=D^{ii}$ has to be interpreted with certain care. One might be inclined to infer from it that the a^i relaxation process is governed by just one relaxation rate k^2D^{ii} instead of two $k^2D_\pm$. Indeed, a straightforward algebraic manipulation of (3.16)

$$S^{11}(k,z)=\frac{-S^{11}(t=0)}{z+ik^2D^{11}+k^4D^{12}D^{21}/(z+ik^2D^{22})}\ ,\quad \mathrm{Im}z>0 \quad (3.18)$$

shows that the single relaxation time approximation to, e.g., the density correlation function is valid only for $k\to 0$ and finite ω since the continuation of the one-mode generalized diffusivity $iD_{11}[1-i(z+ik^2D^{22})^{-1}k^2D^{12}D^{21}/D^{11}]$ into the lower half plane displays a pole of residue $\sim k^2D^{12}D^{21}/D^{11}$. Its influence on the upper half plane is largest at $z=0+i0$. However already for $\omega\lesssim k^2D^{22}$ and appreciable coupling $4D^{12}D^{21}(D^{11}-D^{22})^{-2}$ the third term in the denominator of (3.18) cannot be neglected.

Similarly one should include explicitly any further conserved density which couples to $a^i(\vec{k})$ with sufficient strength to induce in the analytical continuation of $D^{ij}(k,z)$ diffusive poles with large enough residues to cause appreciable additional Lorentzian contributions to (3.16). The Lorentz system has an infinite number of conserved densities $a^{n+1}(\vec{k})=QH_0^n e^{-i\vec{k}\cdot\vec{r}_0}$ with Q ensuring proper orthogonalization. However for $n\geqslant 2$ their coupling strength to number density fluctuations is, at least in hard-sphere potentials, so small that (3.18) is almost unchanged for small k,z.[16,23] Intuitively we expect the effect of higher modes ($n\geqslant 2$) in a continuous potential of scatterers to be even smaller. We are not sure whether nonlinear powers of the energy $H_0=p_0^2/2m+U_0(\{\vec{r}_n\})$ being nonadditive with respect to the scatterers in contrast to $H_0=p_0^2/2m$ being independent of N_s for hard spheres supports our feeling.

In some real many-body systems generalized transport coefficients diverge for $k,z\to 0$ below a critical dimension d_c where the volume element $q^{d_c-1}dq$ around $q=0$ within which products $a(\vec{q})a(\vec{k}-\vec{q})$ of conserved densities are also slow modes becomes sufficiently large. Above the critical dimension, $d_c=2$ for fluids and $d_c=3$ for low-temperature isotropic ferromagnets, such coupled modes cause generalized transport coefficients to display nonanalytic behavior in k,z near the origin. In the Lorentz system such product modes are also slow variables and that not only for $q=0$. However their effect is already properly taken care of by the above discussed set $a^{n+1}(\vec{k})$ of conserved densities each of which can be written as product modes of the basic variables $a^i(\vec{k})$ (3.1). In a strict sense the "hydrodynamic" description of a hard sphere Lorentz system was shown[16] to break down below $d_c=\infty$ as a result of an infinite number of slow modes formed by products of conserved densities being slow for every wave number q.

In real many-body systems the diffusivities of fluctuations of the energy density $\epsilon(\vec{k})$, the temperature $\hat{T}(\vec{k})$, and the heat $Ts(\vec{k})$ are all the same as a consequence of momentum conservation: Only the energy current but not the particle current contributes[20] to Green-Kubo integrands for the diffusivities of linear combinations of energy and number density like $\hat{T}(\vec{k})$ and $s(\vec{k})$. Or stated physically, the relaxation time of such a combination is determined by the slow energy diffusion process. A local-density fluctuation has long been propagated away over such a time. Here both, $\epsilon(\vec{k})$ and $\rho(\vec{k})$, relax slowly, i.e., diffusively, and both of their currents contribute to Green-Kubo integrands so that the Kubo relations yield for different combinations of $\rho(\vec{k})$ and $\epsilon(\vec{k})$ different diffusion constants being related to the D^{ij}. Consider, e.g., fluctuations of the "heat"

$$\begin{aligned} Ts(\vec{k})&=\epsilon(\vec{k})-\frac{(\epsilon(\vec{k})|\mathcal{L}^2|\rho(\vec{k}))}{(\rho(\vec{k})|\mathcal{L}^2|\rho(\vec{k}))}\rho(\vec{k})\\ &=\epsilon(\vec{k})-(\langle H_0\rangle+k_BT)\rho(\vec{k}) \end{aligned} \quad (3.19)$$

defined in analogy to fluids[22,24] with $(s(\vec{k})|s(\vec{k}))=k_Bc_p=k_B(c_v+k_B)$. Via a Kubo relation one obtains for the "heat" diffusivity

$$\frac{D_{ss}}{D^{11}}=\frac{k_B}{c_p}\left(1+\frac{c_v}{k_B}\frac{D^{22}-2k_BTD^{12}}{D^{11}}\right)\ . \quad (3.20)$$

It is amusing to note that in the Lorentz system the ratio of "heat" conductivity $(N_0/V)c_pD_{ss}$ and electrical conductivity $(N_0/V)e^2D_{11}/k_BT$ as defined via an Einstein relation follows within a simple approximation (cf. Sec. III E) Wiedemann-Franz's law.

C. Relaxation kernels

Rather than approximating generalized transport coefficients directly it is advisable[25] to approximate their relaxation kernels or even the kernels thereof. Here the basic kernel is a "stress-stress" correlation matrix of viscosity-type

$$m^{ij}_{\alpha\beta}(\vec{\mathrm{k}},z)=\left(j^i_\alpha(\vec{\mathrm{k}})\left|\mathfrak{L}Q\frac{1}{Q\mathfrak{L}Q-z}Q\mathfrak{L}\right|j^j_\beta(\vec{\mathrm{k}})\right)=\frac{k_\alpha k_\beta}{k^2}m^{ij}_l(k,z)+\left(\delta_{\alpha\beta}-\frac{k_\alpha k_\beta}{k^2}\right)m^{ij}_t(k,z) \tag{3.21}$$

in which Q projects orthogonal to the densities $a^i(\vec{\mathrm{k}})$ and the currents $\vec{\mathrm{j}}^{\,i}(\vec{\mathrm{k}})$. The transverse and longitudinal parts appear via

$$M_{l,t}(k,z)=m_{l,t}(k,z)C^{-1}(t=0) \tag{3.22}$$

in the dispersion-relation representations for the correlation matrices of transverse currents

$$C_t(k,z)=-[z+M_t(k,z)]^{-1}C(t=0) \tag{3.23}$$

and of longitudinal fluctuations

$$C_l(k,z)=-z[z^2-k^2c_0^2+zM_l(k,z)]^{-1}C(t=0)\ , \tag{3.24}$$

$$D(k,z)=-[z+M_l(k,z)]^{-1}c_0^2\ , \tag{3.25}$$

respectively. Equal-time longitudinal and transverse current correlations

$$(j^i_\alpha(\vec{\mathrm{k}})\,|\,j^j_\beta(\vec{\mathrm{k}}))=\delta_{\alpha\beta}C^{ij}(t=0)=\delta_{\alpha\beta}v_{\mathrm{th}}^2\begin{pmatrix}1 & k_BT\\ k_BT & k_B^2T^2(2+c_v/k_B)\end{pmatrix} \tag{3.26}$$

do not differ. They are wave-number independent like the total spectral weight of the generalized diffusivity $D(k,t=0)=C(t=0)S^{-1}(t=0)$

$$c_0^2=C(t=0)S^{-1}(t=0)=v_{\mathrm{th}}^2\begin{pmatrix}1 & \dfrac{1}{Tc_v}\\ k_BT & 1+2k_B/c_v\end{pmatrix}\ , \tag{3.27}$$

which is the analog of the square of the isothermal sound velocity $\lim_{k\to0}k^{-2}(\rho(\vec{\mathrm{k}})|\mathfrak{L}^2|\rho(\vec{\mathrm{k}}))/(\rho(\vec{\mathrm{k}})|\rho(\vec{\mathrm{k}}))$ in fluids.

There are two reasons for investigating also a representation of $M_{l,t}(k,z)$ itself in terms of relaxation kernels: (i) The diffusivity matrix $D=\lim_{\omega\to0}\mathrm{Im}[\omega+M(\omega+i0)]^{-1}c_0^2$ is determined by the inverse of $M_{l,t}$ so that $M_{l,t}(k=0,\omega=0)$ diverges in the localized phase where one matrix element (or more) of D^{ij} vanishes. This might be easier to handle in terms of relaxation kernels of $M_{l,t}(k,z)$ which consequently would vanish. (ii) Also high-frequency excitations are better studied within the dispersion relation representation

$$M_{l,t}(k,z)=-[z+N_{l,t}(k,z)]^{-1}M_{l,t}(k,t=0)\ . \tag{3.28}$$

A straightforward calculation yields

$$M_l(k,t=0)=\Omega_l^2(k)-k^2c_0^2,\quad M_t(k,t=0)=\Omega_t^2(k)\ , \tag{3.29a}$$

$$\Omega_l^2(k)=\Omega_E^2+3k^2c_\infty^2,\quad \Omega_t^2(k)=\Omega_E^2+k^2c_\infty^2\ . \tag{3.29b}$$

The matrix

$$c_\infty^2=v_{\mathrm{th}}^2\frac{c_v}{c_p}\begin{pmatrix}1 & \dfrac{1}{Tc_v}\\ k_BT\left(1-2\dfrac{k_B}{c_v}\right) & 1+4\dfrac{k_B}{c_v}\end{pmatrix} \tag{3.30}$$

contains characteristic velocities for high k,z wavelike excitations and c_p abbreviates c_v+k_B. The matrix

$$\Omega_E^2=\omega_E^2\begin{pmatrix}1-\xi_1\dfrac{k_B}{c_p} & \dfrac{1}{k_BT}\xi_1\dfrac{k_B}{c_p}\\ k_BT\left(\dfrac{c_v}{k_B}(1+\xi_1)-\dfrac{d}{2}-\xi_2\right)\dfrac{k_B}{c_p} & (1+\xi_1+\xi_2)\dfrac{k_B}{c_p}\end{pmatrix} \tag{3.31}$$

is a generalization of the square of the Einstein or Kirkwood frequency

$$\omega_E^2=\frac{(\vec{\mathrm{p}}_0|\mathfrak{L}^2|\vec{\mathrm{p}}_0)}{(\vec{\mathrm{p}}_0|\vec{\mathrm{p}}_0)}=\frac{1}{md}\langle\vec{\nabla}^2U_0\rangle\ , \tag{3.32}$$

which measures the mean-square force $\langle(\dot{\vec{p}}_0)^2\rangle^{1/2}$ on particle 0. The dimensionless quantities

$$\xi_1=\frac{\langle\delta U_0\vec{\nabla}^2U_0\rangle}{k_BT\langle\vec{\nabla}^2U_0\rangle},\quad \xi_2=\frac{\langle(\delta U_0)^2\vec{\nabla}^2U_0\rangle}{k_B^2T^2\langle\vec{\nabla}^2U_0\rangle} \tag{3.33}$$

depending on "temperature" and scatterer density n_s are determined by higher-order correlation functions. However the approximation

$$\xi_2\simeq\frac{\langle(\delta U_0)^2\rangle}{k_B^2T^2}=\frac{c_v}{k_B}-\frac{d}{2},\quad \xi_1\simeq+\sqrt{\xi_2} \tag{3.34}$$

which is consistent with the Cauchy Schwartz inequality $\xi_1^2\leqslant 1+\xi_2$ and which seems to be reasonable does not require additional unknown quantities.

Finally the transverse current correlation functions and their longitudinal counterparts, the generalized diffusivities, read

$$C_t(k,z)=-[z^2-\Omega_t^2(k)+zN_t(k,z)]^{-1}[z+N_t(k,z)]C(t=0)\ , \tag{3.35}$$

$$D(k,z)S(t=0)=-[z^2-(\Omega_l^2(k)-c_0^2k^2)+zN_l(k,z)]^{-1}[z+N_l(k,z)]C(t=0)\ . \tag{3.36}$$

Thus the velocity-correlation matrix

$$\psi(z)=-[z^2-\Omega_E^2+zN(z)]^{-1}[z+N(z)]C(t=0) \tag{3.37}$$

is given in terms of the matrix of restoring forces Ω_E^2 and the frequency-dependent complex relaxation-rate matrix $N(z)=N_{l,t}(k=0,z)$.

D. Diffusion versus localization

To interpret (3.37) let us forget for a moment that the quantities entering (3.37) are matrices—the generalization is straightforward. Then the imaginary part $N''(\bar{\omega})$ measures the lifetime of a velocity fluctuation of frequency $\bar{\omega}$ determined by $\bar{\omega}^2-\Omega_E^2+\bar{\omega}N'(\bar{\omega})=0$. The velocity fluctuation is of diffusive character if $N''(\bar{\omega})/\bar{\omega}>>1$. In the opposite case $N''(\bar{\omega})/\bar{\omega}<<1$ it represents a bounded oscillatory type of motion. Note in particular that a slowing down of the relaxation rate

$$\lambda_D=N''(\omega=0) \tag{3.38a}$$

for zero-frequency velocity fluctuations indicates a phase transition to a bounded type of motion: According to (3.37) the diffusivity

$$D=\Omega_E^{-2}\lambda_Dc_0^2 \tag{3.38b}$$

vanishes if the zero-frequency relaxation rate λ_D vanishes. Then the particle's mean-square displacement grows slower than linearly in time for $t\to\infty$.

We do indeed expect that there exists for finite n_s,T a transition to such a localized phase characterized by $D=0$ despite the initial momentum distribution having tails of high momentum $p_0^2/m>>k_BT$. That will cause only exponentially small escape rates out of the cagelike configurations which are characteristic for high-density environments. In any case, there will exist localization in the sense of experimental physics since in the high-density phase of scatterers corresponding to an amorphous solid the self-diffusion constant determined over experimentally accessible time is zero. Hence, at least in this sense, there will exist a line $T_{\text{loc}}(n_s)$ separating the $T-n_s$ plane into the localization regime where $D(n_s,T\leqslant T_{\text{loc}}(n_s))=0$ and into the diffusion regime where $D(n_s,T>T_{\text{loc}}(n_s))>0$. We furthermore expect all diffusivities D^{ij} to vanish simultaneously at $T_{\text{loc}}(n_s)$ since a blocking of particle diffusion enforces in our system also the energy to be blocked; the latter being transported only by the one moving particle. Since Ω_E^2 and c_0^2 are smoothly varying functions of n_s,T staying finite at $T_{\text{loc}}(n_s)$ the phase change $D\to 0$ to the localized state is indicated by $\lambda_D\to 0$. Hence $\lambda_D(n_s,T)$ is the relevant variable to be approximated.

We will now investigate the low-frequency structure of $\psi(\omega+i0)$. To that end consider the expansion

$$N(\omega+i0)\cong n_1\,\text{sgn}(\omega)|\omega|^{\alpha_1}+i(\lambda_D+n_2|\omega|^{\alpha_2}) \tag{3.39}$$

valid for $\omega\to 0$ with arbitrary $\alpha_1,\alpha_2>0$, e.g., $\alpha_1=1,\alpha_2=2$. Then one obtains

$$\psi(\omega+i0)\cong\Omega_E^{-2}[\omega+n_1\,\text{sgn}(\omega)|\omega|^{\alpha_1}+i(\lambda_D+n_2|\omega|^{\alpha_2})]C(t=0) \tag{3.40}$$

In $d=2,3$ dimensions $\alpha_2=d/2$ ($\alpha_2=2$) has been reported for a different model[10] in the diffusive (localized) regime corresponding to a long-time tail[6] $\psi(t)\sim t^{-d/2-1}$. Whereas $\psi(\omega+i0)$ is well behaved in both regimes its kernel

$$M(\omega+i0)\cong-[\omega+n_1\,\text{sgn}(\omega)|\omega|^{\alpha_1}+i(\lambda_D+n_2|\omega|^{\alpha_2})]^{-1}\Omega_E^2 \tag{3.41}$$

shows an infrared divergence[10] at $T_{\text{loc}}(n_s)$ where the relaxation rate λ_D slows down. Thus it might be advantageous to approximate N rather than M.

E. Simple approximations

A straightforward approximation which proved to be quite successful for current excitation spectra of fluids[19,25,26] is to neglect the frequency dependence of the relaxation kernels $N_{l,t}(k,z) \simeq i\tau_{l,t}^{-1}(k)$ so that

$$D(k,z) \simeq -[z^2 - \Omega_l^2(k) + c_0^2k^2 + iz\tau_l^{-1}(k)]^{-1} \times [z + i\tau_l^{-1}(k)]c_0^2 \ , \qquad (3.42a)$$

$$C_t(k,z) \simeq -[z^2 - \Omega_t^2(k) + iz\tau_t^{-1}(k)]^{-1} \times [z + i\tau_t^{-1}(k)]C(t=0) \ . \qquad (3.42b)$$

The relaxation times $\tau_{l,t}(k)$ can be taken either as fit parameters or they can be expressed in various ways[19,25,26] by spectral sum rules. If one adopts, e.g., the procedure proposed by the de Raedt brothers[27] one obtains in our case

$$\tau_{l,t}^{-1}(k) = \Omega_{l,t}(k) \ , \qquad (3.43)$$

where the matrix product $\Omega_{l,t}^2(k)$ is given by (3.29b). Then the velocity correlation matrix reads

$$\psi(z) \simeq -(z^2 - \Omega_E^2 + iz\,\Omega_E)^{-1}(z + i\,\Omega_E)c_0^2 \qquad (3.44)$$

leading to the diffusivity matrix

$$D \simeq \Omega_E^{-1}c_0^2 \ . \qquad (3.45)$$

By the way, one obtains, up to a factor $\sqrt{\pi/2}$, the same transport coefficients from approximating the spectral matrix of $D(k,z)$ by a Gaussian $D''(k,\omega) \simeq \sqrt{\pi/2}\,\Omega_l^{-1}(k)c_0^2\exp[-\frac{1}{2}\omega^2\Omega_l^{-2}(k)]$ constructed such[28] as to guarantee the lowest two spectral moments. One can not expect the localization transition to be realistically described with (3.45) since the high-frequency moments—i.e., the small-time behavior of the particle—will be almost unaffected by such a phase change. In the diffusive regime however one can obtain, as in simple fluids, a realistic estimate[25,28] of the transport coefficients and from (3.42)–(3.44) a reasonable description of the fluctuation spectra.[25,26]

With the approximation (3.34) $\xi_2 \simeq \langle(\delta U_0/k_BT)^2\rangle = \xi$, $\xi_1 \simeq \sqrt{\xi}$ the diagonal elements of the diffusivity matrix (3.45) are given by a product of v_{th}^2/ω_E with a number depending only on the quotient ξ of potential energy fluctuations and kinetic energy. After some matrix algebra one finds for $\xi = 0.25$ (1, 4)

$$D^{ij} = \frac{v_{\text{th}}^2}{\omega_E}\begin{pmatrix} 0.99(1.1, 1.6) & \frac{1}{k_BT}0.32(0.078, -0.97) \\ k_BT1.0(0.59, -0.67) & 2.7(2.0, 9.1) \end{pmatrix} . \qquad (3.46)$$

The self-diffusion constant D^{11} increases weakly with ξ in the above range while the energy diffusivity D^{22} shows a much more pronounced nonmonotonous dependence on ξ. Even more sensitively depends the coupling $D^{12}D^{21}/(D^{11}-D^{22})^2$ between long-wavelength number and energy-density fluctuations on the quotient ξ.

On the other hand, the velocity-fluctuation spectra $\psi^{ii}(\omega)/\psi^{ii}(\omega=0)$ being reduced by the diffusivities are roughly the same (cf. Fig. 1). For small values of ξ both above spectra are similar to that of a tagged particle in liquid argon.[25] For larger potential fluctuations $\xi = 4$ (or equivalently smaller temperatures) spectral intensity is shifted to larger frequencies such that additional side peaks develop around ω_E. It would be interesting to compare these predictions with computer experiments.

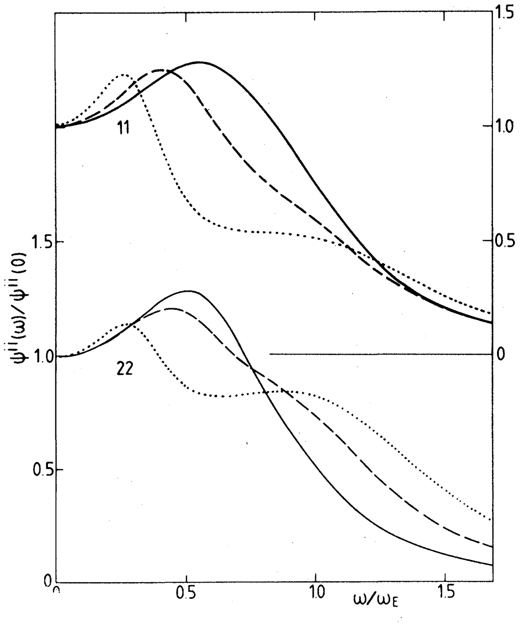

FIG. 1. Reduced velocity fluctuation spectra (3.44) as functions of ω/ω_E for $\xi = \langle(\delta U_0/k_BT)^2\rangle = 0.25$ (full curve), $\xi = 1$ (dashed curve), and $\xi = 4$ (dash-dotted curve).

IV. KINETIC THEORY OF PHASE-SPACE DENSITY FLUCTUATIONS

In this section we present a kinetic theory for phase-space density fluctuations of the two conserved quantities, particle number and energy. Our motivation for doing this is twofold. Approximations formulated within the generalized hydrodynamics framework of Sec. III being constructed such as to ensure the correct low k, ω behavior almost always violate the free-particle limit. The latter can naturally be incorporated in kinetic theories. Furthermore, approximations of comparable quality if formulated within a kinetic theory are superior[25,29] to those formulated within the generalized hydrodynamics framework.

The problem with kinetic theories is to construct "conserving" approximations to collision operators which guarantee the conservation laws for the constants of the motion of the system and thereby ensure the correct low k, ω behavior of their fluctuations. In particular, the restriction imposed by energy conservation upon kinetic theories is so severe that it can be met for real many-body systems only approximately in the low-density, weak-coupling limit. For high-density, strong-coupling systems a satisfactory solution is lacking. The basic reason for this is the potential part of the energy density which, depending on two positions, requires[25,30-34] two-point distribution functions in order to ensure energy conservation. In our system, however, the energy density is dynamically a one-point variable since only one end $[\vec{r}_0(t)]$ of the bonds in the potential part moves. Statistically the energy and its density is a two-point variable because of the statistical behavior of the scatterer environment entering H_0. That renders the construction of energy-conserving approximations tractable without making it trivial. Moreover it offers the present problem a guideline for a generalization to real dynamical systems.

To develop a kinetic theory which manifestly conserves particle number and energy for arbitrary scatterer densities and interaction strengths we introduce the *two* phase-space densities

$$A^i_{\vec{p}}(\vec{k},t) = \frac{1}{b_p}\delta(\vec{p}-\vec{p}_0(t))\,a^i(\vec{k},t) \tag{4.1}$$

of particle number $N_0 = 1$ ($i=1$) and of the energy deviation δH_0 ($i=2$). Both are products of the real-space densities $a^i(\vec{k})$ (3.1) and the momentum space density $\delta(\vec{p}-\vec{p}_0)$ normalized for convenience by the square root of its mean

$$b_p = \langle \delta(\vec{p}-\vec{p}_0)\rangle^{1/2} = \left(\frac{\beta}{2\pi m}\right)^{d/4} e^{-(\beta/2)p^2/2m} \ . \tag{4.2}$$

Integrating $A^i_{\vec{p}}(\vec{k})$ over all momenta with the weight $b_p[b_p\vec{p}/m]$ one obtains the Fourier transformed real-space densities $a^i(\vec{k})$ $[\vec{j}^i(\vec{k})]$. The "continuity" equations (3.7) reflecting conservation of particle number and energy read

$$\int d\vec{p}\, b_p\left(\mathfrak{L} + \frac{\vec{k}\cdot\vec{p}}{m}\right) A^i_{\vec{p}}(\vec{k}) = 0 \ . \tag{4.3}$$

This relation is of central importance for constructing conserving approximations.

A. Correlation functions of the two phase-space densities

The main object of our interest is the dynamical correlation matrix of phase-space density fluctuations.

$$\phi^{ij}_{\vec{p}\,\vec{p}'}(\vec{k},z) = \left(A^i_{\vec{p}}(\vec{k}) \left| \frac{1}{\mathfrak{L}-z} \right| A^j_{\vec{p}'}(\vec{k}) \right) = \phi^{ji}_{\vec{p}'\,\vec{p}}(\vec{k},z) \ . \tag{4.4}$$

These functions summarize all the correlation functions investigated in Sec. III and contain besides that a wealth of additional information. In particular, they describe the relaxation of a fluctuation $\delta A^i_{\vec{p}}(\vec{k},t)$ of the phase-space density towards its mean.

We will interpret

$$\phi_{\vec{p}\,\vec{p}'}(\vec{k},z) = \langle \vec{p}\,|\phi(\vec{k},z)|\,\vec{p}'\rangle \tag{4.5}$$

as matrix elements of an associated operator $\phi(\vec{k},z)$ in the continuous "$\vec{p}$ representation" with $\langle\vec{p}\,|\,\vec{p}'\rangle = \delta(\vec{p}-\vec{p}')$ and $\int d\vec{p}\,|\vec{p}\rangle\langle\vec{p}'| = 1$. Here $\langle\,|$ and $|\,\rangle$ are analogous to Dirac's bra and ket state vectors.[35] We will also consider matrix elements of $\phi(\vec{k},z)$ in the discrete "$\vec{n}$ representation"

$$\langle\vec{n}\,|\phi(\vec{k},z)|\,\vec{m}\rangle = \int d\vec{p}\int d\vec{p}'\,\langle\vec{n}\,|\,\vec{p}\rangle\,\phi_{\vec{p}\,\vec{p}'}(\vec{k},z)\,\langle\vec{p}'\,|\,\vec{m}\rangle \tag{4.6}$$

defined by

$$\langle\vec{n}\,|\,\vec{p}\rangle = \langle\vec{p}\,|\,\vec{n}\rangle = \frac{(a_1^\dagger)^{n_1}\dots(a_d^\dagger)^{n_d}}{\sqrt{n_1!\dots n_d!}}\,b_p \tag{4.7}$$

in terms of Hermite polynomials with $\vec{n} = (n_1, \dots, n_d)$, $n_\alpha = 0, 1, \dots$ so that $\langle\vec{n}\,|\,\vec{m}\rangle = \int d\vec{p}\,\langle\vec{n}\,|\,\vec{p}\rangle\langle\vec{p}\,|\,\vec{m}\rangle = \delta_{\vec{n},\vec{m}}$ and $\sum_{\vec{n}}|\vec{n}\rangle\langle\vec{n}| = 1$. The creation and annihilation operators $[\hat{p}_\alpha = p_\alpha/(\sqrt{2}m v_{\text{th}})]$

$$a_\alpha^\dagger = \frac{1}{\sqrt{2}}\left(\hat{p}_\alpha - \frac{\partial}{\partial\hat{p}_\alpha}\right),\quad a_\alpha = \frac{1}{\sqrt{2}}\left(\hat{p}_\alpha + \frac{\partial}{\partial\hat{p}_\alpha}\right) \tag{4.8}$$

obey the usual commutator algebra.

The matrix elements (4.6) of $\phi(k,z)$ between the lowest "states" $|\vec{0}\rangle$ and $|1_\alpha\rangle = a_\alpha^\dagger|\vec{0}\rangle$ are correlation functions of densities $\langle\vec{0}\,|\phi^{ij}(\vec{k},z)|\,\vec{0}\rangle = S^{ij}(k,z)$ and currents $\langle 1_\alpha|\phi^{ij}(k,z)|1_\beta\rangle = C^{ij}_{\alpha\beta}(\vec{k},z)/v_{\text{th}}^2$. This gives a first hint at the usefulness of the $\vec{n}$ representation.[34,36] Its main advantage however is the possibility to formulate within it a systematic, conserving operator expansion for the collision operator of $\phi(\vec{k},z)$.

B. Kinetic equation for $\phi(\vec{k},z)$

With the standard technique of Sec. II one obtains the equation of motion

$$[z-\omega(\vec{k})+\Sigma(\vec{k},z)]\,\phi(\vec{k},z) = -\chi \tag{4.9}$$

for the correlation matrix of phase-space densities.

The equal time phase-space density correlations χ are wave-number independent. In $\vec{p}$ representation

$$\chi^{ij}_{\vec{p}\,\vec{p}'}=(A^{i}_{\vec{p}}(\vec{k})|A^{j}_{\vec{p}'}(\vec{k}))$$

$$=\delta(\vec{p}-\vec{p}')\begin{pmatrix}1 & \dfrac{\delta p^2}{2m}\\ \dfrac{\delta p^2}{2m} & \left(\dfrac{\delta p^2}{2m}\right)^2+\langle(\delta U_0)^2\rangle\end{pmatrix} \qquad (4.10a)$$

is diagonal with respect to $\vec{p},\vec{p}'$. In $\vec{n}$ representation there are off-diagonal matrix elements

$$\langle\vec{n}|\chi|\vec{m}\rangle=\langle\vec{n}|\begin{pmatrix}1 & \dfrac{\delta p^2}{2m}\\ \dfrac{\delta p^2}{2m} & \left(\dfrac{\delta p^2}{2m}\right)^2+\langle(\delta U_0)^2\rangle\end{pmatrix}|\vec{m}\rangle \qquad (4.10b)$$

since

$$\frac{\delta p^2}{2m}=\frac{p^2-\langle p_0^2\rangle}{2m}=\frac{k_BT}{2}(a^\dagger_\alpha a^\dagger_\alpha+a_\alpha a_\alpha+2a^\dagger_\alpha a_\alpha)\ . \qquad (4.11)$$

The inverse χ^{-1} does not exist in the limiting case $U_0=0$ of a free particle.

With only one particle moving there is no Vlasov term and hence the operator $\omega(\vec{k})$ represents just free streaming. It is diagonal in $\vec{p}$ representation

$$\omega^{ij}_{\vec{p}\,\vec{p}'}(\vec{k})=(A^{i}_{\vec{p}}(\vec{k})|\mathcal{L}|A^{i}_{\vec{p}}(\vec{k}))[\chi^{-1}]^{ij}_{\vec{p}\,\vec{p}'}$$

$$=-\frac{\vec{k}\cdot\vec{p}}{m}\delta(\vec{p}-\vec{p}')\delta^{ij}\ , \qquad (4.12a)$$

while in $\vec{n}$ representation

$$\langle\vec{n}|\omega^{ij}(\vec{k})|\vec{m}\rangle=-k\,v_{\text{th}}\langle\vec{n}|a_1^\dagger+a_1|\vec{m}\rangle\delta^{ij}\ . \qquad (4.12b)$$

there are with our choice (3.5) for the wave-vector off-diagonal elements in the first Cartesian component.

1. Collision kernel $\Sigma(\vec{k},z)$

The collision operator

$$\Sigma(\vec{k},z)=\Gamma(\vec{k},z)\chi^{-1} \qquad (4.13)$$

is a product of a $\vec{k},z$ dependent relaxation kernel and the inverse static susceptibility χ^{-1}. The $\vec{p}$ representation of $\Gamma(\vec{k},z)$

$$\Gamma^{ij}_{\vec{p}\,\vec{p}'}(\vec{k},z)$$

$$=\left(A^{i}_{\vec{p}}(\vec{k})\middle|\mathcal{L}Q_A\frac{1}{Q_A\mathcal{L}Q_A-z}Q_A\mathcal{L}\middle|A^{j}_{\vec{p}'}(\vec{k})\right) \qquad (4.14)$$

with Q_A projecting orthogonal to $A^{i}_{\vec{p}}(\vec{k})$ reveals that the dynamics of the collision operator is determined by fluctuations of the generalized phase-space densities $[d\vec{p}_0(t)/dt]A^{i}_{\vec{p}}(\vec{k},t)$ of the force $d\vec{p}_0/dt$ on the moving particle

$$Q_A\mathcal{L}A^{j}_{\vec{p}}(\vec{k})=Q_A\left(-\frac{\vec{k}\cdot\vec{p}}{m}-i\frac{(\dot{p}_0^{\alpha})a^\dagger_\alpha}{m v_{\text{th}}}\right)A^{j}_{\vec{p}}(\vec{k})$$

$$=-ia^\dagger_\alpha\frac{\dot{p}_0^{\alpha}}{m v_{\text{th}}}A^{j}_{\vec{p}}(\vec{k})\ . \qquad (4.15)$$

Their correlation functions

$$\left(\frac{\dot{p}_0^{\alpha}}{m v_{\text{th}}}A^{i}_{\vec{p}}(\vec{k})\middle|\frac{1}{Q_A\mathcal{L}Q_A-z}\middle|\frac{\dot{p}_0^{\beta}}{m v_{\text{th}}}A^{j}_{\vec{p}'}(\vec{k})\right)$$

$$=\langle\vec{p}|\gamma^{ij}_{\alpha\beta}(\vec{k},z)|\vec{p}'\rangle \qquad (4.16)$$

determine $\Gamma(\vec{k},z)$

$$\langle\vec{p}|\Gamma^{ij}(\vec{k},z)|\vec{p}'\rangle=a^\dagger_\alpha a'^\dagger_\beta\langle\vec{p}|\gamma^{ij}_{\alpha\beta}(\vec{k},z)|\vec{p}'\rangle\ , \qquad (4.17a)$$

$$\langle\vec{n}|\Gamma^{ij}(\vec{k},z)|\vec{m}\rangle=\langle\vec{n}|a^\dagger_\alpha\gamma^{ij}_{\alpha\beta}(\vec{k},z)a_\beta|\vec{m}\rangle\ . \qquad (4.17b)$$

Here $a'^\dagger_\beta$ operates on $\vec{p}'$ and the second line follows with the definitions (4.6) and (4.7) making use of partial integrations. We consider the above force-density correlation functions to be the basic quantity to be approximated.

2. Particle number and energy conservation

The kinetic equation (4.9) guarantees the relations

$$\int d\vec{p}\,b_p\left(z+\frac{\vec{k}\cdot\vec{p}}{m}\right)\phi^{ij}_{\vec{p}\,\vec{p}'}(\vec{k},z)=-\int d\vec{p}\,b_p\,\chi^{ij}_{\vec{p}\,\vec{p}'}\ ,$$

$$z\langle\vec{0}|\phi^{ij}(\vec{k},z)+k_\alpha v_{\text{th}}\langle 1_\alpha|\phi^{ij}(\vec{k},z)=-\langle\vec{0}|\chi^{ij}\ , \qquad (4.18)$$

following from the "continuity" equations (4.3) if and only if the collision operator is such that

$$\langle\vec{0}|\Gamma(\vec{k},z)\chi^{-1}=\langle\vec{0}|\Sigma(\vec{k},z)=0=\Sigma^{\mathrm{T}}(\vec{k},z)|\vec{0}\rangle$$

$$=\chi^{-1}\Gamma(\vec{k},z)|\vec{0}\rangle\ . \qquad (4.19)$$

The energy-conserving criterion is much simpler than in case of a fluid[33] because here the energy-density current is as simple as the number-density current and because the phase-space density of the energy has been introduced explicitly within the 2 × 2 matrix formalism. To formulate the energy conservation requirement within the standard one component description of $A^{1}_{\vec{p}}(\vec{k})$ alone is more difficult. Since the correct collision operator satisfies the conditions $\Gamma(\vec{k},z)|\vec{0}\rangle=\langle\vec{0}|\Gamma(\vec{k},z)=0$ for particle number and energy conservation one concludes from (4.17b) that the operator $\gamma^{ij}_{\alpha\beta}(\vec{k},z)$ is a well-behaved function of the operators a^+ and a.

C. Operator expansion of $\Gamma(\vec{k},z)$

It has been a commonly practiced strategy in kinetic theory[25,37] to approximate dynamical quantities like relaxation kernels while incorporating static correlations as far as possible exactly. We will also stick to this recipe and expand the operator $\Gamma(\vec{k},z)$ [or equivalently $\gamma(\vec{k},z)$] in powers of $a_\alpha^\dagger$ and a_β. Such a polynomial approximation with all creation (annihilation) operators to the left (right) is systematic as shown in Appendix A and conserving.

In this work we keep in the expansion (cf. Appendix A) of $\Gamma^{ij}(\vec{k},z)$ only the lowest term

$$\begin{aligned}\Gamma^{ij}(\vec{k},z) &\simeq a_\alpha^\dagger a_\beta \langle 1_\alpha | \Gamma^{ij}(\vec{k},z) | 1_\beta \rangle \\ &= a_\alpha^\dagger a_\beta \langle \vec{0} | \gamma_{\alpha\beta}^{ij}(\vec{k},z) | \vec{0} \rangle \ ,\end{aligned} \tag{4.20}$$

which is bilinear in $a^\dagger$ and a. The next terms contain at least products of three operators since the coefficients of $a_\alpha^\dagger a_\beta^\dagger$ and $a_\alpha a_\beta$ have to vanish due to the conservation laws $\Gamma|\vec{0}\rangle = 0 = \langle \vec{0}|\Gamma$. The coefficient $\langle \vec{0} | \gamma_{\alpha\beta}^{ij}(\vec{k},z) | \vec{0} \rangle$ is determined by correlations of the generalized real-space densities $(d\vec{p}_0/dt)a^i(\vec{k})$ of the force $d\vec{p}_0/dt$ on the moving particle

$$\begin{aligned}\tilde{m}_{\alpha\beta}^{ij}(\vec{k},z) &= \left(j_\alpha^i(\vec{k}) \,\middle|\, \mathfrak{L} Q_A \frac{1}{Q_A \mathfrak{L} Q_A - z} Q_A \mathfrak{L} \,\middle|\, j_\beta^j(\vec{k}) \right) \\ &= \left(\dot{v}_0^\alpha a^i(\vec{k}) \,\middle|\, \frac{1}{Q_A \mathfrak{L} Q_A - z} \,\middle|\, \dot{v}_0^\beta a^j(\vec{k}) \right) \\ &= v_{\text{th}}^2 \langle 1_\alpha | \Gamma^{ij}(\vec{k},z) | 1_\beta \rangle \ .\end{aligned} \tag{4.21}$$

Note that $\tilde{m}(\vec{k},z)$ differs from $m(\vec{k},z)$ (3.21) because of the projectors Q_A, Q. Whereas the latter projects out only the real-space densities $a^i(\vec{k})$ and $\vec{j}^i(\vec{k})$ the former eliminates phase-space densities $A_{\vec{p}}^i(\vec{k})$. Hence the spectrum $\tilde{m}''(\vec{k},\omega)$ of force density fluctuations is expected to be smoother than that of $m(\vec{k},z)$ which still contains phase-space density excitations. That is not only of academic interest since numerical calculations require to approximate $\tilde{m}_{\alpha\beta}^{ij}(\vec{k},z)$. Their outcome has to decide whether $\tilde{m}(\vec{k},z)$ directly should be approximated—e.g., by some generalized mode-coupling procedure—or whether the self-energy of $\tilde{m}(\vec{k},z)$ is more appropriate for approximations.

We should like to point out that the approximation (4.20) which looks rather simple minded in the $\vec{n}$ representation contains a Fokker-Planck operator in the $\vec{p}$ representation.[34,38] Our approximation is exact for the equal-time relaxation kernel $\Gamma^{11}(\vec{k},t=0) = a_\alpha^\dagger a_\beta \langle 1_\alpha | \Gamma^{11}(\vec{k},t=0) | 1_\beta \rangle$, i.e., the operator expansion terminates with the bilinear term $a^\dagger a$ which still operates in the infinite-dimensional Hilbert space spanned by the Hermite polynomials. The standard expansion procedures employed in kinetic hydrodynamic theory[25] which truncate the space of states are inadequate to reproduce the above feature (cf. Appendix A). Also the expansion which has recently been suggested[39] for a different problem cannot reproduce the correct Fokker-Planck operator structure of the equal-time collision kernel. The other matrix elements

$$\Gamma^{ij}(\vec{k},t=0) = \omega_E^2 a_\alpha^\dagger \begin{pmatrix} 1 & k_B T\left(1+\xi_1+\dfrac{\delta p^2}{2mk_BT}\right) \\ k_B T\left(1+\xi_1+\dfrac{\delta p^2}{2mk_BT}\right) & k_B^2T^2\left[\xi_2+\left(\dfrac{\delta p^2}{2mk_BT}\right)^2+2(1+\xi_1)\left(1+\dfrac{\delta p^2}{2mk_BT}\right)\right] \end{pmatrix} a_\alpha \tag{4.22}$$

would be bilinear in $a^\dagger$ and a as well were it not for the operator $\delta p^2/2m$ (4.11) in the matrix elements containing the phase space density $A_{\vec{p}}^2(\vec{k})$ of the energy.

Our approximation (4.20) can be written for the 1-1 component in the form $\Gamma_{\vec{p}\,\vec{p}'}^{11}(\vec{k},z) \simeq \Gamma_{\vec{p}\,\vec{p}'}^{11} \times (\vec{k},t=0) f(k,z)$ which was suggested earlier on heuristic grounds[38,40] for fluids. However, in contrast to our theory, the function $f(k,z)$ cannot be identified unambiguously by correlation functions of the system. To determine $f(k,z)$ by the lowest matrix elements in the $\vec{n}$ representation which might seem reasonable [and is correct for the above special case in terms of our operator expansion] is not compelling within the above heuristic approach and was not suggested anyhow by the authors.[34,38,40,41] They took for $f(k,z)$ a Lorentzian or a Gaussian with a wave-number-dependent relaxation rate chosen by various *ad hoc* procedures. The resulting density and current correlation spectra agreed remarkably well with experiments.

D. Approximate kinetic equation

With the approximation (4.20) for the relaxation kernel the collision operator

$$\Sigma^{ij}(\vec{k},z) \simeq \frac{1}{v_{\text{th}}^2} \tilde{m}_{\alpha\beta}^{il}(\vec{k},z) a_\alpha^\dagger a_\beta (\chi^{-1})^{lj} \tag{4.23}$$

still contains higher than bilinear combinations of $a^\dagger$ and a. They stem from the operator $\delta p^2/2m$ appearing in the inverse of the static susceptibility (4.10). For the purpose of practical calculations we suggest an additional approximation, namely, expanding (4.23) up to bilinear order which affects the inverse of the static susceptibility. We consider this approximation to be only of technical nature the basic approximation being (4.20). The above expansion $a_\alpha^\dagger a_\beta \chi^{-1} \simeq a_\nu^\dagger a_\mu \langle 1_\nu | a_\alpha^\dagger a_\beta \chi^{-1} | 1_\mu \rangle$ yields

$$\Sigma^{ij}(\vec{k},z) \simeq \sigma_{\alpha\beta}^{ij}(\vec{k},z) a_\alpha^\dagger a_\beta \tag{4.24}$$

with

$$\sigma_{\alpha\beta}^{ij}(\vec{k},z) = \frac{c_v + k_B}{c_v - \frac{1}{2} d k_B} \tilde{m}_{\alpha\beta}^{il}(\vec{k},z) [C^{-1}(t=0)]^{lj} \ , \tag{4.25}$$

where $C^{ij}(t=0)$ are equal-time current correlations.

However, with (4.24) and (4.25) the potential part of the second moment of the current correlation matrix $(j_\alpha^i(\vec{k}) | L^2 | j_\beta^j(\vec{k})) = v_{\text{th}}^2 \langle 1_\alpha | [\omega^2(\vec{k}) + \Sigma(\vec{k},t=0)] \chi | 1_\beta \rangle$ is wrong as a consequence of the approximation χ^{-1}: Whereas (4.23) still guarantees the exact relation

$$v_{\text{th}}^2 \langle 1_\alpha | \Sigma(\vec{k},t=0) \chi | 1_\beta \rangle = \tilde{m}_{\alpha\beta}(\vec{k},t=0) \tag{4.26}$$

our technical approximation for χ^{-1} yields the additional prefactor $(c_v + k_B)(c_v - \frac{1}{2} d k_B)^{-1} = 1 + \frac{1}{2}(d+2)(k_B T)^2 \langle (\delta U_0)^2 \rangle^{-1}$. It measures how much the identity $\chi^{-1} \chi | 1_\beta \rangle = | 1_\beta \rangle$ entering (4.26) is violated by approximating χ^{-1} alone. In the strong-coupling case of dense scatterer environments which is of greatest interest this factor is of minor importance. In the weak-coupling limit or equivalently for large frequencies and wave numbers where free-particle behavior dominates one would prefer a technical approximation for χ^{-1} which guarantees as many moments in a high-frequency expansion as possible. In our case one can demand that a bilinear truncation $\Sigma(\vec{k},z) \simeq \sigma_{\alpha\beta}(\vec{k},z) a_\alpha^\dagger a_\beta$ of the collision kernel (4.23) satisfies (4.26). That yields as an alternative to (4.25)

$$\sigma_{\alpha\beta}^{ij}(\vec{k},z) = \tilde{m}_{\alpha\beta}^{il}(k,z) [C^{-1}(t=0)]^{lj} \ . \tag{4.27}$$

In any case the approximate kinetic equation for $\phi(\vec{k},z)$ reads

$$[z\delta^{il} + v_{\text{th}} k (a_1 + a_1^\dagger) \delta^{il} + a_\alpha^\dagger a_\alpha \sigma^{il}(k,z)] \phi^{lj}(\vec{k},z) = -\chi^{ij} \ . \tag{4.28}$$

Here we have replaced $\sigma_{\alpha\beta}^{ij}(\vec{k},z)$ which is diagonal in α, β by $\delta_{\alpha\beta} d^{-1} \sigma_{\gamma\gamma}^{ij}(k,z)$. Thus longitudinal and transverse parts $\tilde{m}_{l,t}^{ij}(k,z)$ of $\tilde{m}_{\alpha\beta}^{ij}(\vec{k},z)$ were taken to be the same. The solution to (4.28) for the general case can be obtained as well. Since it is only more complicated without offering new insight we will investigate for notational convenience the above simplification. Besides that seems $\tilde{m}_l^{ij}(k,z) \simeq \tilde{m}_t^{ij}(k,z)$ to be reasonable since in the limiting cases $k \to 0$ and for large z [cf. (4.21), (4.22)] longitudinal and transverse parts are the same.

E. Correlation functions of currents and velocities

The correlation-function matrices of densities and currents following from the kinetic equation (4.28) are derived in Appendix B. They are given in terms of integrals related to the incomplete gamma function

$$C_l(k,z) = -v_{\text{th}}^2 z \, \sigma^{-2}(k,z) \int_0^1 dx \, e^{-\lambda^2(1-x)} x^{\zeta-1} (1-x) \times P_4(x;\lambda) \ , \tag{4.29a}$$

$$C_t(k,z) = -v_{\text{th}}^2 \sigma^{-1}(k,z) \int_0^1 dx \, e^{-\lambda^2(1-x)} x^{\zeta} P_4(x;\lambda) \ , \tag{4.29b}$$

with

$$\lambda = -k v_{\text{th}} \sigma^{-1}(k,z), \quad \zeta = z\sigma^{-1}(k,z) - \lambda^2 \ . \tag{4.30}$$

The polynomial $P_4(x;\lambda)$ (B12)

$$P_4(x;\lambda) = v_{\text{th}}^{-2} C(t=0) + (1-x)^2 \lambda^2 \frac{k_B T}{2} \begin{pmatrix} 0 & 1 \\ 1 & 4k_B T \end{pmatrix} + (1-x)^4 \lambda^4 \left(\frac{k_B T}{2} \right)^2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{4.31}$$

contains even terms up to quartic order. At long wavelengths however only the matrix element (B12) between "hydrodynamic" states $\langle 1_1 | \chi | 1_1 \rangle = v_{\text{th}}^{-2} C(t=0)$ enters the theory. Note that λ and ζ are 2×2 matrices depending on $\sigma^{ij}(k,z)$. Thus to evaluate (4.29) numerically for finite k for a particular $\sigma^{ij}(k,z)$ one should determine first the transformation matrix which diagonalizes $\sigma^{ij}(k,z)$ and consequently also λ and ζ. Then one has to integrate, for a particular power λ^n in P_4 (4.31), over the two diagonal elements ($\nu = 1,2$) of the integrands in (4.29) which have typically the form $\exp[-\lambda_{(\nu)}^2 (1-x)] \times x^{\zeta(\nu)} (1-x)^n$.

In the limit $k \to 0$ where λ vanishes the result (4.29) simplifies considerably. One verifies immediately that both current correlation matrices

$$\begin{aligned} C_l(k \to 0,z) &= -z\sigma^{-2}(z) \int_0^1 dx \, x^{z\sigma^{-1}(z)-1} (1-x) C(t=0) = -[z+\sigma(z)]^{-1} C(t=0) \ , \\ C_t(k \to 0,z) &= -\sigma^{-1}(z) \int_0^1 dx \, x^{z\sigma^{-1}(z)} C(t=0) = -[z+\sigma(z)]^{-1} C(t=0) \ , \end{aligned} \tag{4.32}$$

yield the same velocity correlation matrix. Hence the kinetic theory developed here yields for the diffusivity matrix

$$\begin{aligned} D &= -\lim_{\omega \to 0} [\omega + i\sigma(\omega + i0)]^{-1} c_0^2 \\ &= C(t=0)[\tilde{m}''(0,0)]^{-1} c_0^2 \ , \end{aligned} \tag{4.33}$$

where we used (4.27). This has to be compared with the generalized hydrodynamic result $D = C(t=0) \times [m''(0,0)]^{-1} c_0^2$. Presumably $m''(0,0) \neq \tilde{m}''(0,0)$ due to the different projectors in (3.21) and (4.21) although we have not been able to prove it. However, at least within simple approximations, there is no difference. Consider as an example for such an approximation

$$\sigma(k,z) \simeq -[z + i\tilde{\tau}^{-1}(k)]^{-1} \sigma(k,t=0) \ . \tag{4.34}$$

From (4.21) one sees that $\sigma(k,t=0) = \Omega_E^2$ (3.31) is wave number independent. Whether one uses $\tilde{\tau}^{-2}(k) \simeq (j|\mathcal{L}Q_A\mathcal{L}|j)(j|j)^{-1}$ or $\tau^{-2}(k) \simeq (j|\mathcal{L}^2|j) \times (j|j)^{-1}$ for determining the relaxation time matrix does not play a role for $k \to 0$. In both cases one obtains for the diffusivity matrix $D \simeq \Omega_E^{-1} c_0^2$, i.e., the same result as from the equivalent approximation in generalized hydrodynamics theory.

V. SUMMARY

We have investigated the dynamics of a classical particle moving in the potential of randomly fixed scatterers which are thought to be realized by freezing in a fluid in thermal equilibrium with a tagged particle immersed in it. The statistical mechanics of this system is determined via a canonical ensemble average over the phase-space variables remaining after the quench. That implies, in particular, that the energy of the moving particle which is a constant of the motion fluctuates within the ensemble. Moreover, fluctuations of the energy density relax diffusively for low k, ω. They represent a second relevant "hydrodynamic" mode besides number-density fluctuations.

In Sec. III we developed a generalized hydrodynamics theory for the fluctuation spectra of the densities of particle number and energy, of their currents and of their velocities. We used dispersion relation representations for the 2×2 matrices of correlation functions. The diffusivity matrix D^{ij} of the two densities has off-diagonal elements. Due to this coupling between the densities the decay of either fluctuation is characterized by two different relaxation rates: neglecting the coupling to other conserved densities like $H_0^2 e^{-i\vec{k}\cdot\vec{r}_0}$ the low-k, ω excitation spectra of both densities are superpositions of two Lorentzians of widths $k^2 D_\pm$ determined by the eigenvalues $D_\pm$ of the diffusivity matrix. We also investigated dispersion relation representations for the generalized diffusivities, for the transverse current correlation matrix, and for the relaxation kernels of all of them.

The transition to a localized state where the diffusivities vanish is indicated and determined by the slowing down of the zero-frequency relaxation rate of velocity fluctuations. The change in the low-frequency velocity-fluctuation spectrum associated with the phase change can naturally be described within the framework presented here. Excitation spectra of currents and velocities are determined within simple approximations which follow from Lorentzian or Gaussian relaxation kernels and the dependence of the velocity-fluctuation spectra and diffusivities on the ratio of mean potential fluctuations and kinetic energy are discussed.

In Sec. IV we have developed a new type of kinetic theory for the fluctuations of the phase-space densities of the two constants of motion. We derived a matrix kinetic equation for the 2×2 matrix of correlations of the two phase-space densities which manifestly guarantees the exact conservation laws of both, particle number and energy. This was achieved because (i) phase-space density fluctuations of the energy are explicitly taken into account, (ii) they are two-point quantities only in a statistical sense—dynamically the energy phase-space density is a one-point quantity since only one end of the bonds of the potential part moves.

Technically we introduced for the $\vec{p}$, $\vec{p}\,'$ dependent correlation operators in the kinetic equation a well known discrete $\vec{n}$ representation based upon Hermite polynomials. In the space spanned by this $\vec{n}$ basis the operators are functions of creation and annihilation operators acting on the $\vec{n}$ states. In particular, the collision operator can be expanded in a power series of creation and annihilation operators which manifestly ensures particle number and energy conservation. The expansion coefficients are matrix elements of the operator between $\vec{n}$ states the lowest of which are "hydrodynamic" states. Terminating the expansion at some order one obtains a systematic (cf. Appendix A) approximation which is novel in kinetic theory literature.

Unlike conventional expansion schemes for the collision operator the state space is not truncated and thus already the lowest orders guarantee the correct operator structure at small times. In this work terms up to bilinear order in creation and annihilation operators are kept. The expansion coefficient thereof is a correlation function of the generalized densities of the force acting on the moving particle. This correlation function is similar though not equal to a relaxation kernel appearing in the generalized hydrodynamics theory of Sec. III. Our systematic approximation to the collision kernel is similar in structure to one suggested[33,38,40,41] on heuristic grounds which has proven to be quite successful for fluids.[25,29,33] From the solution of the approximate kinetic equation we obtained correlations of currents and densities in terms of integrals related to the incomplete gamma function. In the limit $k \to 0$ they yield a dispersion relation representation of the velocity correlation matrix and an explicit expression for the diffusivity matrix analogous to that obtained from the generalized hydrodynamics theory.

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APPENDIX A: OPERATOR EXPANSION

Let

$$F=\sum_{n=0}^{\infty}{}' \sum_{m=0}^{\infty} |n\rangle F_{nm} \langle m| , \quad \langle n|F|m\rangle = F_{nm} \tag{A1}$$

be any operator acting in the infinite dimensional Hilbert space spanned by the orthonormal state vectors $|n\rangle = (n!)^{-1/2}(a^\dagger)^n|0\rangle$; $n=0,1,\ldots$. The generalization to the case $|\vec{n}\rangle = |n_1,\ldots,n_d\rangle$ being obvious is left out here for the sake of notational convenience. Then the coefficients f_{kl} in the operator expansion

$$\tilde{F}=\sum_{k=0}^{N}\sum_{l=0}^{N}(a^\dagger)^k a^l f_{kl} \tag{A2}$$

can be evaluated in terms of $\{F_{nm}; n \leqslant k,\ m \leqslant l\}$ such that

$$\langle n|F|m\rangle = \langle n|\tilde{F}|m\rangle , \quad \text{for } n,m \leqslant N , \tag{A3}$$

i.e., F and $\tilde{F}$ have the same matrix elements between the states $0,1,\ldots,N$.

To express f_{kl} in terms of $\{F_{nm}\}$ one has to invert the series

$$F_{nm}=\sqrt{n!m!}\sum_{k=\max(0,n-m)}^{n}\frac{1}{(n-k)!}f_{k,k+m-n} , \tag{A4}$$

which follows from (A3). That can be done starting from F_{0n}, F_{n0} then proceeding to F_{1n}, F_{n1} with $n \geqslant 1$ then to F_{2n}, F_{n2} with $n \geqslant 2$ and so on. In this way one obtains, e.g.,

$$f_{0n}=\frac{1}{\sqrt{n!}}F_{0n}, \quad f_{n0}=\frac{1}{\sqrt{n!}}F_{n0} \tag{A5a}$$

and for $n \geqslant 1$

$$\begin{aligned} f_{1n}&=\frac{1}{\sqrt{n!}}F_{1n}-\frac{1}{\sqrt{(n-1)!}}F_{0,n-1} , \\ f_{n1}&=\frac{1}{\sqrt{n!}}F_{n1}-\frac{1}{\sqrt{(n-1)!}}F_{n-1,0} . \end{aligned} \tag{A5b}$$

As noted already is the coefficient f_{kl} determined only by $\{F_{nm}\}$ with $n \leqslant k$, $m \leqslant l$. Thus to improve the approximation $\tilde{F}$ to F from level N to level $N+1$ one merely has to evaluate the additional coefficients $f_{N+1,l}$ and $f_{k,N+1}$ for $k,l \leqslant N+1$.

We are mainly interested in the expansion of F up to powers $N=1$ of $a^\dagger$ and a

$$\begin{aligned} F \simeq{}& \langle 0|F|0\rangle 1 + \langle 0|F|1\rangle a + \langle 1|F|0\rangle a^\dagger \\ &+ [\langle 1|F|1\rangle - \langle 0|F|0\rangle] a^\dagger a + \cdots . \end{aligned} \tag{A6}$$

The Fokker-Planck operator $\Gamma^{11}(\vec{k}, t=0)$ (4.22) is an example for which the expansion (A6) is exact while an expansion $\sum_{n,m}|n\rangle A_{nm}\langle m|$ with a truncation of the form

$$A_{nm} \simeq \begin{pmatrix} A_{00} & A_{01} & & 0 \\ A_{10} & A_{11} & & \\ & & a & \\ & 0 & & \ddots \ a \end{pmatrix}$$

used in standard kinetic theory[25] with $a=0$ or $a \neq 0$ fails.

APPENDIX B: SOLUTION OF THE APPROXIMATE KINETIC EQUATION (4.36)

We will employ algebraic methods[33] (well known from displaced harmonic oscillators) to evaluate the matrix elements of

$$\phi(\vec{k},z) = -[z + v_{\text{th}}k(a_1^\dagger + a_1) + a_\alpha^\dagger a_\alpha \sigma(k,z)]^{-1}\chi \tag{B1}$$

in the $\vec{n}$ representation. Since the linear term in the square bracket causes difficulties it is eliminated by the transformation

$$(U^{-1}a_1^\dagger U)^{ij} = a_1^\dagger \delta^{ij} + \lambda^{ij} , \quad (U^{-1}a_1 U)^{ij} = a_1 \delta^{ij} + \lambda^{ij} \tag{B2}$$

of $a_1^\dagger, a_1$ which is generated by the (nonunitary) operator

$$U^{ij}(a_1^\dagger, a_1) = (e^{\lambda a_1^\dagger} e^{-\lambda a_1})^{ij} . \tag{B3}$$

Here

$$\lambda = -k v_{\text{th}} \sigma^{-1}(k,z) , \tag{B4}$$

$$\zeta = z\sigma^{-1}(k,z) - \lambda^2 , \tag{B5}$$

are complex 2×2 matrices. With (B2) one obtains

$$\phi(\vec{k},z) = -\sigma^{-1}(k,z)U(\zeta + a_\alpha^\dagger a_\alpha)^{-1}U^{-1}\chi . \tag{B6}$$

Current correlation functions are matrix elements of (B6) between the longitudinal current "state vector" $a_1^\dagger|\vec{0}\rangle = |1_1\rangle$ or the transverse current "state vector" $a_2^\dagger|\vec{0}\rangle = |1_2\rangle$. Since U operates only on the longitudinal component of state vectors one readily sees that the longitudinal current correlation matrix is given by

$$v_{\text{th}}^{-2}C_l(k,z) = \langle 1_1|\phi(\vec{k},z)|1_1\rangle = -\sigma^{-1}(k,z)\langle 1_1|U|m_1\rangle(\zeta+m_1)^{-1}\langle m_1|U^{-1}|n_1\rangle\langle n_1|\chi|1_1\rangle \quad , \tag{B7}$$

where summation over n_1,m_1 is implied. With

$$\langle 1_1|U|m_1\rangle = \frac{(-\lambda)^{m_1}}{\sqrt{m_1!}}\left(\lambda - \frac{m_1}{\lambda}\right) \quad , \tag{B8}$$

$$\langle m_1|U^{-1}|n_1\rangle = \left(\frac{m_1!}{n_1}\right)^{1/2}\lambda^{n_1-m_1}\sum_{\mu}\frac{(-\lambda^2)^{\mu}}{\mu!}\binom{n_1+\mu}{m_1} \quad , \tag{B9}$$

and the relation

$$(\zeta+m_1)^{-1} = \int_0^1 dx x^{\zeta-1}x^{m_1} \tag{B10}$$

one obtains after some straightforward algebra

$$v_{\text{th}}^{-2}C_l(k,z) = -z\sigma^{-1}(k,z)\int_0^1 dx e^{-\lambda^2(1-x)}x^{\zeta-1}(1-x)P_4(x,\lambda) \quad . \tag{B11}$$

The polynomial

$$P_4(x,\lambda) = \sum_{n=0}(1-x)^n\lambda^n\frac{\langle (n+1)_1|\chi|1_1\rangle}{\sqrt{(n+1)!}} \tag{B12}$$

contains only even powers up to quartic order. Its lowest-order term is determined by the equal-time current-correlation matrix $C(t=0) = v_{\text{th}}^2\langle 1_1|\chi|1_1\rangle$.

Transverse current correlations are even easier to evaluate with

$$\langle 1_2|U|m_1,1_2\rangle = \frac{(-\lambda)^{m_1}}{\sqrt{m_1!}} = \langle\vec{0}|U|m_1\rangle \quad , \tag{B13}$$

$$\langle m_1,1_2|U^{-1}|n_1,1_2\rangle = \langle m_1|U^{-1}|n_1\rangle \quad , \tag{B14}$$

$$\frac{\langle n_1,1_2|\chi|1_2\rangle}{\sqrt{n_1!}} = \frac{\langle (n+1)_1|\chi|1_1\rangle}{\sqrt{(n_1+1)!}} \quad . \tag{B15}$$

The result is

$$v_{\text{th}}^{-2}C_t(k,z) = -\sigma^{-1}(k,z)\int_0^1 dx e^{-\lambda^2(1-x)}x^{\zeta}P_4(x,\lambda) \quad . \tag{B16}$$

For the sake of completeness we also give the density correlation matrix

$$\langle\vec{0}|\phi(\vec{k},z)|\vec{0}\rangle = S(k,z) = -\sigma^{-1}(k,z)\int_0^1 dx\, e^{-\lambda^2(1-x)}x^{\zeta-1}\sum_{n=0}(1-x)^n\lambda^n\frac{\langle n_1|\chi|\vec{0}\rangle}{\sqrt{n!}} \quad , \tag{B17}$$

which can be obtained either directly from (B6) or, using the continuity equations, from $C_l(k,z)$.

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