Fluctuation and dissipation in classical many-particle systems

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Coarse-grained Langevin-type effective field equations are derived for classical systems of particles. These equations include the effects of thermal fluctuation and dissipation that may arise from coupling to an external bath, as in the Brownian motion of a single particle, or from statistical fluctuations in small parts of an isolated many-particle system, as in sound waves. These equations may provide some guidance for the analysis of mesoscopic or microscopic molecular systems or for systems of hundreds to thousands of subatomic particles produced in high-energy nuclear collisions.
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I. INTRODUCTION

The theoretical description of Brownian motion of a classical particle is well known and widely discussed; it is textbook material [1]. It is used in numerous practical applications, such as evaluating reaction rates at finite temperature in systems where thermal fluctuations are of vital importance [2–5]. Thermal fluctuations and the actual evaluation of fluctuating forces and dissipative coefficients for dense, interacting, classical many-particle systems is somewhat less known; early studies were done by Irving and Kirkwood [6], Green [7], and Mori [8]. Studies of nonlinear systems were initiated by Zwanzig [9].

We were originally motivated to do this study by the physics of nuclear collisions at high energy. In these collisions many subatomic particles are produced, mostly pions that are the main carrier of the nuclear force. The collision may be viewed as a miniature big bang where soon after impact a large amount of the initial translational energy is put into particle creation and entropy production. This system can be roughly characterized by a temperature. As time goes on, the system expands and cools. Eventually collisions become so infrequent that thermal equilibrium is lost and the particles stream freely to infinity and are detected. The properties of a system of pions, numbering in the hundreds or thousands, at high temperature may have very interesting properties. For example, pion fields transform under an internal symmetry group rather analogously to spins in a magnet. During the early stage of the expansion, when the temperature is high, the field may collectively point in a direction different from that in the surrounding vacuum. This is referred to as a disoriented chiral condensate (DCC) [11]. One would like to have coarse-grained field equations to describe the fluctuation and dissipation of DCC domains and their inevitable coalescence and evolution into the surrounding vacuum [12]. A good description is lacking.

Our goal here is to develop some understanding of the DCC problem by considering a collection of classical particles undergoing Brownian motion and generalizations of such. This might appear to be a simple problem, but there are subtle issues relating to the nature of what one considers the heat bath. For a single particle it is relatively straightforward; for a collection of particles it is not. In one limit, the particles of interest may each be coupled to an external heat bath, but they may also interact with each other via forces that are more slowly varying than the ones operative between the particles and the heat bath. In this case Langevin equations of motion can be obtained for time scales that are short compared to the interparticle interaction times but long compared to the interaction times with the heat bath. In another limit, there is no external heat bath; one averages over a macroscopically small but microscopically large number of neighboring particles and seeks a Langevin equation to describe the motion of these subsets of particles over times long compared to the force fluctuation times between subsets. In the real world there may be a continuum of interesting problems lying between these two extremes.

In the following sections we will analyze and contrast the two limiting cases outlined above. In both cases we will do coarse graining to obtain an effective field equation of motion in one and three dimensions. Phenomenological field equations have been found to be very useful in the study of dynamic critical phenomena in atomic and molecular systems [10].

II. EXTERNAL HEAT BATH

A. Recollection of simple Brownian motion

This case is discussed in many textbooks, such as [1], and often repeated in the literature, such as [13]. For a particle of mass m connected to a heat bath and moving under the influence of external potential fields, for example, a small object suspended in a fluid or gas in a gravitational field, and

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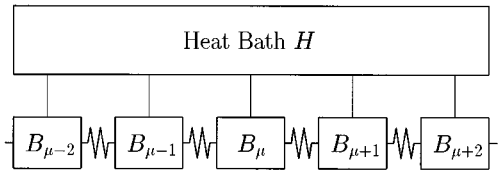

FIG. 1. Series of Brownian particles $B_{\mu-1}$, B_{μ}, $B_{\mu+1}$, ... interacting with a thermal heat bath H with random thermal forces $F_{\mu}(t)$ (thin lines) and with their nearest neighbors via conservative forces (heavy lines).

moving in one dimension, the generalized Langevin equation is

$$m\frac{dv(t)}{dt}=G(t)-\int_{-\infty}^{t}dt'K(t-t')v(t')+F'(t). \quad (1)$$

Here $v(t)$ is the velocity of the particle at time t. The force due to external fields is labeled by G. The force due to the heat bath has been separated into two parts: $F=\overline{F}+F'$, where F' represents the rapidly varying, random, part of the force whose average value is zero and $\overline{F}$ represents the slowly varying part whose average value is not necessarily zero. The separation of these two components depends on the coarse graining time chosen. To be a useful coarse graining, this time must be large compared to the characteristic correlation time $\tau_{\rm cor}$ of the force but small enough on an observational time scale to record the desired coarse-grained trajectory of the particle. For example, if the particle under consideration is immersed in a gas of much lighter particles, $\tau_{\rm cor}$ is the average time between collisions with the gas particles that define the heat bath. The friction kernel is

$$K(s)=\beta\langle F'(0)F'(s)\rangle, \quad (2)$$

where β is the inverse temperature of the heat bath (we use units with $k_B=1$ throughout) and the averaging is carried out with respect to the heat bath. This is referred to as a generalized Langevin equation; the normal Langevin equation is obtained in the approximation that $K(s)=2\alpha\delta(s)$. This may be considered as the limit of the somewhat more general case where

$$K(s)=\frac{\alpha}{\tau_{\rm cor}}\exp(-|s|/\tau_{\rm cor}). \quad (3)$$

Simple Brownian motion in more than one dimension is obvious.

B. Coupled Brownian particles

Consider a set of Brownian particles referred to as B_{μ}, which can move in one dimension and are in thermal interaction with a heat bath referred to as H; see Fig. 1. The thermal interaction is mediated by a fluctuating force $F_{\mu}(t)$, which has a mean period of $\tau_{\rm cor}$. This time $\tau_{\rm cor}$ characterizes the relaxation time needed for H to reestablish its equilibrium configuration if it is perturbed by some sudden small change. We assume that the conservative force connecting Brownian particles is slowly varying compared to $\tau_{\rm cor}$; we will study the change of position and velocity of the Brownian particles assuming that changes are small in a time interval $\tau>\tau_{\rm cor}$.

Suppose that at time t all B_{μ} are in thermal equilibrium with H. Consider a set of macroscopically similar systems forming an ensemble. Then the ensemble average of the fluctuating forces vanishes at this moment

$$\langle F_{\mu}(t)\rangle_0=0. \quad (4)$$

The subscript indicates that the average is taken in thermal equilibrium. Due to a change in the position or velocity of some B_{μ}, the force F_{μ} may change and our system, both B_{μ} and H, may deviate from thermal equilibrium. We have to evaluate this deviation.

Apart from the fluctuating random force $F_{\mu}(t)$ there is another slowly varying, not fluctuating, force $G_{\mu}(t)$. The forces connecting the Brownian particles are of this type. We will be interested in finding the corresponding slowly varying part of the velocity of each B_{μ}. Integrating the equation of motion $m\dot{v}_{\mu}=G_{\mu}(t)+F_{\mu}(t)$ for a short but macroscopic period of time τ, we get, in a particular microscopic configuration,

$$m[v_{\mu}(t+\tau)-v_{\mu}(t)]=G_{\mu}\tau+\int_{t}^{t+\tau}F_{\mu}(t')dt'. \quad (5)$$

Here we have taken into consideration that G_{μ} can be considered constant during the short period of time τ. The microscopic configurations are not under our control; we know only the ensemble average of similarly prepared systems. Taking the ensemble average of both sides of the above equation of motion we obtain

$$m\langle v_{\mu}(t+\tau)-v_{\mu}(t)\rangle=G_{\mu}\tau+\int_{t}^{t+\tau}\langle F_{\mu}(t')\rangle dt'. \quad (6)$$

In general, $\langle F_{\mu}(t')\rangle$ is not independent of the motion of B_{μ}; otherwise it would be always the same as the mean value $\langle F_{\mu}(t)\rangle_0=0$ in thermal equilibrium. We will evaluate the changes in $\langle F_{\mu}(t')\rangle$ following the lines of ([1] Sec. 15.7).

Let us consider the change during the time interval from t to $t+\tau'$. The velocity of B_{μ} changes from $v_{\mu}(t)$ to $v_{\mu}(t+\tau')$. The motion of this particle affects its environment. If τ' is small enough the mean force $\langle F_{\mu}\rangle$ changes, but still depends on its earlier value at t. If τ' exceeds $\tau_{\rm cor}$, the heat bath will reestablish its thermal equilibrium and will be found with equal probability in any of its Ω accessible states. Since the energy of the B_{μ} changes the energy of the heat bath changes as well. The total energy of the heat bath changes by

$$\Delta E(\tau')=\cdots+\Delta E_{\mu-1}(\tau')+\Delta E_{\mu}(\tau')+\Delta E_{\mu+1}(\tau')+\cdots, \quad (7)$$

where $\Delta E_{\mu}(\tau')$ is the energy *given* to the heat reservoir H *by* the particle B_{μ}. Since we consider small time increments only the local environment of B_{μ} is relevant. The number of other Brownian particles influencing the heat bath is not infinite, but extends to some distance comparable to the mean free path or the spatial correlation length. The number of states available to H changes from $\Omega(E_0)$ to

$\Omega(E_0+\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)$. This change of energy of the heat bath will influence the Brownian particles connected to it and modify the populations of microstates r in the ensemble corresponding to B_μ. We will use this information to estimate the change of the fluctuating thermal force acting on B_μ.

The equilibrium probability of the occurrence of a given microstate r for B_μ is proportional to the corresponding number of states available to the heat bath. Here we assume that the total number of microstates of all Brownian particles $B_{\mu-1}, B_\mu, B_{\mu+1}, \ldots$ together is negligibly small compared to the number of microstates of the heat reservoir. Now we can compare the probability distribution over the microstates $W_{r\mu}$ of B_μ at time t and τ' later:

$$\frac{W_{r\mu}(t+\tau')}{W_{r\mu}(t)}=\frac{W_{r\mu}(t+\tau')}{W^{(0)}_{r\mu}}$$
$$=\frac{\Omega(E_0+\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)}{\Omega(E_0)}$$
$$=\exp[\beta(\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)]. \tag{8}$$

Here $\beta\equiv\partial\ln\Omega/\partial E$ is the inverse temperature of the heat bath, assumed to be constant. This means that if more energy is made available to the heat bath the probability to populate a particular microstate r of B_μ increases. This is true even if that particular B_μ takes energy from the heat bath as long as its neighbors add more.

Now we can estimate how population probabilities change with time;

$$W_{r\mu}(t+\tau')$$
$$=W^{(0)}_{r\mu}\exp[\beta(\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)]$$
$$\approx W^{(0)}_{r\mu}[1+\beta(\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)]. \tag{9}$$

We can also evaluate how the ensemble average of the fluctuation force changes during this time interval:

$$\langle F_\mu(t+\tau')\rangle\equiv\sum_r W_{r\mu}(t+\tau')F_{r\mu}$$
$$\approx\sum_r W^{(0)}_{r\mu}[1+\beta(\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)]F_{r\mu}$$
$$=\langle[1+\beta(\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)]\ F_\mu\rangle_0. \tag{10}$$

Since the ensemble average of the fluctuating force vanishes for the thermal equilibrium distribution $W^{(0)}_{r\mu}$, the above expression for the fluctuation force reduces to

$$\langle F_\mu(t+\tau')\rangle=\beta\langle(\cdots+\Delta E_{\mu-1}+\Delta E_\mu+\Delta E_{\mu+1}+\cdots)F_\mu\rangle_0. \tag{11}$$

In this estimate the change of the energy of the heat bath is still undefined. This energy is, however, simply the negative of the work done by the fluctuating force on the Brownian particle B_ν:

$$\Delta E_\nu=-\int_t^{t+\tau'}F_\nu(t'')v_\nu(t'')dt''. \tag{12}$$

Inserting this expression into that for the fluctuating force we obtain

$$\langle F_\mu(t+\tau')\rangle=-\beta\int_t^{t+\tau'}dt''\langle F_\mu(t+\tau')F_\nu(t'')\rangle_0 v_\nu(t''). \tag{13}$$

We use the summation convention where a repeated index is summed over. In this case, the sum on ν runs over the neighbors of B_μ; it is cut off by the range of the forces and by the finite time interval. There is no need to do an ensemble averaging over the velocities because they are much more slowly varying than the fluctuating forces. Thus we have estimated the expectation value of the force F_μ for an ensemble, weakly deviating from a thermal equilibrium, via expectation values obtained in thermal equilibrium. This is, of course, just linear-response theory.

Now the equation of motion for the Brownian particle B_μ can be cast in the form

$$m\langle v_\mu(t+\tau)-v_\mu(t)\rangle=G_\mu\tau-\beta\int_t^{t+\tau}dt'\int_0^{t'-t}ds\langle F_\mu(t')\times F_\nu(t'-s)\rangle_0 v_\nu(t'-s). \tag{14}$$

The ensemble averaging in the expression for the interparticle force may be dropped because the coordinates change much more slowly than the velocities, which are again much more slowly varying than the fluctuating forces.

It is straightforward to perform the above derivation in three dimensions. The forces F_μ and velocities v_μ become three-dimensional vectors $F^i_{\boldsymbol{\mu}}$ and $v^i_{\boldsymbol{\mu}}$ with spatial indices labeled by roman letters and where the bold greek indices now label the position. The work done by particle $B_{\boldsymbol{\nu}}$ will contain the scalar product $v^j_{\boldsymbol{\nu}}F^j_{\boldsymbol{\nu}}$ of its velocity and the random force acting on it. Equation (14) takes the form

$$m\langle v^i_{\boldsymbol{\mu}}(t+\tau)-v^i_{\boldsymbol{\mu}}(t)\rangle=G^i_{\boldsymbol{\mu}}\tau-\beta\int_t^{t+\tau}dt'\int_0^{t'-t}ds\langle F^i_{\boldsymbol{\mu}}(t')\times F^j_{\boldsymbol{\nu}}(t'-s)\rangle_0 v^j_{\boldsymbol{\nu}}(t'-s). \tag{15}$$

The friction kernel is proportional to the correlation function of the random fluctuating force:

$$K^{ij}_{\boldsymbol{\mu\nu}}(s)\equiv\beta\langle F^i_{\boldsymbol{\mu}}(t)F^j_{\boldsymbol{\nu}}(t-s)\rangle_0. \tag{16}$$

Here it is assumed that this function is time translation invariant, as is normally the case in thermal equilibrium. This assumption can be relaxed. We will discuss the properies of time translationally invariant correlation functions a little later.

Now it is useful to separate the fluctuating force into two components. The first component is just the average value of the fluctuating force in the slightly out of equilibrium ensemble:

$$\overline{F^i}_{\boldsymbol{\mu}}(t) = -\int_t^{t+\tau}\frac{dt'}{\tau}\int_0^{t'-t} ds\ K^{ij}_{\boldsymbol{\mu\nu}}(s)\ \ v^j_{\boldsymbol{\nu}}(t'-s). \quad (17)$$

It leads to a damping of the velocity. Note that the right-hand side of this expression involves averages defined with respect to the unperturbed thermal ensemble. We note that the integrand is appreciable only when $s \ll \tau$ because the coarse-graining time τ was chosen to be much bigger than the correlation time of the random forces. The velocity is slowly varying and so it may be evaluated with t replacing t'. [This is just the first term in a Taylor series expansion: $v(t'-s) = v(t-s) + (t'-t)\dot{v}(t-s) + \cdots$.] The upper limit of the s integral may then be sent to infinity yielding the approximation

$$\overline{F^i}_{\boldsymbol{\mu}}(t) = -\int_0^{\infty} ds\ K^{ij}_{\boldsymbol{\mu\nu}}(s) v^j_{\boldsymbol{\nu}}(t-s). \quad (18)$$

The nonlocality reflects the time delay between the motion of the particles and the responding force.

The second component is the most rapidly fluctuating part and is defined by its zero average with respect to the actual out of equilibrium ensemble:

$$F'^{\,i}_{\boldsymbol{\mu}}(t) \equiv F^i_{\boldsymbol{\mu}}(t) - \overline{F^i}_{\boldsymbol{\mu}}(t). \quad (19)$$

The equation of motion including both the drift and the fluctuating parts of the velocity is

$$m\frac{dv^i_{\boldsymbol{\mu}}(t)}{dt} = G^i_{\boldsymbol{\mu}} - \int_0^{\infty} ds\ K^{ij}_{\boldsymbol{\mu\nu}}(s) v^j_{\boldsymbol{\nu}}(t-s) + F'^{\,i}_{\boldsymbol{\mu}}(t). \quad (20)$$

In this analysis the stochastic forces of the external heat bath act on every Brownian particle the same way. The correlation between two forces $K^{ij}_{\boldsymbol{\mu\nu}}(s)$ under normal circumstances is expected to decrease with increasing distance between Brownian particles $B_{\boldsymbol{\mu}}$ and $B_{\boldsymbol{\nu}}$ and with the time difference s. The summation over the neighbors $\boldsymbol{\nu}$ of $B_{\boldsymbol{\mu}}$ extends to infinity in all directions; however, the contribution of more and more distant neighbors is expected to be rapidly decreasing.

C. Continuum limit

Rather than attempting to solve the equations of motion for a macroscopic number of particles it is often useful to approximate them by a continuous medium. This is effectively coarse graining and is accurate so long as the length scales of interest are large enough and the time scales of interest long enough. With this in mind, let us replace the discrete particle labels $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$ with continuous position variables $\mathbf{x}$ and $\mathbf{y}$. Displacement of the particles in the gas will be denoted by $\eta^i(\mathbf{x},t)$. The sum over particle index is replaced by an integral over position. Divide both sides of Eq. (20) by the average volume v_0 per particle. The mass density is $\rho \equiv m/v_0$. Forces per particle then become forces per unit volume and are denoted by a lowercase letter. The Langevin equation then becomes

$$\rho\ \ddot{\eta}^i(\mathbf{x},t) = g^i(\mathbf{x},t) - \int d^3y \int_0^{\infty} ds\ k^{ij}(\mathbf{y},s)\,\dot{\eta}^j(\mathbf{x}-\mathbf{y},t-s) + f'^{\,i}(\mathbf{x},t). \quad (21)$$

Here

$$k^{ij}(\mathbf{y},s) = \beta\langle f^i(\mathbf{x},t) f^j(\mathbf{x}-\mathbf{y},t-s)\rangle_0 \quad (22)$$

is the correlation function for the force densities of the heat bath.

If the medium is isotropic then the friction kernel must have the tensorial structure

$$k^{ij}(\mathbf{y},s) = k_L(y,s)\hat{y}^i\hat{y}^j + k_T(y,s)(\delta^{ij} - \hat{y}^i\hat{y}^j), \quad (23)$$

where $y = |\mathbf{y}|$ and k_L and k_T are longitudinal and transverse correlation functions. When we are interested in lengths greater than those characterizing the friction kernel we can evaluate the velocity at position $\mathbf{x}$ and take it past the y integration. (More generally, $\dot{\boldsymbol{\eta}}$ would be expanded in a Taylor series about $\mathbf{y} = \mathbf{0}$.) Carrying out the averaging over angles gives

$$\rho\,\ddot{\boldsymbol{\eta}}(\mathbf{x},t) = \mathbf{g}(\mathbf{x},t) - \int_0^{\infty} ds\ \ \dot{\boldsymbol{\eta}}(\mathbf{x},t-s) \times \int d^3y \left(\frac{1}{3}k_L(y,s) + \frac{2}{3}k_T(y,s)\right) + \mathbf{f}'(\mathbf{x},t). \quad (24)$$

Usually it happens that correlations fall off exponentially. Then the friction kernel may be parametrized by correlation times, correlation lengths, and strengths:

$$k_L(y,s) = \beta\langle f_L^2\rangle \exp(-s/\tau_L - y/\lambda_L),$$
$$k_T(y,s) = \beta\langle f_T^2\rangle \exp(-s/\tau_T - y/\lambda_T). \quad (25)$$

When our interest is in times greater than those characterizing the friction kernel and when the actual displacement velocity is slowly varying on those scales we can take the velocity outside the s integration to obtain

$$\rho\ \ddot{\boldsymbol{\eta}}(\mathbf{x},t) = \mathbf{g}(\mathbf{x},t) - \rho\gamma\dot{\boldsymbol{\eta}}(\mathbf{x},t) + \mathbf{f}'(\mathbf{x},t), \quad (26)$$

where the damping constant is $\gamma = \frac{1}{3}\gamma_L + \frac{2}{3}\gamma_T$ with

$$\gamma_L = \frac{\langle f_L^2\rangle}{\rho T}\int_0^{\infty} ds \int d^3y\ \exp(-s/\tau_L - y/\lambda_L) = 4\pi\Gamma(3)\frac{\langle f_L^2\rangle \tau_L \lambda_L^3}{\rho T} \quad (27)$$

and a similar expression for γ_T. This is a manifestation of the fluctuation-dissipation theorem.

The interesting feature of this Langevin field equation is that the damping term is linear in the displacement velocity. This is the form that is normally used in phenomenological

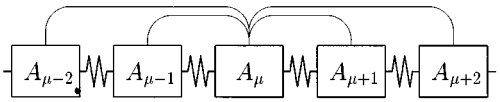

FIG. 2. Series of small subsystems $A_{\mu-1}, A_{\mu}, A_{\mu+1}, \ldots$ interacting with each other via random thermal forces (thin lines). The random forces are classified into the nearest neighbor $F_{\mu}^{(1)}(t)$, next-nearest neighbor $F_{\mu}^{(2)}(t), \ldots,$ and so on. In addition, each subsystem interacts with its nearest neighbors via conservative forces (heavy lines) too.

settings. However, this is certainly not the most general Langevin field equation for the displacement, as may be observed from the truncation of the Taylor expansion in **y** and as we shall see in the next section.

III. INTERNAL HEAT BATH

In this section we remove the external heat bath and group all the particles of the system into small subsystems labeled A_{μ}. Focusing our attention on one subsystem we can think of the all the remaining ones as constituting a heat bath. There will be forces acting among these subsystems as sketched in Fig. 2 These forces can be separated into a part that is rapidly varying on the time scale of interest and a part that is slowly varying.

First consider a one-dimensional system. During a particular time interval of duration τ there will be a net momentum transfer $p_{\mu-1,\mu}$ from $A_{\mu-1}$ to A_{μ} and a net momentum transfer $p_{\mu,\mu+1}$ from A_{μ} to $A_{\mu+1}$ due to the random forces. The net force experienced by A_{μ} due to these is

$$F_{\mu}^{(1)}(t)=\frac{p_{\mu-1,\mu}-p_{\mu,\mu+1}}{\tau}. \tag{28}$$

The averaged equation of motion is just like Eq. (14) except that now the force F originates in the intersubsystem interactions, not with an external heat bath. We make the assumption that there are no correlations between random momentum transfers involving different pairs of subsystems. That is,

$$\langle p_{\mu,\mu+1}(t)p_{\nu,\nu+1}(t-s)\rangle_0=T\tau^2K^{(1)}(s)\delta_{\mu,\nu}, \tag{29}$$

where as before $K^{(1)}(s)$ is expected to fall exponentially with s. Substitution into the equation of motion gives

$$m\langle v_{\mu}(t+\tau)-v_{\mu}(t)\rangle = G_{\mu}\tau+\int_t^{t+\tau}dt'\int_0^{t'-t}ds[v_{\mu+1}(t'-s) -2v_{\mu}(t'-s)+v_{\mu-1}(t'-s)]K^{(1)}(s). \tag{30}$$

Here each subsystem has been assumed to have the same mass m for simplicity.

Next we should allow for the possibility of random forces acting between next-to-nearest neighbors. The arguments exactly parallel those for nearest neighbors. The force is

$$F_{\mu}^{(2)}(t)=\frac{p_{\mu-2,\mu}-p_{\mu,\mu+2}}{\tau}. \tag{31}$$

The correlation functions are

$$\langle p_{\mu,\mu+2}(t)p_{\nu,\nu+2}(t-s)\rangle_0=T\tau^2K^{(2)}(s)\delta_{\mu,\nu}. \tag{32}$$

This may be continued for next-to-next-to-nearest neighbors *ad infinitum*. The averaged equation of motion, taking all of them into account, is

$$m\langle v_{\mu}(t+\tau)-v_{\mu}(t)\rangle = G_{\mu}\tau+\int_t^{t+\tau}dt'\int_0^{t'-t}ds \times\sum_{\sigma=1}^{\infty}[v_{\mu+\sigma}(t'-s)-2v_{\mu}(t'-s) +v_{\mu-\sigma}(t'-s)]K^{(\sigma)}(s). \tag{33}$$

The function $K^{(\sigma)}(s)$ undoubtedly decreases rapidly with increasing σ.

In taking the continuum limit we replace the subsystem labels μ and σ with position coordinates x and y, respectively. We divide the equation by the average length l_0 of each subsystem. The sum over σ gets replaced by an integral over y:

$$\rho\langle v(x,t+\tau)-v(x,t)\rangle = g(x,t)\tau+\int_t^{t+\tau}dt'\int_0^{t'-t}ds\int_0^{\infty}dy\ k(y,s) \times[v(x+y,t'-s)-2v(x,t'-s)+v(x-y,t'-s)]. \tag{34}$$

Here $k(y,s)$ is the continuation of $K^{(\sigma)}(s)/l_0^2$. Generally, the velocity will be more slowly varying with position than the correlation function characterizing the random forces. If that is so, then the difference $v(x+y,t'-s)-2v(x,t'-s)+v(x-y,t'-s)$ is well approximated by $y^2\partial_x^2v(x,t'-s)$. Then

$$\rho\langle v(x,t+\tau)-v(x,t)\rangle = g(x,t)\tau+\int_t^{t+\tau}dt'\int_0^{t'-t}ds\ \partial_x^2v \times(x,t'-s)\int_0^{\infty}dy\ y^2k(y,s). \tag{35}$$

To obtain a Langevin equation we proceed as before. Divide through by τ, replace t' with t in the argument of the velocity on the right-hand side, let the upper limit on the s integration go to infinity, and denote the displacement by the variable $\eta(x,t)$:

$$\rho\ddot{\eta}(x,t)=g(x,t)+\int_0^{\infty}ds\ \partial_x^2\dot{\eta}(x,t-s)\int_0^{\infty}dy\ y^2k(y,s) +f'(x,t). \tag{36}$$

The rapidly fluctuating force per unit length f' is the deviation from the average value in the perturbed system. It is constructed by taking the continuum limit of the sum of random forces acting on the subsystem minus the average of

those forces, similar to Eq. (19). The average is just the second term on the right-hand side of Eq. (36):

$$\frac{1}{l_0}\sum_{\sigma=1}^{\infty} F_\mu^{(\sigma)}(t)-\overline{f}(x,t)\to f'(x,t). \tag{37}$$

In general, it is difficult to find a simple closed expression for f'. One way is to generate it from knowledge of the correlation functions such as Eqs. (29) and (32).

When our interest is on times and lengths greater than those characterizing the friction kernel and when the actual displacement velocity is slowly varying on those scales we can take the velocity outside the integration to obtain

$$\rho\,\ddot{\eta}(x,t)=g(x,t)+\gamma^*\partial_x^2\dot{\eta}(x,t)+f'(x,t), \tag{38}$$

where

$$\gamma^*=\int_0^\infty ds\int_0^\infty dy\; y^2 k(y,s). \tag{39}$$

The essential difference between this equation and the one for an external heat bath is the second space derivative acting on the velocity, which is absent in the latter case. The origin is translational invariance. The external heat bath imposes a particular frame of reference, whereas the absence of an external heat bath means that the system must be invariant under boosts of constant velocity.

The generalization to more than one spatial dimension is straightforward. We assume that random momentum transfers between different pairs of subsystems are uncorrelated and that the system is rotationally invariant, for simplicity:

$$\langle p^i_{\boldsymbol{\mu},\boldsymbol{\mu}+\boldsymbol{\sigma}}(t')p^j_{\boldsymbol{\nu},\boldsymbol{\nu}+\boldsymbol{\rho}}(t'-s)\rangle_0=T\tau^2\delta_{\boldsymbol{\mu},\boldsymbol{\nu}}\delta_{\boldsymbol{\sigma},\boldsymbol{\rho}}K_{ij}^{(\boldsymbol{\sigma})}(s). \tag{40}$$

This can be used to calculate the force-force correlation function

$$\begin{aligned}\beta\langle F^i_{\boldsymbol{\mu}}(t')F^j_{\boldsymbol{\nu}}(t'-s)\rangle_0&=\beta\sum_{\boldsymbol{\sigma},\boldsymbol{\rho}}\langle F^{(\boldsymbol{\sigma})i}_{\boldsymbol{\mu}}(t')F^{(\boldsymbol{\rho})j}_{\boldsymbol{\nu}}(t'-s)\rangle_0\\&=\sum_{\boldsymbol{\sigma}}(2\delta_{\boldsymbol{\mu},\boldsymbol{\nu}}-\delta_{\boldsymbol{\mu}+\boldsymbol{\sigma},\boldsymbol{\nu}}-\delta_{\boldsymbol{\mu}-\boldsymbol{\sigma},\boldsymbol{\nu}})K_{ij}^{(\boldsymbol{\sigma})}(s).\end{aligned} \tag{41}$$

The sum over $\boldsymbol{\sigma}$ runs from $\sigma_1,\sigma_2,\sigma_3=1$ to ∞, and similarly for $\boldsymbol{\rho}$, in order not to double count the number of pairs. Then

$$\begin{aligned}-\beta\langle F^i_{\boldsymbol{\mu}}(t')F^j_{\boldsymbol{\nu}}(t'-s)\rangle_0 v^j_{\boldsymbol{\nu}}(t'-s)&\\=\sum_{\boldsymbol{\sigma}}[v^j_{\boldsymbol{\mu}+\boldsymbol{\sigma}}(t'-s)-2v^j_{\boldsymbol{\mu}}(t'-s)&\\+v^j_{\boldsymbol{\mu}-\boldsymbol{\sigma}}(t'-s)]K_{ij}^{(\boldsymbol{\sigma})}(s).&\end{aligned} \tag{42}$$

This leads to an equation of motion similar to Eq. (33) with spatial indices i and j in the appropriate places and with the scalars μ and σ replaced with location vectors $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$.

We take the continuum limit in the usual way:

$$\begin{aligned}\rho\langle v^i(\mathbf{x},t+\tau)-v^i(\mathbf{x},t)\rangle&\\=g^i(\mathbf{x},t)\tau+\int_t^{t+\tau}dt'\int_0^{t'-t}ds\int_0^\infty dy_1dy_2dy_3k^{ij}(\mathbf{y},s)&\\\times[v^j(\mathbf{x}+\mathbf{y},t'-s)-2v^j(\mathbf{x},t'-s)+v^j(\mathbf{x}-\mathbf{y},t'-s)].&\end{aligned} \tag{43}$$

Because of rotational symmetry, the kernel k has the same structure as in Eq. (23). Expand the velocity to second order in $\mathbf{y}$ and integrate over all directions of $\mathbf{y}$:

$$\begin{aligned}\rho\langle v^i(\mathbf{x},t+\tau)-v^i(\mathbf{x},t)\rangle&\\=g^i(\mathbf{x},t)\tau+\frac{1}{120}\int_t^{t+\tau}dt'\int_0^{t'-t}ds\nabla^2v^i(\mathbf{x},t'-s)&\\\times\int d^3y\; y^2[k_L(y,s)+4k_T(y,s)]&\\+\frac{1}{60}\int_t^{t+\tau}dt'\int_0^{t'-t}ds\,\partial_i\nabla\cdot\mathbf{v}(\mathbf{x},t'-s)&\\\times\int d^3y\; y^2[k_L(y,s)-k_T(y,s)].&\end{aligned} \tag{44}$$

Here $y\equiv|\mathbf{y}|$. Converting this to a Langevin equation in the now familiar way, we get

$$\begin{aligned}\rho\,\ddot{\boldsymbol{\eta}}(\mathbf{x},t)=\mathbf{g}(\mathbf{x},t)+\frac{1}{60}\int_0^\infty ds\nabla[\nabla\cdot\dot{\boldsymbol{\eta}}(\mathbf{x},t-s)]&\\\times\int d^3y\; y^2[k_L(y,s)-k_T(y,s)]&\\+\frac{1}{120}\int_0^\infty ds\nabla^2\dot{\boldsymbol{\eta}}(\mathbf{x},t-s)&\\\times\int d^3y\; y^2[k_L(y,s)+4k_T(y,s)]+\mathbf{f}'(\mathbf{x},t).&\end{aligned} \tag{45}$$

The rapidly fluctuating force $\mathbf{f}'$ may be constructed along the same lines as in one dimension.

In the very-low-frequency limit the velocities can be evaluated at time t and taken past the s integral. The Langevin equation then reduces to the Navier-Stokes equation

$$\rho\frac{d\mathbf{v}}{dt}=-\nabla P+\eta\nabla^2\mathbf{v}+\left(\zeta+\frac{1}{3}\eta\right)\nabla(\nabla\cdot\mathbf{v}) \tag{46}$$

with the addition of the rapidly fluctuating force. By comparison we can determine the shear (η) and bulk (ζ) viscosities

$$\eta=\frac{1}{120}\int_0^\infty ds\int d^3y\ y^2(4k_T+k_L),$$

$$\zeta=\frac{1}{72}\int_0^\infty ds\int d^3y\ y^2(k_L-2k_T). \tag{47}$$

The requirement that the viscosities must be non-negative places a restriction on the relative magnitudes of the moments of the longitudinal and transverse correlation functions.

IV. COMPARISON OF FIELD EQUATIONS AND CONCLUSION

An isotropic gas or liquid can be fully described by a scalar density $\phi\equiv-\nabla\cdot\boldsymbol{\eta}$ characterizing the local relative compression of the matter. The Langevin equation for the cases of external and of internal heat baths can be expressed in terms of ϕ alone without any reference to a vector displacement. But first we should inquire about the effective Lagrangian describing this field in the absence of dissipation and fluctuation.

A real scalar field has the Lagrangian density

$$\mathcal{L}_0=\frac{1}{2}\dot{\phi}^2-\frac{c^2}{2}(\nabla\phi)^2-V(\phi), \tag{48}$$

where $V(\phi)$ is a potential, usually a polynomial. This Lagrangian density does not contain the fluctuations or any dissipative term. For example, if $V=0$ then this describes undamped sound waves with speed c. The equation of motion is

$$\ddot{\phi}=c^2\nabla^2\phi-\partial V(\phi)/\partial\phi. \tag{49}$$

Here we may identify $-\nabla\cdot\mathbf{g}/\rho$ with the right-hand side of Eq. (49). The influence of fluctuations can be included by adding to the Lagrangian density

$$\mathcal{L}_{\rm fluc}=-b'(\mathbf{x},t)\phi. \tag{50}$$

The fluctuating field b' is simply identified with $-\nabla\cdot\mathbf{f}'/\rho$ in both the external and internal heat bath systems. The nature of this stochastic field is determined by the microscopic dynamics of the system expressed in terms of its original degrees of freedom. The frictional term cannot, of course, be written as an additional term in the Lagrangian. It must be added by hand to the equation of motion.

Including the dissipative and the fluctuating terms, the Langevin field equation for an external heat bath is

$$\ddot{\phi}(\mathbf{x},t)=c^2\nabla^2\phi(\mathbf{x},t)-\partial V(\phi)/\partial\phi-\gamma\dot{\phi}(\mathbf{x},t)+b'(\mathbf{x},t), \tag{51}$$

where γ was discussed in Sec. II C. For the internal heat bath

$$\ddot{\phi}(\mathbf{x},t)=c^2\nabla^2\phi(\mathbf{x},t)-\partial V(\phi)/\partial\phi+\gamma^*\nabla^2\dot{\phi}(\mathbf{x},t)+b'(\mathbf{x},t), \tag{52}$$

where

$$\gamma^*=\frac{1}{120\rho}\int_0^\infty ds\int d^3y\ y^2[3k_L(y,s)+2k_T(y,s)]. \tag{53}$$

This is obtained under the assumption that the variation in ϕ is minor during the correlation times of k_L and k_T.

It is important to appreciate the difference between the external and internal heat baths. With an external heat bath there is a preferred frame of reference. The random forces couple individual Brownian particles to the heat bath; it is assumed that there are no random forces between Brownian particles. With an internal heat bath there is no preferred frame of reference. The random forces couple different subsystems. This difference is the origin of the Laplacian in Eq. (52), which is what really distinquishes the two field equations. In fact, if we desired a more fine-grained description we should expand the velocities in Eqs. (15) and (43) to higher order in spatial and temporal variations. The resulting field equation will involve dissipation of the form

$$\sum_{i,j=1}^{\infty}\Gamma_{ij}(\nabla^2)^{i-1}\left(\frac{\partial}{\partial t}\right)^j\phi(\mathbf{x},t). \tag{54}$$

Translational invariance demands that $\Gamma_{1j}=0$. All the coefficients can be determined in terms of moments of the friction kernel. Generally, we would expect that only the first few terms in the sum are required for a good description of a coarse-grained system.

Of course, in realistic situations it is always a matter of judgement whether there is a clear case of external or internal heat bath. It is possible to have different components in the system, where part of this system can be considered as internal while the rest is external. Usually the external heat bath is chosen to be dominant, but this is not necessarily the case and mixed cases may come up in realistic studies.

Although it is not our intention to apply these results to any particular problems in this paper, it is instructive to consider one example. Let $V(\phi)=0$ and look for plane-wave solutions in the absence of significant fluctuations. Denoting the frequency of the wave by ω and the wave vector by q we obtain the dispersion relation

$$\omega=\sqrt{c^2q^2-\gamma^2/4}-i\gamma/2 \tag{55}$$

for the external heat bath and

$$\omega=\sqrt{c^2q^2-\gamma^{*\,2}q^4/4}-i\gamma^*q^2/2 \tag{56}$$

for the internal heat bath. For a real wave vector the frequency in each case has an imaginary part resulting in damping of the wave. Note that for the external heat bath the wave becomes overdamped for wave vectors less than $\gamma/2c$. This is certainly not representative of sound waves in the atmosphere. For the internal heat bath the damping goes to zero as q^2, resulting in the absence of dissipation in this limit so that $\omega\to cq$. This dispersion relation is the same as that obtained for damped sound waves in a gas or liquid by solution of viscous hydrodynamics [14].

In summary, we have derived (in some sense) coarse-grained Langevin-type effective field equations based on the classical dynamics of systems of many particles. We considered two extreme limits: one where the stochastic

forces arose from coupling to an external heat bath and the other where the stochastic forces arose from statistical fluctuations in small parts of the full system. The obvious next steps are to consider quantum-mechanical effects and to apply these results to real atomic, molecular, or nuclear systems.

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