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Ehrenfest's argument extended to a formalism of nonequilibrium thermodynamics

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A general method of constructing dissipative equations is developed, following Ehrenfest's idea of coarse graining. The approach resolves the major issue of discrete time coarse graining versus continuous time macroscopic equations. Proof of the H theorem for macroscopic equations is given, several examples supporting the construction are presented, and generalizations are suggested.

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I. INTRODUCTION

In their seminal paper [1], P. and T. Ehrenfest have given an argument on how irreversibility can be derived from reversible dynamics. Ehrenfest's consideration was based on two important notions: Coarse graining (replacement of a continuous distribution function by a set of averaged values over a system of phase cells), and the H curve (a sequence of values that the entropy takes in the course of a discrete time marching over coarse-grained states). The impact of Ehrenfest's ideas on the long-standing discussions of the foundations of nonequilibrium thermodynamics is enormous [2]. However, to the best of our knowledge, Ehrenfest's approach has never been systematically exploited for the purpose of practical derivations of macroscopic equations. It is the goal of this paper to extend Ehrenfest's argument to a simple and general formalism for such derivations. Starting point of our consideration is the well known quasiequilibrium approximation that, for the sake of completeness, is discussed briefly below. Next, a formalization of Ehrenfest's argument is given. It resolves the major issue, namely, the coarse graining is the discrete time process while the macroscopic dynamics is continuous in time. In most of the earlier approaches based on a coarse graining, transition to the continuous time dynamics is done by introducing much larger time scales. Here we demonstrate that it is possible to reconstruct uniquely the macroscopic dynamics within the time interval between the coarse-graining events. This reconstruction is the main result of our paper, and it leads to a simple formalism in a rather straightforward way. Several examples are considered in order to illustrate the construction. Finally, we discuss how the suggested formalism is related to other well known methods of nonequilibrium thermodynamics, as well as some generalizations.

II. QUASIEQUILIBRIUM APPROXIMATION FOR CONSERVATIVE DYNAMICS

Let us consider a conservative dynamics given by an equation,

$$\dot{f}=J(f), \tag{1}$$

where $f(x,t)$ is the distribution function over the phase space variables x at the time t, and where operator J may be linear or nonlinear. Conservation is understood in the following sense: There exists a concave functional $S(f)$ (the entropy) whose values do not change along solutions to Eq. (1), $\dot{S}\equiv\langle DS(f)|J(f)\rangle=0$, for any f. Here $DS(f)$ is the first differential of S in the state f, and angle brackets denote scalar multiplication. Concavity of S means that the second differential $D^2S(f)$ defines a nonpositive definite quadratic form in each state f. A typical example of dynamics (1) is the Liouville equation for classical particles, and S is the Gibbs-Shannon entropy functional.

Let $M(f)=\{M_k(f)\}$ be a set of linear functionals, where $M_k(f)=\langle m_k|f\rangle$. Values of functionals M are called the macroscopic variables. The quasiequilibrium approximation $f^*(M)$ maximizes the entropy subject to fixed values of M (due to concavity of the entropy, if such a maximizer exists, then it is unique). Dynamics of macroscopic variables in the quasiequilibrium approximation is given by equations,

$$\dot{M}_k=\langle m_k|J^*\rangle. \tag{2}$$

Here $J^*\equiv J(f^*(M))$ is the right hand side of Eq. (1) evaluated in the quasiequilibrium. In the sequel we skip the label of the macroscopic variables k. The quasiequilibrium approximations do not change the type of dynamics: Conservation of the entropy in the microscopic dynamics implies conservation of the macroscopic entropy, $S^*(M)=S(f^*(M))$, in the quasiequilibrium dynamics (2). Quasiequilibrium approximations to the Liouville equation are nondissipative. In the case of the Gibbs-Shannon entropy, the use of quasiequilibrium approximations has been stressed by Jaynes in his well known works [3]. At present, the usefulness of quasiequilibrium approximations is well understood both for entropy-conserving dynamics [4], as well as for the dissipative dynamics [5–7]. Relatively less studied remains the case of open or externally driven systems, where invariant quasiequilibrium manifolds may become unstable [8].

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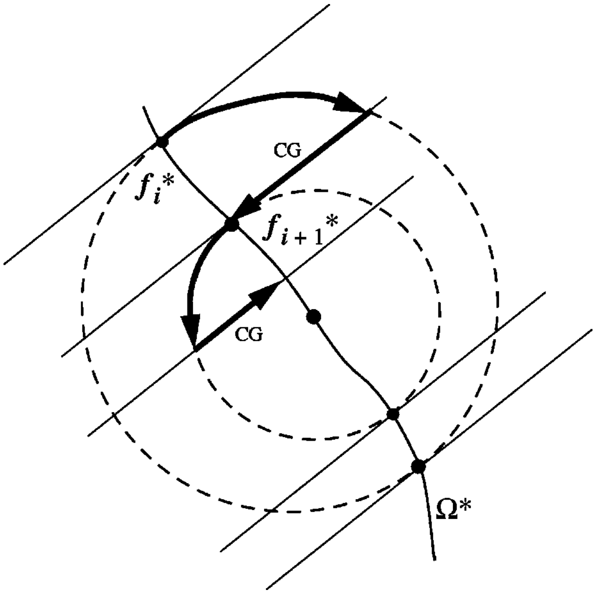

FIG. 1. Entropy-conserving dynamics with periodic coarse graining. The dashed convex curves represent the levels of the entropy. Each straight solid line represents the plane that contains all states with the fixed values of macroscopic parameters. The values of macroscopic parameters are different on different planes. The points where the planes touch levels of the entropy are the quasiequilibrium states. The totality of these tangent points makes up the quasiequilibrium manifold Ω^*. Curved arrows represent the microscopic solutions, straight arrows (CG) represent the coarse-graining.

III. EXTENDED EHRENFEST'S ARGUMENT

Let us now consider an extension of the quasiequilibrium dynamics in order to introduce dissipation. This is achieved by the periodic coarse graining of the microscopic solution with the fixed time step $\tau > 0$. Specifically, a sequence of quasiequilibrium states f^*_s is constructed as the iteration of the following three steps: First, taking the quasiequilibrium state f^*_s as the initial condition to Eq. (1), the solution $f_s(\tau) = T_\tau f^*_s$ is found, where T_τ is the formal solution operator of the Eq. (1). Second, the macroscopic variables M are evaluated with the microscopic solution $f_s(\tau)$ to get $M_{s+1} = \langle m | T_\tau f^*_s \rangle$. Third, the $(s+1)$th quasiequilibrium is defined as

$$f^*_{s+1} = f^*(\langle m | T_\tau f^*_s \rangle). \tag{3}$$

The procedure is then iterated. Periodic coarse graining just described is sufficient to introduce irreversibility, and to prove the discrete-time H theorem: Quasiequilibrium states f^*_s form the Ehrenfest's H curve; if the quasiequilibrium approximation is not the solution to the microscopic dynamics, then the values of the macroscopic entropy *strictly* increase along the H curve, $S^*(M_{s+1}) > S^*(M_s)$. The latter statement is a direct implication of the convexity of the entropy function, and of the noninvariance of the quasiequilibrium approximation with respect to the microscopic dynamics, and it is visualized in Fig. 1.

However, Eq. (3) as it stands does not solve yet the problem of derivation of the macroscopic equations. Indeed, the coarse graining is implemented within a discrete time picture, and the coarse-graining time τ must be finite. Therefore, continuous time equations for macroscopic variables need to be specified by an additional construction, which is the main goal of our paper.

IV. CONSTRUCTION OF THE MACROSCOPIC DYNAMICS

We seek equations for the macroscopic variables in the form,

$$\dot{M} = R(M, \tau), \tag{4}$$

where functions R are yet unknown. They are derived from the requirement that solutions to Eq. (4) with the initial condition $M(t_s)$ coincide at the time $t_s + \tau$ with the macroscopic variables evaluated at the site f^*_{s+1} of the H curve, *to a given accuracy* $O(\tau^n)$, for every $t_s = s\tau$, and for every initial quasiequilibrium condition. This requirement is written as

$$M^{(n)}(t_s + \tau) - \langle m | T^{(n)}_\tau f^*_s \rangle = O(\tau^{n+1}), \tag{5}$$

where the first term is evaluated using an approximation of the macroscopic equation (4), while the second term is evaluated using the corresponding approximation to the microscopic solution. Polynomial approximations employed for this purpose result in a system of recurrently solvable equations. Let us construct explicitly the first two iterations.

The first-order accuracy in Eq. (5) requires only the zero-order accuracy for the function R, and we write $R = R^{(0)}(M) + O(\tau)$. From Eq. (4) and from Eq. (3) it follows, respectively (in order to save notations, we write t instead of t_s),

$$M^{(1)}(t+\tau) = M + \tau R^{(0)} + O(\tau^2),$$

$$\langle m | T^{(1)}_\tau f^* \rangle = M + \tau \langle m | J^* \rangle + O(\tau^2). \tag{6}$$

From Eq. (5) it follows that $R^{(0)} = \langle m | J^* \rangle$. That is, to the lowest order of our construction, the macroscopic dynamics (4) is the quasiequilibrium approximation (2). On the next order, $R = R^{(0)} + \tau R^{(1)} + O(\tau^2)$. By the same pattern,

$$M^{(2)}(t+\tau) = M + \tau R^{(0)} + \tau^2 R^{(1)} + \frac{\tau^2}{2} D_M R^{(0)} \cdot R^{(0)} + O(\tau^3),$$

$$\langle m | T^{(2)}_\tau f^* \rangle = M + \tau \langle m | J^* \rangle + \frac{\tau^2}{2} \langle m | DJ^* \cdot J^* \rangle + O(\tau^3). \tag{7}$$

Here DJ^* is the first differential of the vector field J in the quasiequilibrium, while $D_M R^{(0)}$ is the first differential of the quasiequilibrium vector field with respect to macroscopic variables, and $\cdot$ denote action of corresponding linear operators. Thus,

$$R^{(1)} = \frac{1}{2} [\langle m | DJ^* \cdot J^* \rangle - D_M \langle m | J^* \rangle \cdot \langle m | J^* \rangle]. \tag{8}$$

Higher order approximations are constructed recurrently in entirely the same way. They involve higher order and cross products of differentials of the microscopic vector field and of the macroscopic vector field of lower order approximations. Thus, the macroscopic vector field R in the continuous time Eq. (4) is uniquely constructed as a sequence of polynomial approximations, $R_{(n)}(M,\tau)=\sum_{m=0}^{n}\tau^m R^{(m)}(M)$. This is the main result of our paper: *The macroscopic dynamics is uniquely reconstructed from the condition of matching the microscopic and the macroscopic dynamics at the points of coarse graining.*

The most important consequence of the above construction is that resulting continuous time macroscopic equations retain the dissipation property of the discrete time coarse graining on each order of approximation $n\geqslant 1$. Let us first consider the entropy production formula for the first-order approximation. In order to shorten notations, it is convenient to introduce the quasiequilibrium projection operator, $P^*g=D_M f^*\cdot\langle m|g\rangle$. Direct computation demonstrates that the entropy production, $\dot{S}^*_{(1)}=D_M S^*\cdot[R^{(0)}+\tau R^{(1)}]$, equals

$$\dot{S}^*_{(1)}=-\frac{\tau}{2}\langle(1-P^*)J^*|D^2S^*|(1-P^*)J^*\rangle, \qquad (9)$$

where $D^2S^*=D^2S|_{f=f^*}$ is the second differential of the entropy evaluated in the quasiequilibrium. The entropy production (9) is non-negative definite due to concavity of the entropy. The entropy production (9) is equal to zero only if the quasiequilibrium approximation is the true solution to the microscopic dynamics, that is, if $(1-P^*)J^*\equiv 0$. While quasiequilibrium approximations that solve the Liouville equation are uninteresting objects (except, of course, for the equilibrium itself), vanishing of the entropy production in this case is a simple test of consistency of the theory. Note that the entropy production (9) is proportional to τ.

Though Eq. (9) looks very natural, its existence is rather subtle. Indeed, Eq. (8) is a difference of the two terms, $\langle m|D_f J^*\cdot J^*\rangle$ (contribution of the second-order approximation to the microscopic trajectory), and $D_M\langle m|J^*\rangle\cdot\langle m|J^*\rangle$ (contribution of the second derivative of the quasiequilibrium vector field). Each of these expressions separately gives a positive contribution to the entropy production, and Eq. (9) is the difference of two positive definite expressions. In the higher order approximations, these *subtractions* are more involved, and explicit demonstration of the entropy production formulase becomes a formidable task. Yet, it is possible to demonstrate the increase in entropy without explicit computation, though at a price of smallness of τ. Indeed, let us denote $\dot{S}^*_{(n)}$ the time derivative of the entropy on the nth order approximation. Then

$$\int_t^{t+\tau}\dot{S}^*_{(n)}(s)ds=S^*(t+\tau)-S^*(t)+O(\tau^{n+1}),$$

where $S^*(t+\tau)$ and $S^*(t)$ are true values of the entropy at the adjacent states of the H curve. The difference $\delta S=S^*(t+\tau)-S^*(t)$ is strictly positive for any fixed τ, and, by Eq. (9), $\delta S\sim\tau^2$ for small τ. Therefore, if τ is small enough, the right hand side in the above expression is positive, and

$$\tau\dot{S}^*_{(n)}(\theta_{(n)})>0,$$

where $t\leqslant\theta_{(n)}\leqslant t+\tau$. Finally, since $\dot{S}^*_{(n)}(t)=\dot{S}^*_{(n)}(s)+O(\tau^n)$ for any s on the segment $[t,t+\tau]$, we can replace $\dot{S}^*_{(n)}(\theta_{(n)})$ in the latter inequality by $\dot{S}^*_{(n)}(t)$. The sense of this consideration is as follows: Since the entropy production formula (9) is valid in the leading order of the construction, the entropy production will not collapse in the higher orders at least if the coarse-graining time is small enough. More refined estimations can be obtained only from explicit analysis of higher-order corrections.

Finally, a comment on the mathematical structure of the developed approach is in order. The problem of coarse graining is considered here as the problem of mapping of one (microscopic) dynamic system into another (macroscopic) dynamic system. While we have focused above on the entropy-conserving dynamics (1), it is instructive to contrast it with the dissipative systems. In that case just the mapping of the *vector fields* is sufficient to derive the dissipative macroscopic dynamic system. More specifically, if the microscopic system is dissipative (such as given by the Boltzmann equation, for example), with S its monotonically increasing Lyapunov functional, then the mapping of the vector field J attached to each point of the quasiequilibrium manifold with the help of the quasiequilibrium projector P^* onto the tangent bundle of the quasiequilibrium manifold results in a dissipative macroscopic system. In this case, either through extension of the list of the macroscopic variables, or by constructing corrections to quasiequilibria within the list of chosen variables, one can expect to derive sufficiently accurate dissipative macroscopic models. (see, e. g., Ref. [6,7] where this point is discussed in detail). However, for the entropy-conserving systems just a mapping of the vector fields is not sufficient to derive dissipation. For such systems, neither the enlargement of the list of the macroscopic variables, nor corrections intended to make the quasiequilibrium ''more invariant'' can result in the dissipative macroscopic equations. For this reason, we have considered here a more general *natural projection* based on *segments of trajectories* of both the microscopic and the macroscopic systems, rather than on just the infinitesimal generators thereof. The simplest implementation of this approach as considered above is based on the mapping of Taylor series expansions of the microscopic and the macroscopic trajectories.

V. EXAMPLES

Same as any coarse-graining approach, the extended Ehrenfest's argument is a phenomenological construction. Therefore, the relevance of results can be judged only from examples. We first consider the simplest case of the conservative dynamics, the one-body Liouville equation, $\dot{f}=-v_\alpha\partial_\alpha f$, where $f(\boldsymbol{r},\boldsymbol{v},t)$ is the one-particle distribution function. Subject to appropriate boundary conditions that we assume, this equation conserves the Boltzmann entropy S

$=-k_{\rm B}\int f \ln f d\boldsymbol{v} d\boldsymbol{r}$. The local Maxwell distribution function is the maximizer of the entropy subject to the constraints,

$$M=\{M_0,M_\alpha,M_4\}=\int \{1,v_\alpha,v^2\} f d\boldsymbol{v},$$

where $\alpha=1,2,3$. Macroscopic variables M are related to the usual local hydrodynamic fields. Quasiequilibrium dynamics is given by the Euler equations for nonviscous fluid. In this case,

$$R_0^{(1)}=0, \quad R_\alpha^{(1)}=\frac{\tau}{2}\partial_\beta[n v_T^2 \overline{\partial_\alpha u_\beta}],$$

$$R_4^{(1)}=\frac{5\tau}{8}\partial_\alpha[n T^{-1} v_T^4 \partial_\alpha T]. \tag{10}$$

Here n, $\boldsymbol{u}$, and T are number density, mean velocity, and temperature, overline denotes symmetric traceless dyad, and $v_T=(2k_{\rm B}T/m)^{1/2}$ is the thermal velocity. The first-order approximation is the Navier-Stokes equations, with transport coefficients proportional to the time step τ between coarse-graining events. Thus, in this example, coarse graining is a substitution for particle's collisions, and the time step τ between coarse-graining events corresponds to the mean time between collisions. This is not surprising: the finite-time coarse graining plays here the same role as the relaxation time in the Bhatnagar-Gross-Krook (BGK) model [9] of the Boltzmann collision integral, whereas the outcome (10) corresponds to the first-order approximation of the Chapman-Enskog method for that equation. It is well known that the physical meaning of the relaxation time in the BGK model is the mean collision time.

The next, $O(\tau^2)$ correction in our formalism would correspond to the Burnett-type hydrodynamics [10]. It is well known that the Burnett hydrodynamic equations, as derived from the Boltzmann equation, are exposed to difficulties that preclude the correct entropy production. In particular, small perturbations of the global equilibrium due to the Burnett equations become unstable at a sufficiently short wavelenght [11,12]. It is of interest therefore to address the question of stability of the Burnett-type hydrodynamics in our scheme. It should be also mentioned that the above scheme of derivation in the higher orders requires a modification for systems with local conservation laws. Indeed, the density balance equation,

$$\partial_t M_0 + \partial_\alpha M_\alpha = 0,$$

holds identically for any solution of the one-particle Liouville equation. Therefore, any method of coarse graining should respect this identity. In our case, in the higher-order construction, this amounts to using the Taylor expansion of $M_0(t+\tau)$ only up to the order $O(\tau^2)$.

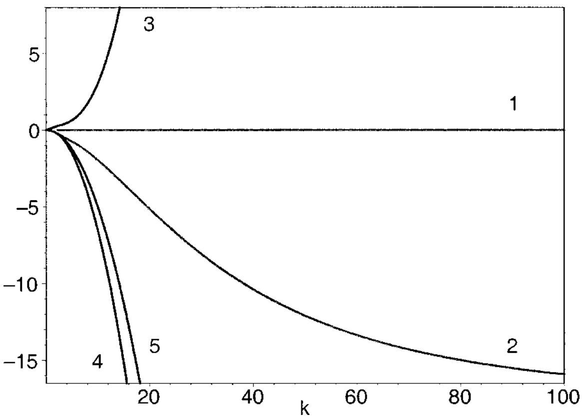

FIG. 2. Dispersion of various modes of the extended hydrodynamic equations (11). The reduced attenuation rates Re ω_i and the frequency Im ω_i of the diffusion mode ω_1, of the two sound modes ω_2, and of the two shear modes ω_3 are given as functions of the reduced wave vector k. 1: Im $\omega_1(k)$, 2: Re $\omega_1(k)$, 3: Im $\omega_2(k)$, 4: Re $\omega_2(k)$, 5: Re $\omega_3(k)$. Stability of dispersion relations means that all functions Re ω_i are nonpositive for any wave vector. For the Burnett hydrodynamics (not shown), function Re ω_2 becomes positive after some value of the wave vector [11].

It is convenient to introduce dimensionless variables, $n'=n/n_0$, $u'_\alpha=u_\alpha/\sqrt{k_{\rm B}T_0/m}$, and $T'=T/T_0$, where n, u_α, and T are small deviations of the number density, of the mean velocity, and of the temperature from their equilibrium values. We also use the reduced time and space variables, $t'=t/\tau$, and $\boldsymbol{r}'=\boldsymbol{r}/\sqrt{k_{\rm B}T_0}m\tau$. Omitting the primes, and using the system of units where $k_{\rm B}/m=1$, the linearized hydrodynamic equations to the order $O(\tau^2)$ are found as follows:

$$\partial_t n = -\partial_\alpha u_\alpha,$$

$$\partial_t u_\alpha = -\partial_\alpha n - \partial_\alpha T + \frac{1}{2}\partial_\beta \overline{(\partial_\alpha u_\beta)} + \frac{1}{9}\Delta\partial_\alpha n + \frac{1}{36}\Delta\partial_\alpha T,$$

$$\partial_t T = -\frac{2}{3}\partial_\alpha u_\alpha + \frac{5}{6}\Delta T + \frac{1}{54}\Delta\partial_\beta u_\beta. \tag{11}$$

Here Δ is the Laplace operator. Direct computation demonstrates that the dispersion relation for the system (11) is stable for arbitrary wave vectors, unlike the Burnett equations (see Fig. 2). Note that this result is different from regularisation of the Burnett approximation obtained by summation of the Chapman-Enskog expansion [13,14].

Another well known quasiequilibrium is the maximizer of the Gibbs-Shannon entropy subject to the one-body distribution function $f(\boldsymbol{p},\boldsymbol{r})$. The quasiequilibrium N-body distribution function is the product of one-body distribution functions. Assuming pair interactions in the N-body Liouville equation, corresponding quasiequilibrium dynamics is given by Vlasov's equation. The correction (8) gives (for smooth and finite pair potentials, all expressions below are well defined):

$$\frac{\partial f}{\partial t} + p_\alpha \frac{\partial f}{\partial r_\alpha} - \nu \frac{\partial f}{\partial p_\alpha}\langle F_\alpha\rangle = D_{\alpha\beta}\frac{\partial^2 f}{\partial p_\alpha \partial p_\beta}. \tag{12}$$

Here $\langle\cdots\rangle$ denotes averaging with f. The (nondissipative) Vlasov terms are on the left hand side while the right hand side is the dissipative correction; ν is the average number density, f is normalized to the total number of particles, F_α is the α component of the force between two particles, while $D_{\alpha\beta}$ is the diffusivity matrix,

$$D_{\alpha\beta}=\frac{\tau}{2}\nu[\langle F_\alpha F_\beta\rangle-\nu\langle F_\alpha\rangle\langle F_\beta\rangle]. \tag{13}$$

This expression clearly indicates that the implementation of the coarse-graining procedure with the finite τ results in a short-memory approximation. Equation (12) is not yet sufficient for the following reason: Since the total energy is not on the list of macroscopic variables, the diffusion term as given in Eq. (12) does not have this conservation law. Therefore, in order to restore the energy conservation, an additional restriction is required. Such a restriction is usually termed a thermostat. In our case, a realization of the thermostat amounts to replacing the right hand side of Eq. (12) with

$$D_{\alpha\beta}\frac{\partial}{\partial p_\alpha}\left\{\frac{\partial f}{\partial p_\beta}+\frac{p_\beta n-j_\beta}{mk_\mathrm{B}T}f\right\}, \tag{14}$$

where j_β is the local average momentum, T is the local kinetic temperature, and n is the local number density. Dissipative terms of the type (14) were derived earlier by many authors [15].

Our final example is the derivation of the hydrodynamic equations from the Vlasov kinetic equation [Eq. (12) with the right hand side equal to zero]. It should be admitted that most of the derivations of the nonequilibrium dynamics from the Liouville equation essentially use the linearity of the latter (see a discussion below), and hence they are formally inapplicable to nonlinear (mean field) conservative systems such as the Vlasov equation. Our approach is applicable to such systems without any modification. The lowest order dissipative equations for the hydrodynamic variables as derived from the Vlasov equation are as follow:

$$\begin{aligned}
\partial_t n&=-\partial_\alpha(nu_\alpha),\\
\partial_t(nu_\alpha)&=-\partial_\alpha\left(\frac{n}{2}v_T^2+u_\alpha u_\beta n\right)+\frac{\tau}{2}\partial_\beta(nv_T^2\overline{\partial_\alpha u_\beta})-\frac{\tau}{2}n\Psi_\alpha\\
&\quad+\frac{\tau}{2}\partial_\beta n(u_\alpha\langle F_\beta\rangle-u_\beta\langle F_\alpha\rangle),\\
\partial_t\varepsilon&=-\partial_\alpha\left(\frac{5}{2}v_T^2nu_\alpha+u^2u_\alpha n\right)+\frac{5\tau}{8}\partial_\alpha(nT^{-1}v_T^4\partial_\alpha T)\\
&\quad+\frac{3\tau}{4}(v_T^2\langle F_\alpha\rangle\partial_\alpha n)+\tau\langle F_\alpha\rangle u_\alpha u_\beta\partial_\beta n-nu_\alpha\Psi_\alpha\\
&\quad+n\langle F_\alpha\rangle\langle F_\alpha\rangle,
\end{aligned} \tag{15}$$

where $\varepsilon=(3/2)nk_\mathrm{B}T$ is the energy density, and

$$\Psi_\alpha=-N\int F_\alpha(\boldsymbol{r},\boldsymbol{r}')\partial'_\beta[nu_\beta(\boldsymbol{r}')]d\boldsymbol{r}'.$$

The set of Eqs. (15) is quite similar to hydrodynamic equations for dense one-component plasma that have been derived from kinetic theory of collision-dominated plasmas by different methods [16]. We defer a further discussion of the above examples to a separate publication.

VI. DISCUSSION AND CONCLUSION

The fundamental Ehrenfest's idea of coarse graining has been followed by many authors [2]. In most of the works, transition to continuous time follows from a consideration of the time scales much larger than the coarse-graining time τ. While these results are very general, they are not directly relevant to the present analysis that concerns the times *within* the coarse-graining time. On the other hand, quasiequilibrium approximations were used by several authors in order to develop a projection operator formalism for systems arbitrary far from equilibrium. In particular, Robertson [17] has used the quasiequilibrium projection operator in order to rewrite the Liouville equation into an equivalent system of equations for the motion along and transverse the quasiequilibrium manifold. Exactness of this and similar transforms has been stressed by many authors [18]. However, any system that is equivalent to the Liouville equation cannot be irreversible, and a version of coarse graining is needed on the later stages of the formalism. Unfortunately, there is no prescription of how to do this in general, and results typically verify Onsager-like symmetry relations but not readily the strict increase in entropy. The H theorem can be demonstrated only in specific examples when system-dependent assumptions are accepted. The same difficulty is present in the well known method of nonequilibrium statistical operator of Zubarev: Though the time asymmetry is explicitly introduced into the Liouville equation, this is done at the expense of a complicated limiting transition, and the H theorem is difficult to prove [19].

Finally, we stress that the correct implementation of the Ehrenfest's coarse graining requires subtraction of the macroscopic component of motion. The natural projection of the segments of trajectories requires that, for any M and given τ,

$$M(t+\tau)=\langle m|T_\tau f^*\rangle. \tag{16}$$

The latter condition should be treated with care because the left hand side of this expression is defined by the *a priori* unknown exact macroscopic equations. In the paper [20], it has been suggested to derive continuous time equations from Eq. (16) as follows:

$$M+\tau\dot{M}\approx\langle m|T_\tau f^*\rangle. \tag{17}$$

In a contrast to our derivation, the latter expression does not attempt to construct a mapping of the microscopic into the macroscopic dynamics. Specifically, Eq. (17) ignores an expansion of the macroscopic equation [more precisely, Eq. (17) implements what is known as the differential pursuit]. In particular, if the second-order approximation is employed in Eq. (17), the entropy production is, $\dot{S}^*=-(\tau/2)\langle J^*|D^2S^*|J^*\rangle$. This expression is positive definite, so an ''increase in entropy'' is present, but, in contrast to the correct Eq. (9), it does not turn into zero when the quasiequilibrium solves the microscopic equation, as it should be.

Therefore, Eq. (17) cannot be valid as a systematic method of derivation of dissipative dynamics.

In conclusion, in this paper, for the first time to the best of our knowledge, the approach of Ehrenfest's has been systematically formalized to a simple and self-consistent tool for derivation of physically sound, clearly dissipative equations. As is, the resulting method qualifies for a class of ''mean free path theories,'' incorporating in itself a simple phenomenological element (coarse graining), and in that respect is close in spirit (but certainly not in the implementation, the present approach is even simpler) to the well known Kirkwood's time averaging approach. There are many ways the present approach can be improved and generalized, in particular, the following.

(i) Going away from the short-memory approximations based on the finite coarse-graining time τ corresponds to taking the limit $\tau\to\infty$ in the Eq. (16). On qualitative grounds, large enough coarse-graining time will allow all correlations to be developed. This point is important and deserves a further study [21]. Here we shall mention only the following result: Let us assume that the microscopic dynamics is defined by a linear equation, $\dot{f}=Lf$, where L is a linear (Liouville) operator. Let us also assume the equilibrium f^{eq}, such that $Lf^{\mathrm{eq}}=0$. For the sake of simplicity, let us also assume that the macroscopic variables M_k are normalized in such a way that $\langle m_k|f^{\mathrm{eq}}m_s\rangle=\delta_{ks}$, and that $m_0=1$ is included in the list of the m_k's. To the first order in the macroscopic variables M, the quasiequilibrium is a linear manifold, $f^*(M)=f^{\mathrm{eq}}(1+\Sigma_{k\neq 0}M_k m_k)$, whereas the quasiequilibrium projector is $P^*=f^{\mathrm{eq}}\Pi$, where $\Pi=\Sigma_k|m_k\rangle\langle m_k|$. The near-equilibrium dynamics of the macroscopic variables M has the form,

$$\dot{M}=AM,$$

where A is yet unknown linear operator. Equation (16) may be written for arbitrary fixed τ as follows:

$$[\exp(\tau A)M]_k=\langle m_k|\exp(\tau L)f^*(M)\rangle.$$

Then, formally,

$$A_{kl}=\left\langle m_k \middle| \lim_{\tau\to\infty}\frac{1}{\tau}\ln[\Pi\exp(\tau L)f^{\mathrm{eq}}\Pi] \middle| m_l\right\rangle, \tag{18}$$

where A_{kl} are the matrix elements of the operator A. Thus, the exact near-equilibrium macroscopic dynamics is expressed in terms of the (operator) Liapunov exponent. Moreover, in the simplest case of a wide separation of time scales of the macroscopic and of the microscopic motions, the more familiar Green-Kubo form can be derived from Eq. (18).

(ii) Without any changes, the method is applicable in the case when the dynamic equation (1) is dissipative, in particular, to the Fokker-Planck equation.

(iii) The use of the thermodynamic projector [6,7] allows to apply the method to nonquasiequilibrium approximations.

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