Nuclear Physics A378 (1982) 375–396

THE INTERPLAY BETWEEN COHERENT AND STOCHASTIC EFFECTS IN DEEPLY INELASTIC COLLISIONS OF HEAVY IONS

(II). Fluctuations in the collective dynamics

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Received 12 October 1981

Abstract: We extend the work developed in paper I of this series, by discussing the dynamics in the collective phase space in terms of a generalized Fokker-Planck equation. We are thus able to discuss fluctuations in the collective motion which were neglected in the mean field theory of paper I. In contrast with the standard derivations of Fokker-Planck equations, we do not assume quasi-equilibrium for the internal system, but rather, describe its evolution in time as it is coupled to the collective system. The transport coefficients appearing in the Fokker-Planck equation are expressed as functionals of the internal density matrix. We use a coarse-grained description to study the development of the internal system as the reaction progresses, and we express the transport coefficients in terms of the above-mentioned coarse-grained variables. Finally, we analyze the balance of energy between the collective and the internal systems.

1. Introduction

In a previous publication in this series of articles [ref. [1]), to be referred to as I], we presented a self-consistent mean-field approximation [2]) for the treatment of dissipative heavy-ion collisions (DIC). The macroscopic degrees of freedom were described by means of classical trajectories. Using a coarse-grained description, the internal system was represented by properly chosen dynamical variables which took into account the rapid excitation in DIC. For these variables a closed set of equations of motion ("reduced equations of motion", REM) was derived. The most severe drawback of the mean field approximation is that the fluctuations in the classical degrees of freedom are neglected. In the present paper we remove this restriction and treat DIC in terms of a generalized Fokker-Planck equation (FPE). The main goal is to express the transport coefficients which appear in the FPE in terms of the internal dynamical variables. A very similar task was undertaken in the

Brownian motion approach to DIC [3]). In the present work, however, we relax the quasi-equilibrium assumption in order to allow also for more rapid changes in the internal system. We obtain therefore a uniform description for DIC, uniform in the sense that the same theory describes both the fast, coherent excitations in the approach phase, and the slower statistical processes which characterize the contact phase. The starting point for the discussion is the semi-classical Liouville equation for the density matrix $\hat{D}(R, P, t)$ [ref. [3])],

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{D}(R,P,t)=\frac{1}{i\hbar}[\hat{H}(R,P),\hat{D}(R,P,t)]_- - \frac{P}{M}\frac{\hat{c}}{\hat{c}R}\hat{D}(R,P,t)-\frac{1}{2}\frac{\hat{c}}{\hat{c}P}[\hat{F}(R),\hat{D}(R,P,t)]_+. \tag{1.1}$$

We use throughout this paper the same notation as was introduced in paper I. Thus, e.g., R and P stand for the collective (macroscopic) degrees of freedom and their conjugate momenta. The operators which act on the internal system are denoted by $\hat{O}$. Also,

$$\hat{H}(R,P)=\hat{h}_0+\hat{V}(R)+\frac{P^2}{2M}\equiv\hat{h}(R)+\frac{P^2}{2M}, \tag{1.2}$$

$$\hat{F}(R)=-\frac{\partial\hat{V}}{\partial R}. \tag{1.3}$$

(Note that due to a printing error, a factor of $\frac{1}{2}$ is missing from the last term in eq. (1.1) of I.) We consider explicitly only one collective variable – the distance between the collision partners. The extension to a larger number of collective degrees of freedom is cumbersome but straightforward.

The self-consistent mean-field approximation is obtained by assuming that $\hat{D}(R, P, t)$ can be factored as

$$\hat{D}(R,P,t)=\hat{\rho}(t)\sigma(R,P,t). \tag{1.4}$$

Once this is accepted, one can show that the dynamics of the collective variables can be described in terms of classical trajectories $R(t)$, $P(t)$, so that

$$\sigma(R,P,t)=\delta(R-R(t))\delta(P-P(t)). \tag{1.5}$$

The reaction is then described by the coupled equations of motion

$$i\hbar\dot{\hat{\rho}}=[\hat{H}(R(t),P(t)),\hat{\rho}]_-, \tag{1.6a}$$

$$\dot{R}=P/M, \tag{1.6b}$$

$$\dot{P}=\langle\hat{F}\rangle_\rho=\mathrm{tr}\,(\hat{\rho}\hat{F}(R)). \tag{1.6c}$$

The main purpose of I was to develop a coarse-grained version of eq. (1.6a). A summary of the relevant results, adapted for the purpose of the formalism presented in this work, is given in sect. 3.

The constraint (1.4) on the form $\hat{D}(R, P, t)$ implies that the correlations between the internal density operator $\hat{\rho}(t)$ and the distribution $\sigma(R, P, t)$ are neglected. In the present paper, we study in detail the correlated part of $\hat{D}(R, P, t)$,

$$\hat{D}_{\mathrm{cor}}(R, P, t) = \hat{D}(R, P, t) - \hat{\rho}(t)\sigma(R, P, t). \tag{1.7}$$

We show in sect. 2 that the inclusion of $\hat{D}_{\mathrm{cor}}$ leads to a generalized FPE for $\sigma(R, P, t)$, similar to the one obtained in the theory of Brownian motion [3]).

In sect. 4 we derive approximate expressions for the transport coefficients in terms of the coarse grained dynamical variables of the internal system. We restrict ourselves to the limit of small diffusion. This is in contrast to the theory of Brownian motion [3]) which holds in the limit of small deviation from thermal equilibrium. In sect. 5 we summarize the results of the paper and discuss the conservation of energy.

2. The generalized Fokker-Planck equation

As mentioned in the introduction, our aim is to derive an equation of motion for the collective distribution function

$$\sigma(R, P, t) = \mathrm{tr}\hat{D}(R, P, t) \tag{2.1}$$

which takes into account the fluctuations in the collective dynamics. We divide the density operator $\hat{D}$ into an uncorrelated and a correlated part,

$$\hat{D}(R, P, t) = \hat{\rho}(t)\sigma(R, P, t) + \hat{D}_{\mathrm{cor}}(R, P, t). \tag{2.2}$$

This is to be considered as a definition of $\hat{D}_{\mathrm{cor}}$ in terms of $\hat{\rho}(t)$, which is as yet an unspecified matrix with $\mathrm{tr}\,\hat{\rho}(t) = 1$. It is convenient to rewrite the semi-classical Liouville equation (1.1) in a tetradic notation,

$$i\dot{\hat{D}} = (L_0 + L_1)\hat{D} \equiv L\hat{D}. \tag{2.3}$$

The density matrices are tetradic vectors, the Liouvilleans

$$L_0 \cdot = \frac{1}{\hbar}[\hat{h}(R), \cdot]_-, \tag{2.4}$$

$$L_1 \cdot = -i\left(\frac{P}{M}\frac{\partial}{\partial R}\cdot + \frac{1}{2}\frac{\partial}{\partial P}[F, \cdot]_+\right) \tag{2.5}$$

tetradic matrices.

We define the time-dependent projector in Liouville space

$$\mathscr{P}(t) \cdot = \hat{\rho}(t)\,\mathrm{tr}\cdot. \tag{2.6}$$

The procedure we follow is similar to that used in the theory of Brownian motion [3]). However, there the projector is constructed with the quasi-static equilibrium density

matrix

$$\hat{\rho}_{\mathrm{eq}}(R) = \exp(-\beta\hat{h}(R))/\mathrm{tr}\,(\exp(-\beta\hat{h}(R))) \tag{2.7}$$

and depends upon R and not t. In our context, we are interested in systems that depart from equilibrium considerably, so that the choice (2.7) is not suitable.

Together with $\mathscr{P}$ we define the projector on the orthogonal subspace

$$\mathscr{Q}(t) = 1 - \mathscr{P}(t), \tag{2.8}$$

with

$$\mathscr{P}(t)\mathscr{Q}(t') = 0 \qquad \text{for any } t, t'. \tag{2.9}$$

The projection operators $\mathscr{P}$ and $\mathscr{Q}$ when operating on the density matrix $\hat{D}$, project out the uncorrelated and correlated parts of $\hat{D}$, respectively:

$$\mathscr{P}\hat{D} = \hat{\rho}\sigma, \qquad \mathscr{Q}\hat{D} = \hat{D}_{\mathrm{cor}}. \tag{2.10}$$

The projection of eq. (2.3) onto $\mathscr{P}$- and $\mathscr{Q}$-space read

$$i\frac{\partial}{\partial t}\mathscr{P}(t)\hat{D}(t) = i\dot{\hat{\rho}}\sigma + \mathscr{P}L\hat{\rho}\sigma + \mathscr{P}L\mathscr{Q}\hat{D}, \tag{2.11}$$

$$i\frac{\partial}{\partial t}\mathscr{Q}(t)\hat{D}(t) = -i\dot{\hat{\rho}}\sigma + \mathscr{Q}L\hat{\rho}\sigma + \mathscr{Q}L\mathscr{Q}\hat{D}. \tag{2.12}$$

In order to eliminate $\mathscr{Q}\hat{D}$, eq. (2.11) is solved formally,

$$\mathscr{Q}(t)\hat{D}(t) = -\int_{t_0}^{t} \mathrm{d}t' \mathscr{G}(t, t')[\mathscr{Q}(t')iL\hat{\rho}(t') + \dot{\hat{\rho}}(t')]\sigma(t'). \tag{2.13}$$

The propagator $\mathscr{G}(t, t')$ is defined by

$$i\frac{\partial}{\partial t}\mathscr{G}(t, t') = \mathscr{Q}(t)L\mathscr{Q}(t)\mathscr{G}(t, t'), \tag{2.14a}$$

$$\mathscr{G}(t, t) = 1. \tag{2.14b}$$

Substituting (2.13) into (2.11) one obtains

$$i\dot{\sigma}(t)\hat{\rho}(t) = \mathscr{P}(t)L\hat{\rho}(t)\sigma(t) - \int_{t_0}^{t} \mathrm{d}t' \mathscr{P}(t)L\mathscr{Q}(t)\mathscr{G}(t, t')\{\mathscr{Q}(t')iL\hat{\rho}(t') + \dot{\hat{\rho}}(t')\}\sigma(t'). \tag{2.15}$$

The various projections are easily written out explicitly,

$$\begin{aligned}
\mathscr{P}(t)iL\mathscr{P}(t)\cdot &= \hat{\rho}(t)\left\{\frac{P}{M}\frac{\partial}{\partial R}\mathrm{tr}\cdot + \langle\hat{F}(R)\rangle_{\rho,t}\frac{\partial}{\partial P}\mathrm{tr}\cdot\right\},\\
\mathscr{P}(t)iL\mathscr{Q}(t)\cdot &= \hat{\rho}(t)\frac{\partial}{\partial P}\mathrm{tr}\,\{\delta_{\rho,t}\hat{F}\cdot\},\\
\mathscr{Q}(t)iL\mathscr{P}(t)\cdot &= iL_0\hat{\rho}(t)\,\mathrm{tr}\cdot + \tfrac{1}{2}[\delta_{\rho,t}\hat{F}, \hat{\rho}]_+\frac{\partial}{\partial P}\mathrm{tr}\cdot,
\end{aligned} \tag{2.16}$$

where

$$\langle \hat{F}(R)\rangle_{\rho,t} = \mathrm{tr}\,(\hat{F}(R)\hat{\rho}(t)), \tag{2.17}$$

$$\delta_{\rho,t}\hat{F}(R) = \hat{F}(R) - \langle \hat{F}(R)\rangle_{\rho,t}. \tag{2.18}$$

With these relations, eq. (2.15) takes the explicit form

$$\begin{aligned}\dot{\sigma}(R,P,t) = &-\frac{P}{M}\frac{\partial}{\partial R}\sigma(R,P,t) - \langle \hat{F}(R)\rangle_{\rho,t}\frac{\partial}{\partial P}\sigma(R,P,t)\\ &+\frac{\partial}{\partial P}\int_{t_0}^{t} \mathrm{d}t'\,\mathrm{tr}\,\{\delta_{\rho,t}\hat{F}\mathcal{G}(t,t')(iL_0\hat{\rho}(t') + \dot{\hat{\rho}}(t'))\}\sigma(R,P,t')\\ &+\frac{\partial}{\partial P}\int_{t_0}^{t} \mathrm{d}t'\,\mathrm{tr}\,\{\delta_{\rho,t}\hat{F}\mathcal{G}(t,t')\tfrac{1}{2}[\delta_{\rho,t'}\hat{F},\hat{\rho}(t')]_+\}\frac{\partial}{\partial P}\sigma(R,P,t'). \end{aligned}\tag{2.19}$$

Eq. (2.19) is still an exact equation. Inspite of the explicit appearance of $\hat{\rho}(t)$ in (2.18), the equation is independent of the choice of $\hat{\rho}(t)$, since $\mathcal{G}(t,t')$ and $\delta_{\rho,t}\hat{F}$ are implicitly dependent on $\hat{\rho}$. In the present context, we define $\hat{\rho}(t)$ in terms of the equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = [\langle \hat{h}\rangle_{\sigma,t}, \hat{\rho}(t)]_-, \tag{2.20}$$

with

$$\langle \hat{h}\rangle_{\sigma,t} = \int \mathrm{d}R\mathrm{d}P\hat{h}(R,P)\sigma(R,P,t), \tag{2.21}$$

and the initial condition

$$\hat{\rho}(t=0) = |0\rangle\langle 0|. \tag{2.22}$$

Here, $|0\rangle$ is the ground state of the two colliding nuclei in the entrance channel. Eq. (2.20) describes the development of the internal system under the mean interaction, and it is the most natural choice for $\hat{\rho}(t)$.

Eqs. (2.19) and (2.20) represent an unsymmetric treatment of the collective and the internal motions. Eq. (2.20) is a self-consistent mean-field equation for the internal density $\hat{\rho}$, whereas eq. (2.19) contains in addition to the effects of the mean field also the fluctuations in the collective distribution function σ. A more symmetric treatment is proposed in ref. [2]). However, due to the complexity of the internal system, an application to the present problem is prohibitive. A more detailed discussion of this point is deferred to appendix B.

The generalized FPE (2.19) finally reads

$$\begin{aligned}\dot{\sigma}(R,P,t) = &-\frac{P}{M}\frac{\partial}{\partial R}\sigma(R,P,t) - \langle \hat{F}(R)\rangle_{\rho,t}\sigma(R,P,t)\\ &+\frac{\partial}{\partial P}\int_{t_0}^{t} \mathrm{d}t'\,\mathrm{tr}\left\{\delta_{\rho,t}\hat{F}(R)\mathcal{G}(t,t')\frac{i}{\hbar}[\delta_{\sigma,t'}\hat{h}(R),\hat{\rho}(t')]\right\}\sigma(R,P,t')\\ &+\frac{\partial}{\partial P}\int_{t_0}^{t} \mathrm{d}t'\,\mathrm{tr}\,\{\delta_{\rho,t}\hat{F}(R)\mathcal{G}(t,t')\tfrac{1}{2}[\delta_{\rho,t'}\hat{F}(R),\hat{\rho}(t')]_+\}\frac{\partial}{\partial P}\sigma(R,P,t'), \end{aligned}\tag{2.23}$$

with

$$\delta_{\sigma,t}\hat{h} = \hat{h} - \langle\hat{h}\rangle_{\sigma,t}. \tag{2.24}$$

The link between the present theory and the mean field approximation of paper I is expressed by eqs. (2.20)–(2.22). We use the methods developed in I, to obtain an approximate, coarse-grained expression for $\hat{\rho}$. This will be used in the evaluation of the integral kernels appearing in eq. (2.23). In the next section we reformulate the results of paper I so that they meet our present requirements. We are then able, in sect. 4, to proceed with the evaluation of (2.23).

To end the present discussion, we compare eq. (2.23) with the generalized FPE which was derived in the Brownian motion approach to DIC [eq. (16) of ref. [3])]. The latter can be rewritten in the form

$$\begin{aligned}\dot{\sigma}(R,P,t) = &-\frac{P}{M}\frac{\partial}{\partial R}\sigma(R,P,t) - \langle\hat{F}\rangle\frac{\partial}{\partial P}\sigma(R,P,t)\\ &+\frac{\partial}{\partial P}\int_{t_0}^{t}\mathrm{d}t'\,\mathrm{tr}\left\{\delta\hat{F}\hat{\mathcal{G}}(t,t')\frac{P}{M}\frac{\partial}{\partial R}\hat{\rho}_{\mathrm{eq}}(R)\right\}\sigma(R,P,t')\\ &+\frac{\partial}{\partial P}\int_{t_0}^{t}\mathrm{d}t'\,\mathrm{tr}\,\{\delta\hat{F}\hat{\mathcal{G}}(t,t')\tfrac{1}{2}[\delta\hat{F},\hat{\rho}_{\mathrm{eq}}(R)]_+\frac{\partial}{\partial P}\sigma(R,P,t'),\end{aligned} \tag{2.25}$$

with $\hat{\rho}_{\mathrm{eq}}(R)$ as defined in (2.7) and

$$\langle\hat{F}\rangle = \mathrm{tr}\,(\hat{F}(R)\hat{\rho}_{\mathrm{eq}}(R)), \qquad \delta\hat{F} = \hat{F} - \langle\hat{F}\rangle. \tag{2.26}$$

Formally, eqs. (2.23) and (2.25) are very similar. The essential difference between the two approaches is the choice of the internal density matrix: in eq. (2.23) the dynamically varying $\hat{\rho}(t)$, in eq. (2.25) the quasi-equilibrium density $\hat{\rho}_{eq}$.

In ref. [3]) it was shown that eq. (2.25) can be further reduced to obtain the standard form of the FPE,

$$\dot{\sigma} = -\frac{P}{M}\frac{\partial}{\partial R}\sigma - \langle F\rangle\frac{\partial}{\partial P}\sigma + \frac{\partial}{\partial P}K\left(\frac{P}{M} + T\frac{\partial}{\partial P}\right)\sigma. \tag{2.27}$$

In the present formalism the diffusion coefficient does not take the simple form $D = KT$, but rather is expressed in terms of the dynamically evolving $\hat{\rho}(t)$. This expression for the diffusion coefficient which is the central result of the present work, is discussed in sect. 4.

3. Reduced description of the internal dynamics

Eqs. (2.20) – (2.22) which define the internal density $\hat{\rho}(t)$, are a generalization of the mean-field equation (1.6a). In I we developed a reduced version of eq. (1.6a). We quote here the relevant results without supplying the proofs. The adiabatic spectrum of the internal system is coarse-grained into groups labelled by n. The $n\nu$th adiabatic

eigenstate of the hamiltonian $\langle \hat{h}(R) \rangle_{\rho, t}$, defined in eq. (2.21) is denoted by $|n\nu\rangle$, where ν stands for all the necessary quantum numbers required to define the state completely. With d_n as the number of states in bin n and $E_{n\nu}(t)$ the energy of state $|n\nu\rangle$, the mean energy of bin n is

$$\bar{E}_n = \frac{1}{d_n} \sum_{\nu \in n} E_{n\nu}. \tag{3.1}$$

The matrix elements of the mean-field coupling in the adiabatic representation read

$$v_{n\nu, m\mu} = \begin{cases} i \cdot \dfrac{\langle n\nu | \dfrac{P}{M} \dfrac{\partial \hat{V}}{\partial R} | m\mu \rangle}{E_{n\nu}(t) - E_{m\mu}(t)} \cdot \dfrac{\sigma, t}{}, & \text{for } n\nu \neq m\nu \\ 0, & \text{for } n\nu = m\mu. \end{cases} \tag{3.2}$$

(For the sake of simplicity we consider transitions between bins only and do not refer to any specific states. The generalization to include them is straightforward.)

The main idea behind the construction of the reduced equations of motion (REM) is the following. Once the (adiabatic) spectrum of the internal system is coarse grained, one should choose a complete set of slow dynamical variables (operators), and develop equations of motion for their expectation values. By means of this process the information content of the theory is reduced and after some necessary smoothing of the fast fluctuations in time, one obtains irreversible relaxation effects in the theory. The search for the complete set of slow dynamical variables is guided by the relevant conservation laws. All variables which contribute to a conserved quantity should be included.

The conservation of probability, $\mathrm{tr}\hat{\rho} = 1$, requires the incorporation of the populations

$$P_n = \sum_{\nu \in n} \rho_{n\nu, n\nu} = \mathrm{tr}\,(\hat{\pi}_n \hat{\rho}) \tag{3.3}$$

with

$$\hat{\pi}_n = \sum_{\nu} |n\nu\rangle\langle n\nu|, \qquad \mathrm{tr}\,\hat{\pi}_n = d_n. \tag{3.4}$$

Since we aim at a theory which should also describe the fast processes in the approach phase of DIC, we go one step further in the Mori hierarchy [4, 5]) and include those operators from which the first derivatives of the $\hat{\pi}_n$ are constructed. That is we consider the coherence operators

$$\hat{\sigma}_{nm} = \sum_{\nu, \mu} |n\nu\rangle v_{n\nu, m\mu} \langle m\mu|. \tag{3.5}$$

The coherences $\mathrm{tr}\,\hat{\rho}^{+}_{nm}\,\hat{\rho}$ represent the probability flux. The norm

$$\gamma^2_{nm} = \sum_{\nu, \mu} |v_{n\nu, m\mu}|^2 \tag{3.6}$$

measures the strength of the coupling between bins n and m. In I we derived REM under the assumption that the populations P_n and the coherences constitute the entire set of slow variables. It turns out that in this approximation energy is not strictly conserved. The energy loss in the relative motion, calculated from the classical trajectory, does not balance the energy gain of the internal system, calculated from the population of the various bins. The physical reason for this unbalance is that we did not properly account for the fact that the total energy is conserved. The set of slow dynamical variables has to be enlarged to include the energies

$$E_n = \sum_\nu E_{n\nu}\rho_{n\nu n\nu} = \bar{E}_n P_n + \delta E_n \tag{3.7}$$

stored in the various bins, or, rather, the deviations δE_n from the mean energies in each bin,

$$\delta E_n = \sum_\nu (E_{n\nu} - \bar{E}_n)\rho_{n\nu,\,n\nu} = \mathrm{tr}\,(\hat{\varepsilon}_n\hat{\rho}), \tag{3.8}$$

with

$$\hat{\varepsilon}_n = \sum_\nu |n\nu\rangle(E_{n\nu} - \hat{E}_n)\langle n\nu|. \tag{3.9}$$

In the same way that we included the coherence operators as the time derivatives of the $\hat{\pi}_n$, we must also take care of the time derivatives of the $\hat{\varepsilon}_n$ corresponding to the energy fluxes. However, within the approximation by which we reduce the exact equation (2.20) the probability and the energy fluxes turn out to be correlated. A detailed discussion of this point will be presented in ref. [6]). The REM only contains the combination

$$S_{nm} = \mathrm{tr}(\hat{\psi}^+_{nm}\hat{\rho}) \tag{3.10}$$

with

$$\hat{\psi}_{nm} = \frac{1}{1+\alpha^2_{nm}} \sum_{\nu,\,\mu} |n\nu\rangle \left\{1 - i\frac{\alpha^2_{nm}}{\hbar\Gamma_{nm}}(E_{n\nu} - \bar{E}_n - E_{m\mu} + \bar{E}_m)\right\} v_{n\nu,\,m\mu}\langle m\mu|. \tag{3.11}$$

Here, Γ_{nm} is the dephasing width of the basic correlation function [cf. (3.32) of I], and

$$\alpha^2_{nm} = \hbar^2\Gamma^2_{nm} \sum_{\nu\mu} |v_{n\nu,\,m\mu}|^2 \Big/ \sum_{\nu\mu} |v_{n\nu,\,m\mu}|^2((E_{n\nu} - \bar{E}_n)^2 + (E_{m\mu} - \bar{E}_m)^2) \tag{3.12}$$

relates this width to the combined rms deviation of the energy spectra in bins n and m. It is assumed throughout that the bin size is chosen in such a way that

$$\sum_{\nu\mu} |v_{n\nu,\,m\mu}|^2(E_{n\nu} - E_{m\mu}) = (\bar{E}_n - \bar{E}_m)\sum_{\nu\mu} |v_{n\nu,\,m\mu}|^2. \tag{3.13}$$

Furthermore, for simplicity

$$\bar{E}_n - \bar{E}_m = \hbar\omega_{nm}, \tag{3.14}$$

where ω_{nm} is defined by (3.32) of I. We do not consider the contribution of the "diabatic force" (that part of the force which comes from the diagonal matrix elements of $\partial\hat{V}/\partial R$). This is equivalent to the assumption that all mean quantities of the adiabatic spectrum do not depend upon t. In particular, $\dot{E}_n = 0$. The effect of the adiabatic force will be discussed in ref. [6]).

The REM for the complete set of slow dynamical variables are

$$\frac{\mathrm{d}}{\mathrm{d}t} P_n = 2 \sum_k \mathrm{Im}\, S_{nk}, \tag{3.15a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \delta E_n = \hbar \sum_k \Gamma_{nk}\, \mathrm{Re}\, S_{nk}, \tag{3.15b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} S_{nk} = \eta_{nk} S_{nk} + i \frac{\gamma_{nk}^2}{1+\alpha_{nk}^2} \left(\frac{P_n}{d_n} - \frac{P_k}{d_k} \right) - \frac{\alpha_{nk}^2}{1+\alpha_{nk}^2} \frac{\gamma_{nk}^2}{\hbar \Gamma_{nk}} \left(\frac{\delta E_n}{d_n} + \frac{\delta E_k}{d_k} \right), \tag{3.15c}$$

with

$$\eta_{nk} = -i\omega_{nk} - \Gamma_{nk} + (\dot{G}_{nk}/G_{nk})^*. \tag{3.16}$$

For the definition of G_{nk} we refer the reader to eq. (3.29) of I. The force $\langle\langle F \rangle\rangle_{\rho,\sigma,t}$ induced on the mean trajectory of the relative motion reads now

$$\langle\langle F \rangle\rangle_{\rho,\sigma,t} = -\langle \nabla U_{\mathrm{opt}} \rangle_{\sigma,t} - \frac{i\hbar}{\dot{R}} \sum_{kl} (\omega_{kl} - i\Gamma_{kl}) S_{kl}. \tag{3.17}$$

With this definition of the force, energy is conserved (on the mean) between the trajectory and the internal system. The correlation between the energy and probability fluxes is apparent from the REM [eqs. (3.15)]. In many ways these equations are analogous to the equations of motion in hydrodynamics where the macroscopic density flux is related to the flow of energy.

Once the expectation values of the dynamical variables are known from the solution of the REM, one has to reconstruct the density matrix $\hat{\rho}$ which enters eq. (2.23). The least biased way to do so [7]) is to use

$$\hat{\rho}_{\mathrm{I}} = \exp\left\{ \sum_n (\lambda_n^{(\pi)} \hat{\pi}_n + \lambda_n^{(\varepsilon)} \hat{\varepsilon}_n) + \sum_{n,m} \lambda_{nm}^{(\psi)} \hat{\psi}_{nm} \right\}, \tag{3.18}$$

where the coefficients $\lambda_n^{(\pi)}$, $\lambda_n^{(\varepsilon)}$ and $\lambda_{nm}^{(\psi)}$ are determined by the condition that $\hat{\rho}_{\mathrm{I}}$ reproduces the expectation values of the corresponding operators (3.12). For $\hat{\rho}(t)$ as it appears under the time integral in eq. (2.23) further simplifications are possible. Because $\hat{\pi}_n$, $\hat{\varepsilon}_n$, Ψ_{nm} represent the Π-space of all slow dynamical variables $\hat{\rho}$ may be just replaced by $\Pi\hat{\rho}$ under the integrals. Furthermore, because the operators Ψ_{nm}

are related to the first time-derivatives of the $\hat{\pi}_n$ and $\hat{\varepsilon}_n$, even the Ψ_{nm} part of $\Pi\hat{\rho}$ may be neglected. Therefore, in order to evaluate the time integrals in eq. (2.23), we use

$$\hat{\rho}(t) = \sum_n \left\{ \frac{P_n}{d_n} \hat{\Pi}_n + \frac{\delta E_n}{\mathrm{tr}(\hat{\varepsilon}_n \hat{\varepsilon}_n)} \hat{\varepsilon}_n \right\}. \tag{3.19}$$

4. The transport coefficients

Eq. (2.23) as it stands cannot be applied to any problem of practical interest because of the complicated integral kernels. In the present chapter, we introduce further approximations by which it becomes possible to reduce these integrals, and express them in terms of already-calculated quantities. To do this, we estimate the transport coefficients to the lowest non-vanishing order in the fluctuations. In this way we take only the first step in improving the results of the mean-field approximation of paper I.

The basic approximation which we make is to neglect the effect of the fluctuations (or width) in the collective phase-space on the internal system during the time interval τ_{cor} which contributes significantly to the integrals in (2.23). From eq. (2.14) we see that τ_{cor} is the average lifetime of a correlation $\mathcal{2}\hat{D}$. In the approach phase the width of the distribution σ is small because of the initial conditions. In the exit channel the fluctuations in σ should remain small because of the large mass of relative motion and the small velocity $\dot{R}$ as compared to the mass and average velocity of the internal nucleonic degrees of freedom. Thus, we assume that the mean-field approximation is sufficient to describe the evolution during short time intervals of the order τ_{cor}. This has the following consequences:

(i) In evaluating the integral kernels in eq. (2.23) we substitute for all phase-space functions $A(R, P, t)$ their σ-averaged values $\langle A(R, P)\rangle_{\sigma, t}$, calculated at the time t in which they appear in the integrands. Consequently the first integral in eq. (2.23) vanishes altogether. We assume that the internal system evolves in time through the influence of the mean field $\langle \hat{h}\rangle_{\sigma, t}$ and that there is no difference between $\hat{h}$ and $\langle \hat{h}\rangle_{\sigma, t}$. Hence in the present theory the "frictional force" is due entirely to the induced force $\langle \hat{F}\rangle_{\rho, t}$.

(ii) In the same spirit, $\delta_{\rho, t}\, \hat{F}(R)$ appearing in the second integral is replaced by

$$\delta_{\rho, t}\langle \hat{F}\rangle_{\sigma, t} = \langle \hat{F}\rangle_{\sigma, t} - \langle\langle \hat{F}\rangle\rangle_{\rho, \sigma, t}. \tag{4.1}$$

The above approximation allows us to evaluate the $\mathcal{2}$-space propagator $\mathcal{G}$ (t, t') of eq. (2.3). During the short times τ_{cor} we replace the Liouvillean by its mean field analogue:

$$\langle L\rangle_t = \langle L_0\rangle_t + \langle L_1\rangle_t, \tag{4.2a}$$

$$\langle L_0\rangle_t \cdot = \frac{1}{\hbar}[\langle \hat{h}\rangle_{\sigma, t}, \cdot\,]_-, \tag{4.2b}$$

$$\langle L_1\rangle_t \cdot = -\left\langle \frac{P}{M} \right\rangle_{\sigma, t} \frac{\partial}{\partial R} \cdot - \langle\langle F\rangle\rangle_{\rho, \sigma, t} \frac{\partial}{\partial P} \cdot . \tag{4.2c}$$

Since,

$$\mathcal{Q}\langle L\rangle\mathcal{Q} = \langle L\rangle\mathcal{Q}, \tag{4.3}$$

$$[\langle L_1\rangle_t, \langle L_0\rangle_{t'}]_- = 0, \tag{4.4}$$

$\mathcal{G}(t, t')$ can be expressed as a product of two propagators $\mathcal{G}_0(t, t')$ and $\mathcal{G}_1(t, t')$ which solve equations analogous to eq. (2.13):

$$i\frac{\partial}{\partial t}\mathcal{G}_0(t, t') = \langle L_0\rangle_t \mathcal{G}_0(t, t'), \tag{4.5a}$$

$$\mathcal{G}_0(t, t) = 1, \tag{4.5b}$$

$$i\frac{\partial}{\partial t}\mathcal{G}_1(t, t') = \langle L_1\rangle_t \mathcal{G}_1(t, t'), \tag{4.6a}$$

$$\mathcal{G}_1(t, t) = 1. \tag{4.6b}$$

The propagator $\mathcal{G}_0(t, t')$ describes the propagation of the internal system under the (self-consistent) mean field $\langle\hat{h}\rangle_{\sigma,t}$. On the other hand $\mathcal{G}_1(t, t')$ propagates each phase-space point R, P along a classical trajectory parallel to the most probable trajectory. It is subjected to the mean velocity $\langle P/M\rangle_{\sigma,t}$ and the mean force $\langle\langle F\rangle\rangle_{\rho,\sigma,t}$.

Implementing these results in (2.23) we obtain for the last term in (2.23)

$$\frac{\partial}{\partial P}\int_{t_0}^{t} dt' \mathrm{tr}\{\delta_{\rho,t}\langle\hat{F}\rangle_{\sigma,t}\mathcal{G}_0(t, t')\tfrac{1}{2}[\delta_{\rho,t'}\langle\hat{F}\rangle_{\sigma,t''}\hat{\rho}(t')]_+\mathcal{G}_1(t, t')\frac{\partial}{\partial P}\sigma(R, P, t')\}. \tag{4.7}$$

Making use of

$$\mathcal{G}_1(t, t')\frac{\partial}{\partial P}\sigma(R, P, t') = \frac{\partial}{\partial P}\mathcal{G}_1(t, t')\sigma(R, P, t') \approx \frac{\partial}{\partial P}\sigma(R, P, t) \tag{4.8}$$

we can write (4.7) as

$$\frac{\partial}{\partial P} D \frac{\partial}{\partial P}\sigma(R, P, t), \tag{4.9}$$

with the diffusion coefficient

$$D(t) = \int_{t_0}^{t} dt' \,\mathrm{tr}\{\delta_{\rho,t}\langle\hat{F}\rangle_{\sigma,t}\mathcal{G}_0(t, t')\tfrac{1}{2}[\delta_{\rho,t'}\langle\hat{F}\rangle_{\sigma,t''}\hat{\rho}(t')]_+\}. \tag{4.10}$$

Here $\mathcal{G}_0(t, t')$ is identical with $U(t, t')$ which was introduced in I. In performing the integral (4.10) we use its lowest-order approximation, namely

$$\mathcal{G}_0(t, t')_{a\alpha,\, b\beta;\, c\gamma,\, d\delta} = \delta_{a\alpha,\, c\gamma}\delta_{b\beta,\, d\delta}\exp\left\{-\frac{i}{\hbar}\int_{t'}^{t} dt''(E_{a\alpha}(t'') - E_{b\beta}(t''))\right\}. \tag{4.11}$$

This, together with the result (3.19) for $\hat{\rho}(t)$ can now be substituted into (4.10) to yield the desired expression for the diffusion coefficient D in terms of the variables $P_n(t)$ and δE_n which characterize the dynamics of the internal system.

Leaving technical details to appendix A, the result reads

$$D(t) = \frac{1}{2}\sum_{nm}\int_{t_0}^{t} dt' \Phi_{nm}(t,t')\left\{\frac{P_n(t')}{d_n} + \frac{P_m(t')}{d_m} - \frac{i}{2}\hbar\Gamma_{nm}\left(\frac{\delta E_n(t')}{\varepsilon_n^2} - \frac{\delta E_m(t')}{\varepsilon_m^2}\right)\right\}, \quad (4.12)$$

with the correlation function

$$\Phi_{nm}(t,t') = \sum_{\nu\mu} F^*_{n\nu,m\mu}(t) F_{n\nu,m\mu}(t') \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} dt''(E_{n\nu} - E_{m\mu})\right], \quad (4.13)$$

and $\varepsilon_n^2 = \sum_\nu (E_{n\nu} - \tilde{E}_n)^2$.

The dissipative part of the mean induced force (3.17) or, rather, the related energy rate can be written in a corresponding way. As shown in appendix A, we obtain

$$\langle\langle \dot{R}F\rangle\rangle_{\text{diss}} = \sum_{nm}\int_{t_0}^{t} dt' \Delta_{nm}(t,t')\frac{i}{1+\alpha_{nm}^2} \times \left\{\frac{P_n(t')}{d_n} - \frac{P_m(t')}{d_m} + \frac{i\alpha_{nm}^2}{\hbar\Gamma_{nm}}\left(\frac{\delta E_n(t')}{d_n} + \frac{\delta E_m(t')}{d_m}\right)\right\}, \quad (4.14)$$

with

$$\Delta_{nm}(t,t') = -i\sum_{\nu\mu} \dot{R}(t) F^*_{n\nu,m\mu} \frac{\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt''(E_{n\nu} - E_{m\mu})\right]}{E_{n\nu}(t') - E_{m\mu}(t')} \dot{R}(t') F_{n\nu,m\mu}(t'). \quad (4.15)$$

The similarity between the expressions for the diffusion coefficient and the dissipative energy rate clearly manifests the intimate link between fluctuation and dissipation. The relation to the Brownian motion approach [3]) and to the fluctuation-dissipation theorem is discussed in appendix A.

A simple form of $D(t)$ is obtained by evaluating the integral in (4.12) in a Markovian approximation. As shown in appendix A we obtain

$$D(t) = \frac{1}{2}\sum_{nm}\sum_{n\nu} |F_{n\nu,n\mu}(t)|^2 \frac{\Gamma_{nm}}{\omega_{nm}^2 + \Gamma_{nm}^2}\left\{\frac{P_n(t)}{d_n} + \frac{P_m(t)}{d_m} - \tfrac{1}{2}\hbar\omega_{nm}\left(\frac{\delta E_n(t)}{\varepsilon_n^2} - \frac{\delta E_m(t)}{\varepsilon_m^2}\right)\right\}, \quad (4.16)$$

which holds for large Γ_{nm}.

5. Summary

In the preceeding chapters we developed a theory for the description of DIC, in which the fluctuations in the collective phasespace are taken into account. The resulting set of equations are written down in terms of the distribution function

$\sigma(R, P, t)$, and a set of dynamical variables with which we obtain a coarse-grained description of the internal dynamics.

The final reduced equations of motion for the system are summarized as

$$\frac{\partial}{\partial t}\sigma(R,P,t) = -\frac{P}{M}\frac{\partial}{\partial R}\sigma - \langle \hat{F}(R)\rangle_{\rho,t}\frac{\partial}{\partial P}\sigma + D(t)\frac{\partial^2}{\partial P^2}\sigma, \tag{5.1a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}P_k = 2\sum_n \mathrm{Im}\, S_{nk}, \tag{5.1b}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\delta E_k = \hbar\sum_n \Gamma_{nk}\,\mathrm{Re}\, S_{nk}, \tag{5.1c}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}S_{nk} = \eta_{nk}S_{nk} + i\frac{\gamma_{nk}^2}{1+\alpha_{nk}^2}\left(\frac{P_n}{d_n} - \frac{P_k}{d_k}\right) - \frac{\alpha_{nk}^2}{1+\alpha_{nk}^2}\frac{\gamma_{nk}^2}{\hbar\Gamma_{nk}}\left(\frac{\delta E_n}{d_n} + \frac{\delta E_k}{d_k}\right). \tag{5.1d}$$

The parameters α_{nk}, γ_{nk}, Γ_{nk} and η_{nk} are explained in sect. 3. For the induced force $\langle \hat{F}\rangle_{\rho,t}$ one may take as first guess the σ-mean induced force

$$\langle\langle \hat{F}\rangle\rangle_{\rho,\sigma,t} = -\langle \nabla U_{\mathrm{opt}}\rangle_{\sigma,t} - \frac{i\hbar}{R}\sum_{kl}(\omega_{kl} - i\Gamma_{kl})S_{kl}. \tag{5.2}$$

With the relation between the diffusion coefficient $D(t)$ entering eq. (5.1a) and the internal dynamical variables as given by eq. (4.12) or in an approximate fashion by eq. (4.16), eqs. (5.1) and (5.2) constitute a set of coupled, self-consistent equations of motion for the internal and relative motion. Eq. (5.1a) is a proper Fokker-Planck equation for the distribution function $\sigma(R, P, t)$.

The set of reduced equations (5.1) represents the most simplified version of our theory as indicated in the appendix. It is straightforward, though sometimes cumbersome, to calculate the diffusion coefficient $D(t)$ and the induced force $\langle F(R)\rangle_{\rho,t}$ in more detail. Also the inclusion of explicit states $|I\rangle$ poses no additional problem.

In practice, one can simplify the generalized FP equation by assuming a gaussian distribution for $\sigma(R, P, t)$. Then eq. (5.1a) reduces to two sets of ordinary differential equations for the mean trajectory and the corresponding variances. At each time t, this form of $\sigma(R, P, t)$ is used to construct the mean internal hamiltonian $\langle \hat{h}\rangle_{\sigma,t}$, and the mean force operator $\langle \hat{F}\rangle_{\sigma,t}$, in terms of which the propagation of the REM [eq. (5.1)] can be calculated to give the mean force $\langle\langle \hat{F}\rangle\rangle_{\rho,\sigma,t}$, eq. (5.2), and the diffusion coefficient D, eq. (4.16), which in turn are required for the propagation of $\sigma(R, P, t)$. The computational effort that should be invested in such calculations does not exceed by much that which is needed to follow the REM in the mean-field approximation (see I). Such calculations are easily carried out now and will be reported in a later publication [6]).

The self-consistent treatment of the internal and the collective degrees of freedom guarantees the conservation of the total amount of energy in the system. This quantity is written as

$$E(t) = \int \mathrm{d}R\mathrm{d}P\mathrm{tr}(\hat{H}(R_1, P)\hat{D}(R, P, t). \tag{5.2}$$

By writing $\hat{D}(R, P, t)$ in terms of its correlated and non-correlated components [eq. (2.8)] we can express $E(t)$ as a sum of the mean-field contribution and the energy stored in the correlations,

$$E_{\mathrm{mean}}(t) = \int \mathrm{d}R\mathrm{d}P\mathrm{tr}(\hat{H}(R, P)\sigma(R, P, t)\hat{\rho}(t) = \langle\langle h\rangle\rangle_{\rho,\sigma,t} + \left\langle \frac{P^2}{2M} \right\rangle_{\sigma,t} \tag{5.3}$$

$$E_{\mathrm{cor}}(t) = \int \mathrm{d}R\mathrm{d}P\mathrm{tr}(\hat{H}(R, P)\hat{D}_{\mathrm{cor}}(R, P, t)). \tag{5.4}$$

Concentrating first on $E_{\mathrm{mean}}(t)$, we write $\langle\langle\hat{h}\rangle\rangle_{\rho,\sigma,t}$ in terms of the dynamical variables which were introduced in sect. 3,

$$\langle\langle\hat{h}\rangle\rangle_{\rho,\sigma,t} = E_{\mathrm{int}}(t) = \sum_{n\nu} E_{n\nu}(t)\rho_{n\nu,n\nu}(t) = \sum_n \hat{E}_n P_n(t) + \sum_n \delta E_n(t). \tag{5.5}$$

The rate of change of the internal energy can be easily written as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} E_{\mathrm{int}} &= -i\sum_{nm} \bar{E}_n(S_{mn} - S_{nm}) + \sum_{nm} \hbar\Gamma_{nm}S_{mn} \\ &= i\hbar\sum_{nm} (\omega_{nm} - i\Gamma_{nm})S_{nm} = -\langle\langle\dot{R}\hat{F}\rangle\rangle_{\rho,\sigma,t}. \end{aligned} \tag{5.6}$$

The rate of change of the mean kinetic energy can be calculated by using the FP equation (5.1a),

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \frac{P^2}{2M} \right\rangle_{\sigma,t} = \int \mathrm{d}R\mathrm{d}P \frac{P^2}{2M}\dot{\sigma}(R, P, t) = \langle\langle\dot{R}\hat{F}\rangle\rangle_{\rho,\sigma,t} + D(t)/M. \tag{5.7}$$

Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t} E_{\mathrm{mean}}(t) = \frac{1}{M} D(t), \tag{5.8}$$

where $D(t)$ is the diffusion coefficient (4.10).

We now show that within the framework of approximations introduced in sect. 4, the rate of change of E_{mean} is balanced by the rate of energy due to the correlated

part of $\hat{D}(R, P, t)$,

$$\frac{\mathrm{d}}{\mathrm{d}t} E_{\mathrm{cor}}(t) = \int \mathrm{d}R\mathrm{d}P \mathrm{tr}\{\hat{H}(R, P)\mathcal{Q}(t)iL\hat{D}(R, P, t)\}$$

$$= -\int \mathrm{d}R\mathrm{d}P \mathrm{tr}\{\delta_{\rho,t}\hat{H}iL\hat{D}(R, P, t)\}$$

$$= -\int \mathrm{d}R\mathrm{d}P \mathrm{tr}\left\{\delta_{\rho,t}\hat{h}\left(\frac{P}{M}\frac{\partial\hat{D}}{\partial R} + \tfrac{1}{2}\left[\hat{F}, \frac{\partial\hat{D}}{\partial P}\right]_+\right)\right\}$$

$$= -\int \mathrm{d}R\mathrm{d}P \mathrm{tr}\left\{\delta_{\rho,t}\hat{F}\frac{P}{M}\hat{D}(R, P, t)\right\}. \tag{5.9}$$

Using eq. (2.12) for $\mathcal{Q}\hat{D}(R, P, t)$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t} E_{\mathrm{cor}}(t) = \int \mathrm{d}r\mathrm{d}P \frac{P}{M} \int_{t_0}^{t} \mathrm{d}t' \mathrm{tr}\{\delta_{\rho,t}\hat{F}\mathcal{G}(t, t')(\mathcal{Q}(t')iL\hat{\rho}(t') + \dot{\hat{\rho}}(t'))\}\sigma(R, P, t'). \tag{5.10}$$

By following the sequence of approximations of sect. 4, we arrive at

$$\frac{\mathrm{d}}{\mathrm{d}t} E_{\mathrm{cor}}(t) = \int \mathrm{d}R\mathrm{d}P \frac{P}{M} D(t) \frac{\partial}{\partial P}\sigma(R, P, t) = -\frac{1}{M} D(t). \tag{5.11}$$

The loss of correlation energy is equal to the gain of the diffusive part of the mean energy (5.8). Eq. (5.11) seems to give an unlimited increase of the (negative) correlation energy. However, we calculated the transport coefficients in the limit for small widths of $\sigma(R, P, t)$ (cf. sect. 4). Therefore, eq. (5.11) gives the slope of $E_{\mathrm{cor}}(t)$ for small widths (times) only.

We conclude that the total energy is conserved in our formalism. However, we are unable to calculate directly the correlated part of the total density matrix $\hat{D}(R, P, t)$, nor to obtain an expression for the energy stored in these correlations. We are only able to identify $E_{\mathrm{cor}}(t)$ by its rate of change, using the *exact* relations (5.8) and (5.10). We are not able to show explicitly the influence $E_{\mathrm{cor}}(t)$ may have on the dynamics. This could have been achieved by considering E_{cor} as an explicit dynamical degree of freedom (like, e.g., δE_n), which will result in a non-Markovian diffusion coefficient.

In paper I we have used some arguments based on smoothing the fast fluctuations in the internal system by the introduction of a coarse-grained description in the time variable (see eq. (3.17) in I and the discussion which preceeds and follows it). A more quantitative discussion of this point was deferred to the present paper. A more natural place to discuss this matter seems to be in the next paper of this series. There we reconsider the space of slowly varying dynamical variables and discuss the effects of the energy conservation on the REM.

We would like to express our appreciation of the hospitality extended to us by

the Weizmann Institute and the Hahn-Meitner-Institut, and for their support of this collaboration. We gratefully acknowledge valuable comments of W. Nörenberg.

Appendix A

In this appendix we evaluate the diffusion coefficient (4.10) with $\mathscr{G}_0(t, t')$ given by eq. (4.11),

$$D(t) = \tfrac{1}{2}\,\mathrm{tr}\,\delta_\rho\langle\hat{F}\rangle_{\sigma,t}\int_{t_0}^{t} \mathrm{d}t'\mathscr{G}_0(t,t')[\delta_\rho\langle\hat{F}\rangle_{\sigma,t'},\hat{\rho}(t')]_+. \tag{A.1}$$

In tetradic notation, $\delta_\rho\langle\hat{F}\rangle_{\sigma,t}$ reads

$$\delta_\rho\langle F\rangle_{\sigma,t,n\nu,m\mu} = F_{n\nu,m\mu}(t) - \langle\langle F(t)\rangle\rangle\delta_{n\nu,m\mu}, \tag{A.2}$$

where

$$\langle\langle F(t)\rangle\rangle = \sum_{\nu\mu} F^*_{n\nu,m\mu}(t)\rho_{n\nu,m\mu}(t) \tag{A.3}$$

is the mean induced force. The quantity $\delta_\rho\langle\hat{F}\rangle$ in front of the integral in eq. (A.1) may be replaced by $\langle F(t)\rangle$, because the factor multiplying $\langle\langle F(t)\rangle\rangle$ vanishes.

Under the integral we use for $\hat{\rho}(t)$ the diagonal form (3.19). Consistently, there $\langle\langle F(t')\rangle\rangle$ is to be read as the mean diagonal force, only. Explicitly,

$$\begin{aligned} D(t) = {} & \sum_{\nu\mu} F_{n\nu,n\nu}(t)\int_{t_0}^{t}\mathrm{d}t'(F_{n\nu,n\nu}(t') - \langle\langle F(t')\rangle\rangle)\rho_{n\nu,n\nu}(t') \\ & + \sum_{n\nu,m\mu}{}' \tfrac{1}{2}F^*_{n\nu,m\mu}(t)\int_{t_0}^{t}\mathrm{d}t'\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}(E_{n\nu}-E_{m\mu})\mathrm{d}t''\right] \\ & \times F_{n\nu,m\mu}(t')(\rho_{n\nu,n\nu}(t') + \rho_{m\mu,m\mu}(t')). \end{aligned} \tag{A.4}$$

Σ' runs over non-diagonal elements of F, only.

The sum over the diagonal elements of F is to be neglected. It contains the deviations of the diagonal elements $F_{n\nu,n\nu}$ from the mean adiabatic force. We neglected similar terms in the REM by disregarding the adiabatic forces in each bin and replacing the mean adiabatic force by $-\langle\nabla U_{\mathrm{opt}}\rangle_{\sigma,t}$ eq. (5.2). Into the remaining sum over the non-diagonal elements of F we introduce eq. (3.19),

$$\begin{aligned} D(t) = \frac{1}{2}\int_{t_0}^{t}\mathrm{d}t'\sum_{nm}\{ & \Phi_{nm}(t,t')\left(\frac{P_n(t')}{d_n}+\frac{P_m(t')}{d_m}\right) \\ & + \tfrac{1}{2}(i\hbar\overset{(\cdot)}{\Phi}_{nm}(t,t') - (\bar{E}_n-\bar{E}_m)\Phi_{nm}(t,t'))\left(\frac{\delta E_n(t')}{\varepsilon_n^2}-\frac{\delta E_m(t')}{\varepsilon_m^2}\right) \\ & + \tfrac{1}{2}(\Psi_{nm}(t,t') - (\bar{E}_n+\bar{E}_m)\Phi_{nm}(t,t'))\left(\frac{\delta E_n(t')}{\varepsilon_n^2}+\frac{\delta E_m(t')}{\varepsilon_m^2}\right)\Big\}, \end{aligned} \tag{A.5}$$

with

$$\varepsilon_n^2 = \mathrm{tr}\,(\varepsilon_n \varepsilon_n) = d_n(\bar{E}_n^2 - \bar{E}_n^2).$$

The various correlation functions are

$$\Phi_{nm}(t,t') = \sum_{\nu,\mu} F^*_{n\nu,m\mu}(t) \exp\left[-\frac{i}{\hbar}\int_{t'}^{t}(E_{n\nu}-E_{m\mu})\mathrm{d}t''\right] F_{n\nu,m\mu}(t'), \tag{A.6}$$

$$\overset{(\cdot)}{\Phi}_{nm}(t,t') = -\frac{i}{\hbar}\sum_{\nu,\mu} F^*_{n\nu,m\mu}(t) \exp\left[-\frac{i}{\hbar}\int_{t'}^{t}(E_{n\nu}-E_{m\mu})\mathrm{d}t''\right] F_{n\nu,m\mu}(t')(E_{n\nu}(t')-E_{m\mu}(t')), \tag{A.7}$$

$$\Psi_{nm}(t,t') = \sum_{\nu,\mu} F^*_{n\nu,m\mu}(t) \exp\left[-\frac{i}{\hbar}\int_{t'}^{t}(E_{n\nu}-E_{m\mu})\mathrm{d}t''\right] F_{n\nu,m\mu}(t)(E_{n\nu}(t')+E_{m\mu}(t')). \tag{A.8}$$

$\Phi_{nm}(t,t')$ is intimately related to the force-force-correlation function which plays a fundamental role in both linear response theory and the theory of Brownian motion [3]. Once the matrix elements $F_{n\nu,m\mu}$ are given, the three functions Φ, $\overset{(\cdot)}{\Phi}$ and Ψ can be calculated directly. In analogy to the derivation of the REM [1, 6], we may, however, simplify the evaluation of eq. (A.5) by the approximations

$$\overset{(\cdot)}{\Phi}_{nm}(t',t')/\Phi_{nm}(t,t') = -i\omega_{nm} - \Gamma_{nm}, \tag{A.9}$$

$$\Phi_{nm}(t,t') \cong \mathrm{e}^{(-i\omega_{nm}-\Gamma_{nm})(t-t')}\sum_{\nu\mu} F^*_{n\nu,m\mu}(t)F_{n\nu,m\mu}(t'), \tag{A.10}$$

$$\Psi_{nm}(t,t') \cong \mathrm{e}^{(-i\omega_{nm}-\Gamma_{nm})(t-t')}\sum_{\nu\mu} F^*_{n\nu,m\mu}(t)F_{n\nu,m\mu}(t')(\mathrm{E}_{n\nu}(t')+E_{m\mu}(t'))$$

$$= (\bar{E}_n + \bar{E}_m)\Phi_{nm}(t,t'). \tag{A.11}$$

The last equality in (A.11) follows from the assumption of random matrix elements.

At this point, caution is in order. In principle, all correlation functions should be calculated independently and directly from their microscopic definitions. It should be noted that in the REM only *ratios* of correlation functions, like $\overset{(\cdot)}{I}/I$, $\overset{(\cdot)}{J}/J$ enter. They were simplified in analogy to eq. (A.9) [refs. [1, 6]]. The diffusion coefficient (A.5) is the first place where a correlation function enters explicitly. This is because for its derivation we had to use the COP [chronological ordering prescription [8]], leading to explicit time-integrals. The REM were obtained by following the POP [particle ordering prescription [8]]. They are local in time and only ratios of the correlation functions appear [1, 6].

Inserting the explicit expression (A.10) and (A.11) into (A.5) is a further simplification. Using it naively in other places may lead to unphysical results.

The final result for the diffusion coefficient reads

$$D(t) = \frac{1}{2}\sum_{nm}\int_{t_0}^{t} dt' \Phi_{nm}(t,t')\left\{\frac{P_n(t')}{d_n} + \frac{P_m(t')}{d_m} - \tfrac{1}{2}i\hbar\Gamma_{nm}\left(\frac{\delta E_n(t')}{\varepsilon_n^2} - \frac{\delta E_m(t')}{\varepsilon_m^2}\right)\right\}. \tag{A.12}$$

For large Γ_{nm} the exponential decay of Φ_{nm} dominates the integrand and we obtain the Markovian approximation

$$D(t) = \frac{1}{2}\sum_{nm}\sum_{\nu\mu}|F_{n\nu,\,m\mu}(t)|^2 \frac{\Gamma_{nm}}{\omega_{nm}^2+\Gamma_{nm}^2}\left\{\frac{P_n(t)}{d_n} + \frac{P_m(t)}{d_m} - \tfrac{1}{2}\hbar\omega_{nm}\left(\frac{\delta E_n(t)}{\varepsilon_n^2} - \frac{\delta E_m(t)}{\varepsilon_m^2}\right)\right\}. \tag{A.13}$$

In order to investigate the relations between dissipation and fluctuation we may also evaluate the rate of energy due to the dissipative part of the mean induced force (3.17),

$$\langle\langle \dot{R}\hat{F}(t)\rangle\rangle_{\rm diss} = \hbar\sum_{nm}(-i\omega_{nm}-\Gamma_{nm})S_{nm}(t). \tag{A.14}$$

For $S_{nm}(t)$ we formally solve eq. (3.15c) and obtain

$$\langle\langle \dot{R}\hat{F}(t)\rangle\rangle_{\rm diss} = \sum_{nm}\int_{t_0}^{t} dt' \Delta_{nm}(t,t')\frac{i}{1+\alpha_{nm}^2}\left\{\frac{P_n(t')}{d_n} - \frac{P_m(t')}{d_m} + \frac{i\alpha_{nm}^2}{\hbar\Gamma_{nm}}\left(\frac{\delta E_n(t')}{d_n} + \frac{\delta E_m(t')}{d_m}\right)\right\}, \tag{A.15}$$

with the correlation function

$$\Delta_{nm}(t,t') = (-i\omega_{nm}-\Gamma_{nm})\hbar e^{(-i\omega_{nm}-\Gamma_{nm})(t-t')}\sum_{\nu\mu} v^*_{n\nu,\,m\mu}(t)v_{n\nu,\,m\mu}(t'). \tag{A.16}$$

In analogy to the discussion of sect. 4 of I[†] this may be interpreted as

$$\Delta_{nm}(t,t') = \sum_{\nu\mu}(-i)\dot{R}(t)F^*_{n\nu,\,m\mu}(t)\frac{\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}(E_{n\nu}-E_{m\mu})dt''\right]}{E_{n\nu}(t')-E_{m\mu}(t')}\dot{R}(t')F_{n\nu,\,m\mu}(t'). \tag{A.17}$$

The correspondence between the diffusion coefficient (A.12) with the correlation function (A.6) and the energy rate (A.15) with the correlation function (A.17) is striking. It manifests the close link between dissipation and fluctuation. It may be further supported by a comparison with the results of the Brownian motion approach [3]) where, in a Markovian approximation, the well-known fluctuation-dissipation theorem holds.

In lowest-order pertubation theory, the generalized friction kernel appearing in eq. (16) of ref. [3]) reads

$$\mathcal{K} = \int_0^{\beta} d\lambda \,\mathrm{tr}\{\delta\hat{F}e^{-(i/\hbar)\hat{H}_0(t-\tau)}e^{-\beta\tilde{H}}e^{\lambda\tilde{H}}\delta\hat{F}e^{-\lambda\tilde{H}}e^{(i/\hbar)H_0(t-\tau)}\}. \tag{A.18}$$

[†] In eqs. (4.15), (4.16) of I the sum should run over $n > m$, only. In eq. (4.16) the states $n\nu$, $m\mu$ should be interchanged in the matrix elements.

After some algebra we find

$$\mathscr{K} = \sum_{nm}\sum_{\nu\mu} |\delta F_{n\nu,m\mu}|^2 \frac{e^{-(i/\hbar)(E_{n\nu}-E_{n\mu}-i\eta)(t-\tau)}}{E_{n\nu}-E_{m\mu}-i\eta}(\rho_{n\nu,n\nu}-\rho_{m\mu,m\mu}). \tag{A.19}$$

Similarly, the diffusion kernel

$$\mathscr{D} = \mathrm{tr}\{\delta\hat{F}e^{-(i/\hbar)H_0(t-\tau)}\tfrac{1}{2}[\delta\hat{F}, e^{-\beta\tilde{H}}]_+ e^{(i/\hbar)H_0(t-\tau)}\} \tag{A.20}$$

reads

$$\mathscr{D} = \sum_{nm}\sum_{\nu\mu} |\delta F_{n\nu,m\mu}|^2 e^{-(i/\hbar)(E_{n\nu}-E_{m\mu}-i\eta)(t-\tau)}\tfrac{1}{2}(\rho_{n\nu,n\nu}+\rho_{m\mu,m\mu}). \tag{A.21}$$

Here $\rho_{n\nu,n\nu} = e^{-\beta E_{n\nu}}/\sum_{n\nu} e^{-\beta E_{n\nu}}$. η is an infinitesimal increment.

In our present approach, $\rho_{n\nu,n\nu} = P_n/d_n + (E_{n\nu}-\bar{E}_n)\delta E_n/\varepsilon_n^2$.

We see a close correspondence between eq. (A.19) and eqs. (A.15), (A.17) as well as between (A.21) and (A.12), (A.6).

In a Markovian approximation, the Brownian motion approach leads to the fluctuation-dissipation theorem

$$\int_0^\infty \mathscr{D}(t)\mathrm{d}t = T\int_0^\infty \mathscr{K}(t)\mathrm{d}t.$$

No such theorem can hold in the present dynamical theory for $\hat{\rho}(t)$, since a temperature is not introduced.

Appendix B

RELATION TO THE WORK OF WILLIS AND PICARD [2])

In their paper [2]) Willis and Picard treat the formal reduction of the coupled von Neumann equation for some "matter" degrees of freedom m with some other "field" degrees of freedom f. A reduced and coupled set of equations of motion is deduced for both systems in a symmetrical fashion. In this appendix we want to discuss the similarities and differences between the two reduction schemes.

We sketch the reduction scheme of Willis and Picard applied to our semiclassical Liouville equation (1.1)

$$\frac{\partial}{\partial t}\hat{D}(R,P,t) = \frac{1}{i\hbar}[\hat{H},\hat{D}]_- - \frac{P}{M}\frac{\partial}{\partial R}\hat{D} - \frac{1}{2}\left[\hat{F},\frac{\partial}{\partial P}\hat{D}\right]_+ \tag{B.1}$$

with

$$\hat{H} = \hat{h}_0 + \hat{V}(R) + \frac{P^2}{2M}. \tag{B.2}$$

We choose R and P as the field degrees of freedom and the internal as the matter

degrees of freedom, and define

$$\sigma(R,P,t) = \mathrm{tr}\hat{D}(R,P,t), \tag{B.3a}$$

$$\hat{\rho}(t) = \int \mathrm{d}r\mathrm{d}P\hat{D}(R,P,t). \tag{B.3b}$$

Notice that σ is defined as in (2.1) but $\hat{\rho}\,(t)$ is different from the choice taken in eq. (2.20).

The Willis and Picard projector is given as

$$\mathscr{P}_{\mathrm{WP}}(t) = \hat{\rho}\mathrm{tr} + \sigma \int - \hat{\rho}\sigma \int \mathrm{tr}, \tag{B.4}$$

$$\mathscr{Q}_{\mathrm{WP}}(t) = 1 - \mathscr{P}_{\mathrm{WP}}(t) \tag{B.5}$$

with the properties

$$\mathrm{tr}\mathscr{P}_{\mathrm{WP}}\cdot = \mathrm{tr}\cdot, \qquad \int \mathscr{P}_{\mathrm{WP}}\cdot = \int \cdot. \tag{B.6}$$

We define the following Liouville operators:

$$L = L_m + L_f + L', \tag{B.7a}$$

$$L_m\cdot = \frac{1}{\hbar}[h_0, \cdot\,]_-, \tag{B.7b}$$

$$L_f\cdot = -\frac{P}{M}\frac{\partial}{\partial R}\cdot, \tag{B.7c}$$

$$L'\cdot = \frac{1}{\hbar}[\hat{V}, \cdot\,]_- - \tfrac{1}{2}i\left[\hat{F}, \frac{\partial}{\partial P}\cdot\right]_+, \tag{B.7d}$$

$$\langle L'\rangle_{f,t}\cdot = \frac{1}{\hbar}[\langle V\rangle_{\sigma,t}\cdot\,]_-, \tag{B.7e}$$

$$\langle L'\rangle_{m,t} = -i\langle\hat{F}\rangle_{\rho}\frac{\partial}{\partial P}\cdot, \tag{B.7f}$$

$$\Delta_t L' = L' - \langle L'\rangle_{f,t} - \langle L'\rangle_{m,t}, \tag{B.7g}$$

$$\Delta_t L'\cdot = \frac{1}{\hbar}[\delta_{\sigma,t}\hat{V}, \cdot\,]_- - \frac{i}{2}\left[\delta_{\rho,t}\hat{F}, \frac{\partial}{\partial P}\cdot\right]_+, \tag{B.7h}$$

with

$$\delta_{\sigma,t}\hat{V} = \hat{V} - \langle \hat{V} \rangle_{\sigma,t}, \tag{B.8a}$$

$$\delta_{\rho,t}\hat{F} = \hat{F} - \langle \hat{F} \rangle_{\rho,t}. \tag{B.8b}$$

These definitions are the ones given by Willis and Picard [2]) generalized to the present case of a mixed quantal and classical von Neuman equation (B.1).

The final Willis and Picard coupled reduced equations of motion for $\hat{\rho}\ (t)$ and $\sigma(R, P, t)$ are

$$\frac{\partial}{\partial t}\sigma = -\frac{P}{M}\frac{\partial}{\partial R}\sigma - \langle \hat{F} \rangle_{\rho,t}\frac{\partial}{\partial P}\sigma - \frac{\partial}{\partial P}\int_{t_0}^{t} \mathrm{d}t' \mathrm{tr}$$

$$\times \left(\delta_{\rho,t}\hat{F}\mathcal{G}_{\mathrm{WP}}(t, t') \left\{ \frac{1}{i\hbar}[\delta_\sigma \hat{H}, \hat{\rho}]_- - \tfrac{1}{2}[\delta_\rho \hat{F}, \hat{\rho}]_+ \frac{\partial}{\partial P} \right\}_{t'} \right) \sigma(t'), \tag{B.9a}$$

$$\frac{\partial}{\partial t}\hat{\rho}(t) = \frac{1}{i\hbar}[\langle \hat{h} \rangle_{\sigma}, \hat{\rho}]_- - \int_{t_0}^{t} \mathrm{d}t' \int \mathrm{d}R \mathrm{d}P \frac{1}{\hbar}\delta_{\sigma,t}\hat{H}\mathcal{G}_{\mathrm{WP}}(t, t')\{\ \}\sigma(t'), \tag{B.9b}$$

where the curly brackets { } symbolize the same term as in eq. (B.9a) and $\mathcal{G}_{\mathrm{WP}}(t, t')$ is defined by

$$i\frac{\partial}{\partial t}\mathcal{G}_{\mathrm{WP}}(t, t') = \mathcal{Q}_{\mathrm{WP}} L \mathcal{Q}_{\mathrm{WP}} \mathcal{G}_{\mathrm{WP}}(t, t'), \qquad \mathcal{G}_{\mathrm{WP}}(t, t) = 1. \tag{B.10}$$

Eq. (B.9a) is formally identical to our eq. (2.14). Of course the propagator $\mathcal{G}_{\mathrm{WP}}$ is different from our $\mathcal{G}$ due to the different projector $\mathcal{Q}_{\mathrm{WP}}$. The reduced equation (B.9b) for $\hat{\rho}\ (t)$ is entirely different from our mean field one (2.20), which is the first part of eq. (B.9b) only. The additional second term on the r.h.s. of eq. (B.9b) represents the fluctuations induced into the internal system via the coupling to the R-P motion.

The calculation of $\hat{\rho}(t)$ is of course the key to any treatment of deep inelastic collisions (DIC). The internal system has $6A-6$ degrees of freedom. Therefore any useful equation for $\hat{\rho}(t)$ must be simple. Eq. (B.9b) is by far too complicated. We do not see any possibility of solving it by reducing it further. Therefore, we have to abandon the aesthetical appeal of having symmetrical equations for $\sigma\ (t)$ and $\hat{\rho}\ (t)$. The difficulties are not distributed symmetrically either. It is possible to have a complicated equation for the "simple" R-P motion but we need a simple equation for the complicated internal motion. That is the kind of "symmetry" we have to take into account, and this is achieved in the present paper.

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