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TIME-DEPENDENT SHELL-MODEL THEORY OF DISSIPATIVE  
 HEAVY-ION COLLISIONS

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## Abstract

A transport theory is formulated within a time-dependent shell-model approach. Time averaging of the equations for macroscopic quantities lead to irreversibility and justifies weak-coupling limit and Markov approximation for the (energy-conserving) one- and two-body collision terms. Two coupled equations for the occupation probabilities of dynamical single-particle states and for the collective variable are derived and explicit formulas for transition rates, dynamical forces, mass parameters and friction coefficients are given. The applicability of the formulation in terms of characteristic quantities of nuclear systems is considered in detail and some peculiarities due to memory effects in the initial equilibration process of heavy-ion collisions are discussed.

## 1. Introduction

The initial stage of a heavy-ion collision is characterized by the mutual approach of the nuclei in their ground states. Because of the long mean free path during this stage of the collision, the motion of the nucleons is expected to be governed by their self-consistent mean potential which evolves in time. This stage should therefore be well described by the time-dependent Hartree-Fock (TDHF) theory [1]. By residual interactions the Slater determinant of time-dependent single-particle states decays to more complex configurations. This decay leads possibly to a local statistical equilibrium where the system occupies the total phase space (total configuration space) which is 'locally' available, i.e. available for fixed values of the macroscopic (collective) degrees of freedom. The time necessary for this decay, i.e. the local equilibration time  $\tau_{loc}$  has been estimated to be of the order of  $10^{-21}$  s [2,3].

In the spirit of this discussion the inclusion of residual two-body collisions in a self-consistent mean-field theory (generalized TDHF theories) is a natural step for a more realistic description of heavy-ion collisions [4-10]. However, because of the numerical difficulties involved in such approaches, these attempts are still rudimental. Current transport theories (for a review cf. [11]) like the linear response theory [12], the window - and wall theory [13] and the non-perturbative transport theories [14-16] assume implicitly local statistical equilibrium throughout the collision. Therefore, these theories are not expected to describe properly the initial stage of the collision process where memory effects due to the local equilibration process are expected. Some memory effects have recently been considered within the linear response theory [17,18].

Memory effects due to the local equilibration process have been studied phenomenologically within macroscopic dynamical models [19,20] and microscopically

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within the Fermi-gas model and the harmonic oscillator model [3,21]. By these studies a new dissipation mechanism in large-amplitude collective nuclear motion has been introduced, the *dissipative diabatic dynamics*. The energy dissipation for example is characterized by a two-step process: The diabatic single-particle motion in the time-dependent mean field leads primarily to the storage of collective kinetic energy as a conservative potential. Subsequently, this potential energy is irreversibly dissipated by two-body collisions during the local equilibration. A remarkable dependence of angular and energy distributions on the size of the local equilibration time has been demonstrated [20].

The following study is devoted to the rigorous formulation of a transport theory within a time-dependent shell-model approach which allows for the explicit treatment of local equilibration and contains in some limit the dissipative diabatic dynamics. We start out from a dynamical single-particle basis (cf. § 2) which incorporates main parts of the interaction quantum-mechanically. A master equation for the single-particle occupation probabilities is derived in the weak-coupling limit by a suitable time-averaging procedure (cf. § 3). From the condition of total energy conservation we derive in § 4 an equation of motion for the collective variable with expressions for the potential energy, the mass parameter and the friction coefficient. In § 5 the applicability of the formulation to the initial equilibration process of heavy-ion collisions is discussed. We summarize and discuss in § 6 the main conclusions drawn from this formulation.

This paper was originally thought to form part III of the series "Transport Theory of Dissipative Heavy-Ion Collisions". However, in the course of developing the theory, the subject presented below, finally turned out to be rather independent from the previous published papers [22,23].

## 2. Dynamical single-particle basis

For simplicity we consider only a single collective variable  $q$ , for example the distance between the centers of the two colliding nuclei, and treat it as a classical variable  $q(t)$  which is a function of time  $t$ . The generalization to an arbitrary number of collective variables is straightforward.

A set of stationary single-particle wave functions  $\phi_\alpha(q)$  is formally defined by

$$H_0(q) \phi_\alpha(q) = \epsilon_\alpha(q) \phi_\alpha(q). \quad (2.1)$$

In order to obtain some criteria for optimizing this definition for a given dynamical situation we consider the time-dependent Schrödinger equation

$$i\hbar \psi(t)/\partial t = H(q(t))\psi(t) \quad (2.2)$$

for the total one-body Hamiltonian

$$H(q) = H_0(q) + H'(q). \quad (2.3)$$

In (2.2) we have absorbed  $\hbar^{-1}$  in the time variable, thus measuring times in  $\text{MeV}^{-1}$  (corresponding to  $6.6 \cdot 10^{-22}$  s). Expanding  $\psi(t)$  as

$$\psi(t) = \sum_{\alpha} c_{\alpha}(t) \phi_{\alpha}(q,t) \quad (2.4)$$

in terms of the states

$$\phi_{\alpha}(q,t) = \phi_{\alpha}(q) \exp \left[ -i \int_{\alpha}^t \epsilon_{\alpha}(t') dt' \right] \quad (2.5)$$

we obtain the set

$$i \frac{\partial}{\partial t} c_{\beta}(t) = \sum_{\alpha} U_{\beta\alpha}(t) c_{\alpha}(t) \quad (2.6)$$

of coupled differential equations for the expansion coefficients  $c_{\alpha}(t)$ .

The coupling matrix elements are determined by

$$U_{\alpha\beta}(t) = \langle \phi_{\beta}(q) | H' - i\dot{q} \frac{\partial}{\partial q} | \phi_{\alpha}(q) \rangle \exp[-i \int_0^t \omega_{\alpha\beta}(t') dt'] \quad (2.7)$$

with  $\omega_{\alpha\beta} \equiv \epsilon_{\alpha} - \epsilon_{\beta}$ . The diagonal elements of  $H'$  vanish (i.e. are included in  $H_0$ ). The diagonal elements of  $\partial/\partial q$  vanish by the proper choice of phases for the wave functions.

An optimal choice of the basis states  $\phi_{\alpha}(q)$  would leave the coupling small such that an expansion in powers of  $U_{\alpha\beta}(t)$  becomes meaningful. We want to consider slow collective nuclear motions with collective velocities sufficiently smaller as compared to the Fermi velocity, in order to allow the nucleonic states to adjust continuously to the actual nuclear shape. The first thought would be to choose the adiabatic basis defined by  $H_0 = H$  and hence  $H' = 0$ . However, it has been shown [3,24] that for realistic values of the collective velocities in fission and heavy-ion collisions the nucleonic motion near quasi-crossings [25,26] is far from the adiabatic limit. Rather than within adiabatic states the individual nucleons move in diabatic (i.e. crossing) states across the quasi-crossing. The reason for this behaviour is that each nucleon tries to keep the nodal structure of its wave function. The lower limit for the collective energy per nucleon where the diabatic behaviour becomes dominant has been estimated to be around 0.03 MeV [3]. Remarkable diabatic effects have been obtained even at smaller energies in the fission process [24]. A suitable diabatic basis may be constructed from adiabatic states by connecting states of maximum overlap or by taking out from the total one-body Hamiltonian  $H(q)$  some symmetry breaking parts  $H'$  [27]. In general the optimal basis depends implicitly on the collective velocity  $\dot{q}$ . With increasing  $\dot{q}$  this basis becomes more and more diabatic in the sense that an increasing number of quasicrossings are changed into crossings of the corresponding diabatic states. Such a dynamical single-particle basis is used in the following formulation.

The use of dynamical basis states  $\chi_{\alpha}(q,t)$  which do not depend on  $\dot{q}$  explicitly (cf. (2.1) and (2.5)), may not be always sufficient. In order to reduce the dynamical coupling  $\langle \phi_{\beta} | \dot{q} \partial/\partial q | \phi_{\alpha} \rangle$  it might be appropriate to introduce according to [25] a common phase factor in  $\chi_{\alpha}$  as

$$\chi_{\alpha}(q,\dot{q};t) = \phi_{\alpha}(q) \exp[-i \int_0^t \epsilon_{\alpha}(t') dt' + M\Phi] \quad (2.8)$$

where  $M(q)$  and  $\Phi(q,\dot{q},t)$  denote the effective mass and the velocity potential of the incompressible irrotational flow which corresponds to the collective (shape-) degree of freedom  $q$ . The use of (2.8) instead of (2.5) is expected to be particularly useful in the diabatic limit of single-particle motion where the nodal structure of the wave functions is essentially preserved. In first approximation the nodes and magnitudes of the wave functions are carried along with the irrotational incompressible fluid velocity. The implications of such common phase factors have been studied by several authors [9,28-30]. For simplicity we restrict our following formulation to the basis states (2.5).

### 3. Transport equation for the one-body occupation probabilities

We consider the one-body density matrix

$$\rho_{\alpha\beta}(t) = c_{\alpha}(t) c_{\beta}^*(t) \quad (3.1)$$

in the representation of the dynamical single-particle states  $x_{\alpha}(q,t)$  defined by (2.1) and (2.5). Using (2.6) we obtain the Liouville equation

$$i\frac{\partial}{\partial t} \rho_{\alpha\beta}(t) = \sum_{\gamma\delta} L_{\alpha\beta,\gamma\delta}(t) \rho_{\gamma\delta}(t) \quad (3.2)$$

with the Liouville matrix defined by

$$L_{\alpha\beta,\gamma\delta}(t) = U_{\alpha\gamma}(t)\delta_{\beta\delta} - U_{\delta\beta}(t)\delta_{\alpha\gamma}. \quad (3.3)$$

It is convenient for the following formal manipulations to introduce a superspace spanned by the vectors  $|\alpha\beta\rangle$  which are independent of  $t$  (interaction picture), and define the density vector  $|\rho(t)\rangle$  and the Liouville operator  $L(t)$  in superspace by their matrix elements  $(\alpha\beta|\rho(t)) \equiv \rho_{\alpha\beta}(t)$  and  $(\alpha\beta|L(t)|\gamma\delta) \equiv L_{\alpha\beta,\gamma\delta}(t)$ . With these notations [3] the Liouville equation (3.2) reads

$$i\frac{\partial}{\partial t} |\rho(t)\rangle = L(t)|\rho(t)\rangle. \quad (3.4)$$

Using a projection technique we derive in §3.1 a generalized master equation and obtain in §3.2 the transport equation for the occupation probabilities  $\rho_{\alpha\alpha}(t)$  by time-averaging. In §§ 3.3 and 3.4 we discuss the inclusion of residual interactions and the energy conservation in the collision terms.

#### 3.1 Generalized master equation

In order to obtain a closed equation for the diagonal elements of the density matrix we use the projection technique as described by Zwanzig [31]. Multiplying the Liouville equation with the (time-independent) projectors

$$P = \sum_{\alpha} |\alpha\alpha\rangle\langle\alpha\alpha| \quad (3.5)$$

and  $Q = 1 - P$  we obtain the coupled equations

$$i\frac{\partial}{\partial t} P|\rho(t)\rangle = PL(t)\{P|\rho(t)\rangle + Q|\rho(t)\rangle\} \quad (3.6)$$

$$i\frac{\partial}{\partial t} Q|\rho(t)\rangle = QL(t)\{P|\rho(t)\rangle + Q|\rho(t)\rangle\} \quad (3.7)$$

for the diagonal components  $P|\rho(t)\rangle$  and the non-diagonal components  $Q|\rho(t)\rangle$  of the density matrix. The second equation (3.7) may be solved formally as

$$Q|\rho(t)\rangle = G(t,t_0)Q|\rho(t_0)\rangle - i \int_0^{t-t_0} dt' G(t,t-t')QL(t-t')P|\rho(t-t')\rangle \quad (3.8)$$

with the intermediate propagator in  $Q$ -space

$$G(t,t-t') = Q - i \int_0^{t-t'} dt'' QL(t-t-t'')QG(t-t-t'',t-t'). \quad (3.9)$$

Inserting the expression (3.8) into (3.6) we obtain

$$i\frac{\partial}{\partial t} P|\rho(t)\rangle = PL(t)G(t,t_0)Q|\rho(t_0)\rangle - i \int_0^{t-t_0} dt' PL(t)G(t,t-t')QL(t-t')P|\rho(t-t')\rangle \quad (3.10)$$

where we have used that  $PL(t)P$  vanishes (cf. the definition (3.3) of the Liouville operator). By projection on  $\langle\alpha\alpha|$  this equation yields the generalized master equation (pre-master equation) for the occupation probabilities  $\rho_{\alpha\alpha}(t)$

$$\frac{\partial}{\partial t} \rho_{\alpha\alpha}(t) = I_{\alpha\alpha}(t,t_0) + \sum_{\beta} \int_0^{t-t_0} dt' M_{\alpha\alpha,\beta\beta}(t,t')\rho_{\beta\beta}(t-t') \quad (3.11)$$

with the initial correlation term

$$I_{\alpha\alpha}(t,t_0) \equiv -i\langle\alpha\alpha|L(t)G(t,t_0)Q|\rho(t_0)\rangle \quad (3.12)$$

and the memory kernel

$$M_{\alpha\alpha,\beta\beta}(t,\tau) \equiv -\langle\alpha\alpha|L(t)G(t,t-\tau)QL(t-\tau)|\beta\beta\rangle. \quad (3.13)$$

The initial correlation term represents the contribution from non-diagonal elements of  $\rho$  at the initial time  $t_0$  well before the nuclear interaction starts.

If the basis states coincide with the shell-model states for the separated nuclei, contributions to  $Q[\rho(t_0)]$  result only from the slow collective motion (virtual excitations) or from the residual interactions (ground-state correlations) and hence are small. In general, however,  $Q[\rho(t_0)]$  depends on the choice of the basis states and therefore, need not to be small. The second term on the r.h.s. of (3.11) is usually referred to as the collision term and describes the change of the occupation probabilities due to the coupling  $U_{\alpha\beta}(t)$  between the single-particle states.

### 3.2 Time-averaging

In general the memory kernel (3.13) may produce fast oscillating contributions in the generalized master equation (3.11). Since we are only interested in the smooth behaviour of the occupation probabilities we eliminate such oscillations by taking an average over time. The time average of a quantity  $A(t)$  is defined by

$$\bar{A}(t) \equiv \int_{-\infty}^{+\infty} dt' w(t-t') A(t') \quad (3.14)$$

where the weight function may be chosen for example of Gaussian or Lorentzian shape. By partial integration it is seen immediately that  $\partial \bar{A} / \partial t = \partial A / \partial t$ .

In performing the time average over the r.h.s. of eq. (3.11) we write  $\rho = \bar{\rho} + \delta$  and consider first that part with  $\bar{\rho}$ . The neglect of  $\delta$  in the integral results in

$$\frac{\partial}{\partial t} \bar{\rho}_{\alpha\alpha}(t) = \sum_{\beta} \int_{-\infty}^{+\infty} dt' w(t-t') \{ I_{\alpha\alpha}(t', t_0) + \int_0^{t'-t_0} dt M_{\alpha\alpha, \beta\beta}(t', \tau) \bar{\rho}_{\beta\beta}(t-\tau) \} \quad (3.15)$$

which is considered in more detail. Since we start out in a heavy-ion collision with the ground-state occupation probabilities, i.e.  $\bar{\rho}_{\beta\beta}(t_0) = 0$ , we have only to worry if oscillatory terms can build up during the collision process and affect the mean value  $\bar{\rho}$ .

We consider the weak-coupling limit where the intermediate propagator (3.9) is approximated by unity. The justification of this approximation will be discussed below. Inserting (3.3) in (3.13) yields the memory kernel in the form

$$M_{\alpha\alpha, \beta\beta}(t, \tau) = U_{\alpha\beta}(t) U_{\beta\alpha}(t-\tau) - \delta_{\alpha\beta} \int_{\alpha\gamma} U_{\alpha\gamma}(t) U_{\gamma\alpha}(t-\tau) + c.c. \quad (3.16)$$

Thus we have to examine terms of the form

$$\int_{-\infty}^{+\infty} dt' \frac{e^{i\theta/\tau}}{(t-t')^2 + \theta^2} \int_0^{t'-t_0} dt'' U_{\alpha\beta}(t') U_{\beta\alpha}(t'-\tau) \exp[-i \int_{t'-\tau}^{t'} dt'' w_{\beta\alpha}(t'')] \quad (3.17)$$

where we have introduced a Lorentz curve of width  $2\theta$  for  $w(t-t')$  and used (2.7) with the notation

$$U_{\alpha\beta}(t) = \langle \phi_{\alpha}(q) | H^1 - i q \frac{\partial}{\partial q} | \phi_{\beta}(q) \rangle_{q=q(t)} \quad (3.18)$$

The largest variation in  $\tau$  is expected from the exponential. Using a linear approximation to  $\omega_{\beta\alpha}(t'')$  around  $t''=t$  we obtain for the argument  $-i[\omega_{\beta\alpha}(t) + \dot{\omega}_{\beta\alpha}(t)(t'-t)]\tau$  where the term proportional to  $\tau^2$  is neglected. Performing the integration over  $t'-t$  replaces  $i\dot{\omega}_{\beta\alpha}(t)(t'-t)$  by the decay constant

$$\Gamma_{\beta\alpha}^{-1}(t) = |\dot{\omega}_{\beta\alpha}(t)|_{\theta = (\tau_{\text{corr}}^{\beta\alpha})^{-1}} \quad (3.19)$$

which is the inverse of the correlation time  $\tau_{\text{corr}}^{\beta\alpha}$  and limits the integration over  $\tau$  essentially to  $\tau \leq \tau_{\text{corr}}^{-1}$ . The neglect of the  $\tau^2$ -term in the argument imposes the condition  $|\dot{\omega}_{\beta\alpha}| \tau^2 / 2 \ll \pi$  or with  $\tau \approx \tau_{\text{corr}}^{-1}$  and (3.19)

$$\Gamma_{\beta\alpha}^{-1} = \tau_{\text{corr}}^{\beta\alpha} \ll 2\pi\theta \quad (3.20)$$

Furthermore, by replacing  $\bar{\rho}_{\beta\beta}(t-\tau)$  by  $\bar{\rho}_{\beta\beta}(t) \equiv n_{\beta}(t)$  in the integral on the r.h.s. of (3.15) we imply the conditions

$$\tau_{\text{corr}}^{\beta\alpha} \ll \tau_{\text{loc}}^{\beta\alpha} \quad (3.21)$$

where  $\tau_{loc}$  denotes the relaxation time of the occupation probabilities  $n_\alpha(t)$ . Within these limits we obtain from (3.15) the master equation

$$\frac{3}{3t} \dot{n}_\alpha(t) = \sum_\beta W_{\alpha\beta}(t) [n_\beta(t) - n_\alpha(t)] \quad (3.22)$$

for the occupation probabilities with the transition rate

$$W_{\alpha\beta}(t) = 2 \operatorname{Re} \int_0^\infty d\tau \overline{U_{\alpha\beta}(t)} \overline{U_{\beta\alpha}(t-\tau)} \quad (3.23)$$

$$= 2 \operatorname{Re} \int_0^\infty d\tau \overline{U_{\alpha\beta}(t)} \overline{U_{\beta\alpha}(t-\tau)} \exp[-i\omega_{\beta\alpha}(t)\tau - \Gamma_{\beta\alpha}(t)\tau] \quad (3.24)$$

In writing down (3.22) we have neglected the initial correlation term. This and the replacement of the upper limit in (3.23) by  $\infty$  is justified for  $|t-t_0| \gg \tau_{corr}$ . The relation (3.23) is more general than (3.24) where we assume in addition that the matrix elements are smooth over the averaging interval  $\theta$ . This imposes the restriction

$$\theta \ll \tau_{matrix} \quad (3.25)$$

where  $\tau_{matrix}$  denotes the characteristic time interval for a significant variation of the matrix elements  $U_{\alpha\beta}(t)$ . We note in passing that  $W_{\alpha\beta}(t)$  as given by (3.23) and (3.24) is symmetric in the indices, i.e.  $W_{\alpha\beta}(t) = W_{\beta\alpha}(t)$ . Thus (3.22) conserves the total occupation probability  $\sum_\alpha n_\alpha(t) = A$ .

So far we have treated only the contribution from  $\overline{\rho_{\beta\beta}}(t-\tau)$  on the r.h.s. of (3.15). A fluctuating part  $\hat{\rho}_{\beta\beta}$  is produced whenever the system passes a crossing of diabatic levels where the argument of the exponential in (3.17) becomes stationary. The contribution from a crossing at  $\tau = \tau_c$  is proportional to the oscillating factor  $\exp[-i\omega_{\beta\alpha}(t-t_c)^2]$  with  $t_c = t-\tau_c$ . The frequency of these oscillations increases with increasing distance from the crossing and hence, the contribution to  $\hat{\rho}_{\alpha\alpha}(t) = \int dt' \partial_{\alpha\alpha}^2 / \partial t'$  dies out. It is for this reason that such oscillations in  $\partial \rho_{\alpha\alpha} / \partial t$  do not contribute to  $\overline{\rho_{\alpha\alpha}}$ . Only a coherent superposition of contributions from different level crossings could build up a significant contribution to  $\overline{\rho_{\alpha\alpha}}$ . This, however, is unlikely to occur because of the random location of crossings as function of  $q$ .

We may check the master equation (3.22) by considering the Landau-Zener-Stueckelberg (LZS) model [25,26] of two crossing levels  $\alpha, \beta$  with constant interaction matrix element  $U_{\alpha\beta} = H'_{\alpha\beta}$ . From (3.24) we obtain for the transition rate

$$W_{\alpha\beta}(t) = |H'_{\alpha\beta}|^2 \frac{2\Gamma_{\alpha\beta}}{\omega_{\alpha\beta}^2(t) + \Gamma_{\alpha\beta}^2} \quad (3.26)$$

Integrating across the level crossing we find for the jump probability from level  $\beta$  to level  $\alpha$

$$\int_{-\infty}^{+\infty} dt W_{\alpha\beta}(t) = 2\pi |H'_{\alpha\beta}|^2 / |\dot{\omega}_{\alpha\beta}| \quad (3.27)$$

where  $\omega_{\alpha\beta} = \dot{\omega}_{\alpha\beta} t$  has been used. The result is independent of the time-smoothing interval  $\theta$  and agrees to quadratic order in  $H'_{\alpha\beta}$  with the exact solution  $1 - \exp(-2\pi |H'_{\alpha\beta}|^2 / |\dot{\omega}_{\alpha\beta}|)$ .

In this subsection we have considered the memory kernel (3.13) in the weak-coupling limit by replacing the propagator by unity. The validity of this treatment may be checked by evaluating the next order corrections to 1. The second order correction to this diagonal element is given according to (3.9) by

$$-\sum_{\gamma\delta} \int_0^{\tau} d\tau_1 \int_0^{\tau_1} d\tau_2 L_{\alpha\beta, \gamma\delta}(t-\tau+\tau_1) L_{\gamma\delta, \alpha\beta}(t-\tau+\tau_2) \quad (3.28)$$

Introducing the expressions (2.7), (3.3) and (3.18) we obtain

$$\sum_{\gamma} (|U_{\alpha\gamma}(t)|^2 + |U_{\beta\gamma}(t)|^2) (\tau_{corr}^{\alpha\beta})^2 \quad \text{for } \omega_{\alpha\gamma}^{-1}, \omega_{\beta\gamma}^{-1} \gg \tau_{corr}$$

and

$$\sum_{\gamma} (\omega_{\alpha\gamma}^{-1} |U_{\alpha\gamma}(t)|^2 + \omega_{\beta\gamma}^{-1} |U_{\beta\gamma}(t)|^2) \tau_{corr}^{\alpha\beta} \quad \text{for } \omega_{\alpha\gamma}^{-1}, \omega_{\beta\gamma}^{-1} \ll \tau_{corr}$$

In between these two limits the behaviour as function of  $\omega_{\alpha\gamma} \tau_{corr}^{\alpha\beta}$  and  $\omega_{\beta\gamma} \tau_{corr}^{\alpha\beta}$  is more or less wiggling. In order to obtain a simple closed-form expression we smoothly join the two limits by a simple interpolation function and obtain as a condition for the validity of the weak-coupling limit

$$\sum_{\gamma} \left( \frac{|U_{\alpha\gamma}(t)|^2}{\gamma + \omega_{\alpha\gamma} \tau_{corr}^{\alpha\beta}} + \frac{|U_{\beta\gamma}(t)|^2}{1 + \omega_{\beta\gamma} \tau_{corr}^{\alpha\beta}} \right) (\tau_{corr}^{\alpha\beta})^2 \ll 1 \quad (3.29)$$

The consideration of the linear terms of  $G$  leads to a less restrictive condition. Usually one regards the condition  $\sum_{\beta} M_{\alpha\beta}(t) \tau_{\text{corr}}^{\alpha\beta} \ll 1$  which is equivalent to  $\tau_{\text{corr}}^{\alpha\beta} \ll \tau_{\text{loc}}$  of (3.21) as sufficient for the validity of the weak-coupling limit. Introducing the expression (3.26) leads to

$$2 \sum_{\beta} |U_{\alpha\beta}(t)|^2 \cdot \frac{(\tau_{\text{corr}}^{\alpha\beta})^2}{1 + (w_{\alpha\beta} \tau_{\text{corr}}^{\alpha\beta})^2} \ll 1 \quad (3.30)$$

which seems to be somewhat less restrictive than (3.29) because of the smaller contributions from high frequencies ( $w_{\alpha\beta} \tau_{\text{corr}}^{\alpha\beta} \gg 1$ ).

### 3.3 Inclusion of two-body collisions

In the previous sections residual two-body interactions have been neglected. The collision term on the r.h.s. of (3.22)

$$K_{\alpha}^{(1)}(t) = \int_{\beta} 2 \operatorname{Re} \int_0^{\infty} d\tau \frac{U_{\alpha\beta}(t) U_{\beta\alpha}(t-\tau)}{V_{\alpha\beta}(t) V_{\beta\alpha}(t-\tau)} \quad (3.31)$$

$$\cdot [(1-n_{\alpha}(t)) n_{\beta}(t) - n_{\alpha}(t)(1-n_{\beta}(t))]$$

describes the transitions due to one-body couplings only. In this subsection we obtain the two-body collision term diagrammatically in analogy to the one-body expression. A rigorous derivation within the time-averaging procedure will be published separately [32]. The gain or loss terms of  $K_{\alpha}^{(1)}$  can be associated with the diagram shown in Fig. 1a. The corresponding two-body diagram is given in Fig. 1b where  $V_{\alpha\gamma, \beta\delta}(t)$  denote the two-body matrix elements  $\langle \chi_{\alpha} \chi_{\gamma} | V | \chi_{\beta} \chi_{\delta} \rangle$  taken with the single-particle states  $\chi_{\alpha}$ , cf. (2.5).

Taking all exchange terms into account we find the corresponding analytical expression

$$K_{\alpha}^{(2)}(t) = \int_{\beta, \gamma, \delta} 2 \operatorname{Re} \int_0^{\infty} d\tau \left\{ \frac{V_{\alpha\gamma, \beta\delta}(t) V_{\beta\delta, \alpha\gamma}(t-\tau)}{V_{\alpha\gamma, \beta\delta}(t) V_{\beta\delta, \alpha\gamma}(t-\tau)} - \frac{V_{\alpha\gamma, \beta\delta}(t) V_{\beta\delta, \alpha\gamma}(t-\tau)}{V_{\alpha\gamma, \beta\delta}(t-\tau) V_{\beta\delta, \alpha\gamma}(t)} \right\} \cdot [(1-n_{\alpha}(t))(1-n_{\gamma}(t)) n_{\beta}(t) n_{\delta}(t) - n_{\alpha}(t) n_{\gamma}(t)(1-n_{\beta}(t))(1-n_{\delta}(t))] \quad (3.32)$$

Mixed terms containing  $U$  and  $V$  are neglected because they do not add up coherently and therefore are expected to give only a small contribution to  $\partial n_{\alpha} / \partial t$ . By performing the time average in analogy to the derivation of (3.22) to (3.24) we find

$$\frac{V_{\alpha\gamma, \beta\delta}(t) V_{\beta\delta, \alpha\gamma}(t-\tau)}{V_{\alpha\gamma, \beta\delta}(t) V_{\beta\delta, \alpha\gamma}(t-\tau)} \exp[-i w_{\delta\gamma\beta\alpha}(t) \tau - \Gamma_{\delta\gamma\beta\alpha}(t) \tau] \quad (3.33)$$

with

$$w_{\delta\gamma\beta\alpha}(t) = w_{\delta\gamma} + w_{\beta\alpha} = (\epsilon_{\beta} + \epsilon_{\gamma} - \epsilon_{\alpha} - \epsilon_{\delta}) / \hbar, \quad (3.34)$$

$$\Gamma_{\delta\gamma\beta\alpha}(t) = |w_{\delta\gamma\beta\alpha}| \Theta. \quad (3.35)$$

We note that the correlation time for the two-body matrix elements is determined by the difference in the slopes of all four energy levels. As in the case of one-body couplings we have assumed in deriving (3.33) that the corresponding two-body matrix elements  $V_{\alpha\gamma, \beta\delta}(t)$  evaluated with the single-particle wave functions  $\phi_{\alpha}$  are smooth as compared to the phase factors.

The two-body collision term (3.32) appears to be quite similar to the expressions derived recently [6,10] in connection with extensions of TDHF. However, there are considerable differences in detail. In [6,10] the collision term has been evaluated by applying statistical assumptions about the two-body matrix elements. It is shown in [6] that the ensemble average of the full correlation function  $V_{\alpha\gamma, \beta\delta}(t) V_{\beta\delta, \alpha\gamma}(t-\tau)$  leads to a fast decay in  $\tau$ . The subsequent treatment leads essentially to an expression where our  $\tau_{\delta\gamma\beta\alpha}$  of (3.35) is replaced by the sum of the single-particle decay widths. In [10] and in our time-averaging procedure, the memory of the collision integrals is determined by the time-dependence of the single-particle levels. This also gives rise to a small correlation time for the full correlation function. However, the application of an ensemble average as performed in [10] and our time average leads to different results with respect to energy conservation in the collision term (cf. next subsection and §6).



### 3.4 Energy conservation in the collision terms

The transition rates for the one- and two-body collisions are of the form (cf. (3.23) and (3.32))

$$W_{fi}(t) = 2 \operatorname{Re} \int_0^\infty d\tau v_{if}(t)v_{fi}(t-\tau) \exp \left[ -i \int_{t-\tau}^t dt' \omega_{fi}(t') \right] \quad (3.36)$$

where  $\omega_{fi}$  is the difference in the initial and final single-particle energies as defined in (2.7) and (3.34). By definition, the coupling matrix elements  $v_{if}(t)$  are slowly varying in time. Performing the time average we obtain

$$W_{fi}(t) = 2 \operatorname{Re} \int_0^\infty d\tau v_{if}(t)v_{fi}(t-\tau) \exp \left[ -i\omega_{fi}(t)\tau - \Gamma_{fi}(t)\tau \right]. \quad (3.37)$$

By considering the leading term of the expansion

$$v_{fi}(t-\tau) = v_{fi}(t) - \tau \partial v_{fi}/\partial t + \dots \quad (3.38)$$

and returning to the time average we can rewrite (3.36) as

$$W_{fi}(t) = 2 \operatorname{Re} \int_0^\infty d\tau \frac{|v_{if}(t)|^2 \exp[-i\omega_{fi}(t)\tau - n\tau]}{|v_{if}(t)|^2 \exp[-i\omega_{fi}(t)\tau - n\tau]} \quad (3.39)$$

with  $n \rightarrow +0$ . Integration over  $\tau$  yields

$$W_{fi}(t) = 2\pi \frac{|v_{if}(t)|^2 \delta(\omega_{if}(t))}{|v_{if}(t)|^2 \delta(\omega_{if}(t))} \quad (3.40)$$

which looks quite similar to the transition rate obtained from standard perturbation theory for time-independent interactions and energies. The energy conservation in the collision terms as expressed by (3.40) is an attractive feature of the time-averaging procedure. It suggests the interpretation that the energy is conserved instantaneously in the time-averaged transition rates.

Due to the time average, however, the transition rate is essentially non-zero as long as the energy levels are close within a range given by  $\Gamma_{fi}(t)$ , cf. (3.24) and (3.33). The same effect would be obtained by smearing the energy levels according to  $\Gamma_{fi}$ . Thus, the more correct statement is that the collision terms conserve energy in the mean (time average).

From the similarity of the expression (3.40) for two-body collisions with the transition rate in the usual Boltzmann collision term we can draw some important conclusions about the mean free path of nucleons in a time-dependent mean field as compared to stationary fields. Without the time dependence of the single-particle levels the transition rate would be the same as for a dilute Fermi gas of the same density. However, due to the shifts of the single-particle levels in time and the time average in (3.40) the transition rate differs from the Fermi-gas expression by a smearing of the single-particle energies. This smearing can be accounted for by replacing in the Boltzmann collision term the temperature  $T$  in the Fermi-distribution functions for the occupation probabilities by an effective temperature  $T_{\text{eff}} > T$ . Since  $T_{\text{eff}}$  has to account also for the smearing due to the time-dependence of the single-particle levels, it is determined by the total excitation energy including the energy stored by the shifts of the single-particle levels. Thus we conclude that the mean free path of nucleons in time-dependent mean fields is practically the same as in the stationary case if only the total excitation energy is taken for calculating the temperature. In this way calculations of the mean free path of nucleons in nuclear matter or finite nuclei are also reasonable estimates for the motion of nucleons in time-dependent mean fields. We will return to this point in connection with estimates for  $\tau_{\text{loc}}$  in § 5.

So far we have considered only the leading term of the expansion (3.38) in the transition rate (3.36). Higher-order terms give rise to real and virtual transitions between states with different energies and hence, describe the exchange of intrinsic and collective energy. They can be studied systematically term by term. However, this will not be done here for the transition rates. Instead we will take up this expansion in the following § 4 in connection with the derivation of an equation of motion for the collective variable.

4. Equation of motion for the collective variable

So far we have introduced the collective variable  $q(t)$  as a free parameter which has to be determined from some general property of the system under consideration. Since we describe a closed system with no external interactions it is necessary to determine  $q(t)$  such as to conserve the total energy, i.e.

$$dE/dt = 0. \quad (4.1)$$

Within the shell-model approach the total energy of the system is

$$E = E^0 + \text{Tr} \{H(q)[\rho(t) - \rho^0(q)]\} \quad (4.2)$$

where  $\rho^0(q)$  denotes the ground-state density matrix. Thus (4.1) becomes

$$\begin{aligned} & \dot{q} \frac{\partial E}{\partial q} + \text{Tr} \{ \dot{q} \frac{\partial H}{\partial q} [\rho(t) - \rho^0(q)] \} \\ & = -\text{Tr} \{ H(q) [\dot{\rho} - \dot{q} \frac{\partial \rho^0}{\partial q}] \} = 0. \end{aligned} \quad (4.3)$$

The r.h.s. is zero (i) because  $\dot{\rho} = [H, \rho]$  and the invariance of the trace with respect to cyclic permutation and (ii) because  $\text{Tr} [H(q) \frac{\partial \rho^0}{\partial q}] = 0$  as is obvious in the basis of eigenstates of  $H(q)$ . In writing down (4.3) we have neglected the time-derivative of correction terms like rearrangement energies and correlation energies resulting from residual two-body interactions.

In order to obtain an equation of motion for  $q(t)$  we expand (4.3) in powers of  $\dot{q}$  and  $\ddot{q}$  as

$$\begin{aligned} \frac{dE}{dt} &= -\dot{q} F(q,t) + \dot{\epsilon}(q,t) \dot{q}^2 + \frac{d}{dt} \left[ \frac{1}{2} M \dot{q}^2 \right] + \dots \\ &= \dot{q} [-F + \dot{\epsilon} q + M \dot{q} + \frac{1}{2} \frac{dM}{dt} \dot{q} + \dots] = 0 \end{aligned} \quad (4.4)$$

and identify the coefficients of the lowest-order terms with the force  $F(q,t)$ , the friction coefficient  $\dot{\epsilon}(q,t)$  and the mass parameter  $M(q,t)$  of collective motion. The neglect of all other (higher-order) terms gives the classical equation of motion

$$M \ddot{q} + \dot{\epsilon} \dot{q} = -\frac{\partial E}{\partial q} + F + \frac{1}{2} \frac{dM}{dt} \dot{q} \quad (4.5)$$

for the collective variable  $q(t)$ . In the following we evaluate the dynamical force  $F$ , the friction coefficient  $\dot{\epsilon}$  and the mass  $M$  by considering the lowest-order terms in  $\dot{q}$  and  $\ddot{q}$  of (4.3) explicitly. The ground-state energy  $E^0(q)$  can be calculated for example by employing the method of Strutinsky [33]. The next subsections are concerned with the derivation of general expressions (§ 4.1) and the discussion of the adiabatic and diabatic limits (§ 4.2).

4.1 General expressions

As in § 3.2 we consider the time average of  $\text{Tr} \{ (\partial H / \partial q) [\rho(t) - \rho^0(q)] \}$  in order to eliminate fast oscillating terms which should not enter the equation of motion for the collective variable. We evaluate the trace for the basis states  $\chi_{\alpha} (q,t)$  as defined in (2.5),

$$\begin{aligned} \text{Tr} \{ (\partial H / \partial q) [\rho(t) - \rho^0(q)] \} &= \sum_{\alpha\beta} \langle \alpha | \partial H / \partial q | \beta \rangle \int_{\alpha\beta} \rho_{\alpha\beta}^0(t) \delta_{\alpha\beta} - \rho_{\alpha\beta}^0(q) \\ &+ \sum_{\alpha\beta\gamma} \langle \alpha | \frac{\partial H}{\partial q} | \gamma \rangle \rho_{\beta\gamma}^0(t) \end{aligned} \quad (4.6)$$

where  $\langle \alpha | \beta \rangle$  denote matrix elements of  $A$  with respect to the state  $\phi_{\alpha} \phi_{\beta}$  defined by (2.1). The matrix elements  $\rho_{\alpha\beta}^0(q)$  of the ground-state density is also defined with respect to the basis states  $\phi_{\alpha}$ . Using (3.8) for the non-diagonal elements of  $\rho(t)$  we obtain in analogy to (3.22) and within the same approximations for the r.h.s. of (4.6)

$$\begin{aligned} & \sum_{\alpha} \langle \alpha | \partial H / \partial q | \alpha \rangle \rho_{\alpha\alpha}^0(t) - \partial E^0(q) / \partial q \\ & + \sum_{\alpha\beta\gamma} \ln_{\beta} \langle \alpha | \rho_{\alpha\beta}^0(t) \rangle \text{Re} \int_{\alpha\beta} \frac{\partial H}{\partial q} \rho_{\beta\gamma}^0(t-\tau) \rho_{\gamma\alpha}^0(t,\tau) \end{aligned} \quad (4.7)$$

with

$$g_{\beta\alpha}(t, \tau) = \exp \left[ -i \int_{t-\tau}^t dt' \omega_{\beta\alpha}(t') \right] \quad (4.8)$$

and  $\tilde{E}(q)$  denoting the (time-smoothed) ground-state sum of the adiabatic single-particle energies. Since the coupling matrix elements  $U_{\beta\alpha}(t-\tau)$  are expected to be smooth over time-intervals  $\tau_{\beta\alpha}^{-1}$  we consider the expansion

$$U_{\beta\alpha}(t-\tau) = U_{\beta\alpha}(t) - \tau \partial U_{\beta\alpha} / \partial t + \dots \quad (4.9)$$

up to first order in  $\tau$ . From (3.16) and (4.9) we obtain the desired expansion (4.7) in powers of  $\dot{q}$  and  $\ddot{q}$ , and hence, by comparison with (4.4) the following expressions for the dynamical force  $F'(q, t)$ , the friction coefficient  $\xi(q, t)$  and the mass parameter  $M(q, t)$ ,

$$F'(q, t) = - \sum_{\alpha} \langle \alpha | \partial H / \partial q | \alpha \rangle n_{\alpha}(t) + \sum_{\alpha \neq \beta} [n_{\beta}(t) - n_{\alpha}(t)] \quad (4.10)$$

$$\cdot \operatorname{Re} \int_0^{\infty} d\tau i \langle \alpha | \frac{\partial H}{\partial q} | \beta \rangle \langle \beta | H' | \alpha \rangle g_{\beta\alpha}(t-\tau),$$

$$M(q, t) = \sum_{\alpha \neq \beta} [n_{\beta}(t) - n_{\alpha}(t)] \operatorname{Re} \int_0^{\infty} d\tau (-\tau) \langle \alpha | \frac{\partial H}{\partial q} | \beta \rangle \langle \beta | \frac{\partial}{\partial q} | \alpha \rangle g_{\beta\alpha}(t, \tau), \quad (4.11)$$

$$\xi(q, t) = \sum_{\alpha \neq \beta} [n_{\beta}(t) - n_{\alpha}(t)] \operatorname{Re} \int_0^{\infty} d\tau \left\{ \langle \alpha | \frac{\partial H}{\partial q} | \beta \rangle \langle \beta | \frac{\partial}{\partial q} | \alpha \rangle - i \tau \langle \alpha | \frac{\partial H}{\partial q} | \beta \rangle \langle \beta | H' | \alpha \rangle \right\} g_{\beta\alpha}(t, \tau). \quad (4.12)$$

In these expressions we have neglected terms which result from  $\partial H' / \partial q \cdot \tau \partial U / \partial t$  because they are small in fourth order if we regard  $\langle \alpha | \partial H' / \partial q | \beta \rangle$  and  $U_{\alpha\beta}$  to be small of first order, and  $\langle \alpha | \partial H' / \partial q | \beta \rangle$  and  $\tau \partial U_{\alpha\beta} / \partial t$  to be small of second order. If we want to obtain a consistent result in fourth order, we have to retain the next order term in the expansion (4.9). However, this is not our aim here.

In the expressions (4.10) to (4.12) for the dynamical force, the mass parameter and the friction coefficient, there the occupation probabilities  $n_{\alpha}(t)$

enter which are determined by the master equation

$$\frac{\partial n_{\alpha}(t)}{\partial t} = K_{\alpha}^{(1)}(t) + K_{\alpha}^{(2)}(t) = K_{\alpha}(t) \quad (4.13)$$

with the one- and two-body collision terms given by (3.31) and (3.32).

The formal integration from a time  $t_0$  before the nuclear interaction between the nuclei starts, to  $t$ ; i.e.

$$n_{\alpha}(t) = \int_0^{t-t_0} dt K_{\alpha}(t-\tau) \quad (4.14)$$

introduces retarded expressions for all the quantities (4.10) to (4.12).

The retardation or memory is given by the local equilibration time  $\tau_{loc}$  which is necessary to establish an equilibrium distribution of the occupation probabilities  $n_{\alpha}$  for fixed  $q$ -value. Memory effects of this kind are expected to have considerable effects at the initial stage of a heavy-ion collision. We will discuss this point later in section 5. In the next subsection we want to discuss the two limits of adiabatic and diabatic single-particle motion.

#### 4.2 Limits of adiabatic and diabatic single-particle motion

In this subsection we consider the expressions (4.10) to (4.12) in the limits of adiabatic and diabatic single-particle motion. These limits are defined by different characteristics about the  $q$ -dependence of the single-particle energies and the coupling matrix elements. Explicit formulas are obtained by applying the averaging procedure of (3.17) with a Lorentz curve of width  $2\theta$ .

(a) The *adiabatic limit* is defined by  $H'_0 = H$ ,  $H' = 0$  (cf. § 2). Assuming, as usual, the matrix elements  $\langle \beta | \partial H / \partial q | \alpha \rangle$  to be essentially constant, we perform the time averages and obtain from (4.10) to (4.12)

$$F'(q) = - \sum_{\alpha} (\partial E_{\alpha} / \partial q) n_{\alpha} + \partial E / \partial q \quad (4.15)$$

$$M(q) = \sum_{\alpha, \beta} \langle n_{\beta} - n_{\alpha} \rangle \langle \alpha | \frac{\partial H}{\partial q} | \beta \rangle \left| \frac{\omega_{\alpha\beta}^3 - 3\omega_{\alpha\beta} \Gamma_{\alpha\beta}^2}{[\omega_{\alpha\beta}^2 + \Gamma_{\alpha\beta}^2]^3} \right| \quad (4.16)$$

$$\xi(q) = \sum_{\alpha, \beta} \langle n_{\beta} - n_{\alpha} \rangle \langle \alpha | \frac{\partial H}{\partial q} | \beta \rangle \left| \frac{2\omega_{\alpha\beta} \Gamma_{\alpha\beta}}{(\omega_{\alpha\beta}^2 + \Gamma_{\alpha\beta}^2)^2} \right| \quad (4.17)$$

where the relation  $\langle \beta | \partial/\partial q | \alpha \rangle \omega_{\alpha\beta} = \langle \beta | \partial H/\partial q | \alpha \rangle$  has been used. In the limit of uniform motion (translation, rotation) we have  $\Gamma_{\alpha\beta} = 0$  (since  $\partial\omega_{\alpha\beta}/\partial q = 0$ ) and hence, the familiar result for  $M(q)$  as in the cranking model and  $\xi(q) = 0$  (because  $\omega_{\alpha\beta} \neq 0$ ) is obtained. In the general case of adiabatic single-particle motion the applicability of the formulas is restricted to extremely slow collective motion. This is due to the assumption of constant matrix elements  $\langle \alpha | \partial H/\partial q | \beta \rangle$ . More precisely, the characteristic time for the change of these matrix elements is given by  $|\dot{\omega}_{\alpha\beta}|/|\dot{\omega}'_{\alpha\beta}|$  as is obvious for the Landau-Zener crossing [25,26]. This time has to be large compared to the averaging interval  $\theta$  and the correlation time  $\tau_{\alpha\beta}^{-1} = (|\dot{\omega}_{\alpha\beta}|/\theta)^{-1}$ . Thus  $|\dot{\omega}_{\alpha\beta}|/|\dot{\omega}'_{\alpha\beta}| \ll \tau_{\alpha\beta} \ll |\dot{\omega}_{\alpha\beta}|$  leading again to  $M(q) \approx M_{\text{cranking}}$  and  $\xi(q) \approx 0$ . However, the collective motion is restricted to extremely small velocities as implied by the condition  $|\dot{\omega}_{\alpha\beta}|/|\dot{\omega}'_{\alpha\beta}| \ll |\dot{\omega}_{\alpha\beta}|$ . For a quasi-crossing of two adiabatic levels this amounts to zero jump probability, cf. (3.27). This is consistent with the observation [24] that any perturbation theory for the jump probability between adiabatic levels is not justified, in contrast to the jump probability for diabatic levels as discussed in § 3.2.

(b) As mentioned in § 2 the *diabatic limit* is of large practical importance in heavy-ion collisions whenever the collective energy is larger than  $\approx 0.03$  MeV per nucleon. Diabatic states are generally constructed in such a way as to keep the nodal structure unchanged. As a result these states have rather constant matrix elements  $\langle \alpha | \partial/\partial q | \beta \rangle$ . Moreover, for neighbouring levels we have  $\langle \alpha | \partial/\partial q | \beta \rangle \approx 0$ , in evaluating the time averages for  $F'(q)$ ,  $M(q)$  and  $\xi(q)$

we consider the matrix elements  $\langle \alpha | \partial/\partial q | \beta \rangle$ ,  $\langle \alpha | \partial H'/\partial q | \beta \rangle$  as constant over the time intervals  $\theta$  and  $\tau_{\alpha\beta}^{-1}$  and use the relation  $\langle \alpha | \partial H'/\partial q | \beta \rangle = \omega_{\beta\alpha} \langle \alpha | \partial/\partial q | \beta \rangle$ . The results are

$$F'(q) = \sum_{\alpha} \langle \partial e_{\alpha} / \partial q + \langle \alpha | \partial H'/\partial q | \alpha \rangle \rangle n_{\alpha} + \partial E / \partial q \quad (4.18)$$

$$M(q) = \sum_{\alpha, \beta} \langle n_{\beta} - n_{\alpha} \rangle \langle \alpha | \partial/\partial q | \beta \rangle \left| \frac{\omega_{\alpha\beta}}{\omega_{\alpha\beta}^2 + \Gamma_{\alpha\beta}^2} \right| \quad (4.19)$$

$$\xi(q) = \sum_{\alpha, \beta} \langle n_{\beta} - n_{\alpha} \rangle \langle \alpha | \partial H'/\partial q | \beta \rangle \left| \frac{2\omega_{\alpha\beta} \Gamma_{\alpha\beta}}{(\omega_{\alpha\beta}^2 + \Gamma_{\alpha\beta}^2)^2} \right| \quad (4.20)$$

where terms are neglected which do not add up coherently in the double sum over  $\alpha, \beta$ . In the limit of uniform motion ( $H' = 0$ ,  $\Gamma_{\alpha\beta} = 0$ ) the results become equal to the cranking model for the mass parameter and  $\xi(q) = 0$ . It is important to note that the leading term of  $\xi(q)$  which is proportional to  $|\langle \alpha | \partial/\partial q | \beta \rangle|^2$  vanishes identically. The expression (4.20) is small in fourth order and hence, according to the discussion below (4.12), should not be considered here. Furthermore, we expect  $\partial H'/\partial q \neq 0$  by construction of the neighbouring ( $|\dot{\omega}_{\alpha\beta}| \leq \tau_{\alpha\beta}$ ) diabatic states, such that the friction coefficient generally becomes negligibly small in the diabatic limit.

5. Application to the initial equilibration process

In this section we consider the application of our formalism developed in the previous sections, to the initial stage of the collision process. We discuss the magnitudes of the characteristic quantities which enter the conditions for the applicability of the theory. We find that the diabatic single-particle motion accompanied with two-body collisions constitutes the major mechanism of energy dissipation. These dissipative diabatic dynamics turn out to be well justified for the initial stage, but also seems to have some relevance for the later (damped) stages of a heavy-ion collision.

5.1 Diabaticity of single-particle motion

For convenience we consider the radial motion (coordinate  $r$ ) between the centers of the colliding nuclei. A typical value for the radial kinetic energy is 1 MeV per nucleon which corresponds to  $\dot{r} = 0.05 c$  for the radial velocity in units of the light velocity  $c$ . The diabaticity may be checked from the jump probability at quasicrossings. From (3.27) we find the diabaticity condition

$$\frac{\dot{r}}{c} \gg \frac{2\pi}{c} \left| H_{\alpha\beta}'' \right|^2 \left| \frac{\partial \omega_{\alpha\beta}}{\partial r} \right|^{-1} = 0.01 \quad (5.1)$$

obtained with  $c = 197 \text{ fm} \cdot \text{MeV}$  and some typical values  $H_{\alpha\beta}'' = 0.5 \text{ MeV}$  and

$$\left| \frac{\partial \omega_{\alpha\beta}}{\partial r} \right| = 1 \text{ MeV/fm} \quad (5.2)$$

resulting from numerical studies of a two-center shell-model [27]. Of course, for  $H_{\alpha\beta} = 0$ , i.e. for states with different quantum numbers, diabaticity is generally fulfilled. This is important to note because the initial stage of the collision is characterized by axial symmetry.

An upper limit for  $\dot{r}$  is given by the condition  $\dot{r} \ll v_F = 0.28 c$  (Fermi velocity) which is necessary for the applicability of any single-particle

model. Thus diabatic single-particle motion is expected to be realistic within the range

$$0.01 \ll \dot{r}/c \ll 0.3 \quad (5.3)$$

for the radial velocity and hence, within the range

$$0.04 \text{ MeV} \ll E_{\text{rad}}/A \ll 40 \text{ MeV} \quad (5.4)$$

for the radial kinetic energy per particle ( $A = \text{total mass}$ ). These values show that the velocities during the dissipation process of practically all the radial kinetic energy are sufficiently large as to justify the diabatic approach for the single-particle motion.

5.2 Local equilibration time

We consider the local equilibration time  $\tau_{\text{loc}}$  as determined from two-body collisions. Contributions from the one-body collision term are assumed to be negligible due to a proper choice of the single-particle basis. As discussed in § 3.4 we do not expect the mean free path of nucleons to differ for a time-dependent mean field from the results for a stationary mean field. We therefore can apply the nuclear matter calculations of Bertsch [2] resulting in

$$\tau_{\text{loc}}^{-1} = 72 \epsilon^*/\epsilon_F \text{ MeV} \quad (5.5)$$

where a reduced value of 26 mb for the nucleon-nucleon cross-section is used in order to be consistent with mean-free-path values deduced from the imaginary part of the optical potential, cf. [3]. The quantity  $\epsilon^*/\epsilon_F$  denotes the energy per particle in units of the Fermi energy  $\epsilon_F$  which is stored as intrinsic excitation energy, i.e. the sum of heat and diabatic distortion energy.

Although this result has been deduced in [2] only for pure quadrupole distortions of the Fermi sphere, we think it is applicable also in our more general context.

The inverse local equilibration times for  $e^{\#}/\epsilon_F = 0.005, 0.01, 0.02$  and  $0.04$  (which e.g. correspond to total excitation energies of 50, 100, 200 and 400 MeV for  $A = 250$ ) are, respectively,  $\tau_{10c}^{-1} = 0.36, 0.72, 1.44$  and  $2.9$  MeV. These values for the inverse local equilibration time are approximately equal to the estimates from the mean free path as given in [3].

### 5.3 Averaging interval

With respect to the diabatic single-particle basis we can consider an averaging interval  $\kappa$  for the coordinate  $q = r$ . This interval  $\kappa$  must be small enough to justify the linear approximation for  $\omega_{\alpha\beta}(q)$  and the stationarity of the coupling matrix elements  $U$  and  $V$  (cf. (3.25)) as assumed in the derivations of §§ 3 and 4. Numerical studies of the diabatic basis [27] show that  $\kappa = 2\text{fm}$  is reasonable. With (5.2) we thus obtain

$$\Gamma_{\alpha\beta} = |\omega_{\alpha\beta}|e = |\omega_{\alpha\beta}/r|\kappa \approx 2 \text{ MeV} \quad (5.6)$$

for the mean inverse correlation time (3.19) where  $\kappa = \partial r$  has been used.

The condition for the justification of the weak-coupling limit and the Markov approximation of the collision terms in §§ 3.2 and 3.3 is (cf. (3.21))

$$\Gamma_{\alpha\beta} \tau_{10c}^{-1} \gg 1. \quad (5.7)$$

From the values for  $\tau_{10c}^{-1}$  given in § 5.2 we find  $\Gamma_{\alpha\beta} \tau_{10c} = 6.2, 8, 1.4$  and  $0.7$  for  $e^{\#}/\epsilon_F = 0.005, 0.01, 0.02$ , and  $0.04$ , respectively. Thus the condition on the averaging interval is satisfied roughly for collisions which lead up to 1 MeV per nucleon energy dissipation, i.e. for example up to 250 MeV above the Coulomb plus centrifugal barrier for the total mass  $A = 250$  of a heavy-ion collision.

The averaging interval  $\kappa$  in coordinate space  $r$  corresponds to a time interval  $\theta = \kappa/\dot{r}$ . For the initial stage of a heavy-ion collision we have  $\dot{r} \approx 0.05 c$  and hence  $\theta \approx 0.2 \text{ MeV}^{-1}$  ( $\approx 1.3 \cdot 10^{-22} \text{ s}$ ). This value satisfies

the condition (3.20) and increases with decreasing velocities. However, an upper limit (cf. (3.21)) is given by the local equilibration time because we have excluded the occupation probabilities  $\bar{n}_{\alpha\alpha}(t) \equiv n_{\alpha}(t)$  from the averaging process.

The derivation of the equation of motion in § 4.1 also imposes an upper limit on the averaging interval  $\kappa$  or  $\theta = \kappa/\dot{r}$ . Since the average leaves the terms up to first order in  $t$  unchanged we expect the choice  $\kappa = 2 \text{ fm}$  to be sufficiently small such that the collective motion is described correctly by (4.5) with (4.10) to (4.12).

### 5.4 Qualitative discussion of the initial energy dissipation

We conclude from (5.3) that the initial stage of a heavy-ion collision is characterized by the diabatic single-particle motion until the radial velocity has been slowed down to  $\dot{r} \approx 0.01 c$ . According to § 4.2b this diabatic motion is essentially *free from ordinary friction* which could dissipate energy. Thus, kinetic energy can only be lost through the dynamical force  $F_i$  given by (4.18) which is non-conservative because of the explicit time dependence of  $n_{\alpha}(t)$ . Introducing the retarded solution (4.14) for the occupation probabilities this force is given by

$$F_i(q_i, t) = - \sum_{\alpha} \int_0^{t-t_0} dt' K_{\alpha}(t, t-t') + \partial E/\partial q \quad (5.8)$$

which formally can be divided into conservative and dissipative parts by considering the time-reversible and time-irreversible contributions. The non-locality is determined by the local equilibration time.

The energy dissipation can be pictured as follows. Starting with some equilibrium distribution for the occupation probabilities (e.g. corresponding to the ground state if we consider the initial stage of a heavy-ion collision)

$$n_\alpha(t) = \bar{n}_\alpha(q(t)) - \int_0^{t-t_0} dt' \exp[-\int_{t-t'}^t dt''/\tau_{loc}(t'')] (\frac{\partial \bar{n}_\alpha}{\partial q})_{t-t''} \quad (5.10)$$

Inserting this in (4.18) for the force we obtain

$$F'(q) = - \sum_\alpha \frac{\partial \epsilon_\alpha}{\partial q} \bar{n}_\alpha + \frac{\partial E}{\partial q} + \int_0^{t-t_0} dt' \exp[-\int_{t-t'}^t dt''/\tau_{loc}(t'')] (\frac{\partial \epsilon_\alpha}{\partial q})_{t-t''} (\frac{\partial \bar{n}_\alpha}{\partial q})_{t-t''} \quad (5.11)$$

where we have neglected for convenience the small contributions  $\langle \alpha | \partial H' / \partial q | \alpha \rangle$ . The first two terms account for the difference between the ground-state (adiabatic) force and the force at local equilibrium. Apart from contributions of higher order in  $\dot{q}$ , the last term in (5.11) is repulsive as is obvious by measuring  $\epsilon_\alpha$  with respect to the chemical potential and noting that  $\partial \bar{n}_\alpha / \partial \epsilon_\alpha < 0$ . This *retarded friction force* gives rise to a repulsive oscillator force proportional to  $q - q_0$  for  $\int_{t_0}^t dt' / \tau_{loc}(t') \ll 1$ . The corresponding vibration has been identified with an isoscalar giant vibration in [3]. For  $\int_{t_0}^t dt' / \tau_{loc}(t') \gg 1$  and slowly varying  $\dot{q}$  and  $\tau_{loc}$  the retarded friction force becomes an ordinary friction force

$$F_{friction} = -\tau_{loc} \sum_\alpha (\frac{\partial \epsilon_\alpha}{\partial q}) (\frac{\partial \bar{n}_\alpha}{\partial q}) \dot{q} \quad (5.12)$$

In the limit of slow motion the system will always be close to local equilibrium, such that according to (5.5)  $\tau_{loc} \propto T^{-2}$ . Thus the friction coefficient has the same temperature dependence as the viscosity coefficient for large systems.

According to this discussion we can distinguish three time intervals and three corresponding stages in a heavy-ion collision.

(i) *Quasi-elastic stage:*

This initial time interval is defined by  $\int_{t_0}^t dt' / \tau_{loc}(t') \ll 1$  where  $t_0$  denotes a time well before the collision. This stage is characterized by the diabatic single-particle motion and hence, by elastic collective motion.

the diabatic single-particle motion will produce a repulsive force on the collective motion which is due to the diabatic excitation of particle-hole states. Thus kinetic energy is temporarily stored as a conservative potential. However, this diabatic potential part is destroyed by two-body collisions which try to establish a new equilibrium distribution for the occupation probabilities at a larger excitation energy. The local equilibration via two-body collisions is a time-irreversible process which leads to the dissipation of collective energy. The dynamical process is simultaneously characterized by the diabatic single-particle motion and the dissipative two-body collisions and hence, may be called *dissipative diabatic dynamics*. Beside the two-body collisions also one-body collisions add to the decay of the conservative diabatic potential. However, by a proper choice of the single-particle basis the one-body couplings can be minimized and hence, this contribution to dissipation is expected to be less important.

The temporary storage of collective kinetic energy as a conservative potential and the subsequent dissipation by one- and two-body collisions gives rise to the memory effects implied in (5.8). These memory effects can be illustrated by approximating the collision terms in the master equation (4.13) by a simple relaxation term as

$$\frac{\partial n_\alpha}{\partial t} = - \frac{1}{\tau_{loc}} (n_\alpha - \bar{n}_\alpha) \quad (5.9)$$

which describes the approach (with  $\tau_{loc}(t)$  as decay time) of  $n_\alpha$  towards the local equilibrium distribution  $\bar{n}_\alpha$ , i.e. the equilibrium distribution for a fixed value of the collective coordinate  $q$ . Temperature and chemical potential of  $\bar{n}_\alpha$  are determined by the total excitation energy and the total mass. Essentially due to the  $q$ -dependence of the single-particle energies,  $\bar{n}_\alpha$  is strongly varying with  $q(t)$ . Integration of (5.9) with the initial value  $n_\alpha(t_0) = \bar{n}_\alpha(q(t_0))$  results in

For collisions close to grazing where the interaction time  $\tau_{int}$  is considerably smaller than  $\tau_{loc}$ , we therefore expect undamped collective motion to dominate. This does not mean that the collision is elastic.

Since the diabatic motion corresponds to isoscalar giant vibrations, such modes can be strongly excited in the collision.

(i) *Dissipation stage:*

This stage is connected with the time interval around  $\int_{t_0}^t dt'/\tau_{loc}(t') \approx 1$  where the essential dissipation of collective kinetic energy takes place.

(iii) *Local equilibrium stage:*

For  $\int_{t_0}^t dt'/\tau_{loc}(t') \gg 1$  the system is always close to local equilibrium. The large collective energies have been dissipated during the dissipation stage such that the collective motion is slow. Furthermore the temperature is high and correspondingly  $\tau_{loc}$  is small. In this stage the ordinary friction force as given by (5.12) should be a good approximation to the retarded friction term. All completely damped components of deeply inelastic collisions are expected to go through this stage.

6. Summary and conclusion

We have introduced a theory of dissipative heavy-ion collisions within a time-dependent shell-model approach taking the residual interactions into account. The time-dependence of the mean field is described by a single collective variable  $q(t)$ . The generalisation to a set of collective variables is straightforward. The formulation has two important ingredients: (i) a time-dependent single-particle basis and (ii) a time-averaging procedure.

The time-dependent single-particle basis is defined according to the collective motion in such a way as to reduce considerably the one-body coupling terms in the Liouville equation. With the introduction of these dynamical basis states a major part of the interaction is treated quantum-mechanically. An important feature of the dynamical single-particle levels is the frequent occurrence of level crossings for realistic values of the collective velocity. Thus, for fixed values of the single-particle occupation probabilities, the time-dependence of the single-particle levels is responsible for the direct transformation of collective kinetic energy into intrinsic energy which acts as a conservative potential on the collective variable.

Time averaging is introduced as a natural procedure to apply on the macroscopic or collective motion which by definition should be the slow modes of the system. In connection with the time-dependence of the single-particle levels the time average introduces irreversibility in the macroscopic equations of motion and justifies the use of the weak-coupling limit and the Markov approximation in the basic collision terms. These collision terms conserve not only the total occupation probability (i.e. conservation of total mass and charge) but also the total energy.

The time-averaging procedure applied here is different from the iterative time smoothing introduced by Ballian and Veneroni [34] in their extension of TDHF. We use time averaging in order to eliminate from the macroscopic



quantities some residual fluctuations. The iterative time smoothing of Balian and Veneroni is tailored for taking care of effects from two-body collisions. These two-body collisions are accounted for explicitly in our approach.

Our time-averaging procedure has some advantage over ensemble averages which have been applied extensively in the formulation of transport theories [11,16] and recently also in the derivation of two-body collision terms [9,10]. Whereas the use of random-matrix ensembles is well justified for the complicated many-body states, one has some doubts for the few two-body matrix elements between the relevant single-particle states around the Fermi surface. More important, however, ensemble averages do not lead to energy conservation in the collision terms [9-11,16]. Instead one has to include the correlation energies in order to guarantee total energy conservation. Thus one of the main improvements obtained by time averaging is the mean energy conservation directly in the one- and two-body collision terms. This property leads to the important conclusion that the mean free path of nucleons in time-dependent mean fields is principally the same as in stationary fields for the same total excitation energy. Therefore, calculations of the mean free path of nucleons in nuclear matter or finite nuclei apply also to time-dependent mean fields.

As a result of the formulation we have obtained two coupled equations. The occupation probabilities for the dynamical single-particle states are determined by a master equation (4.13) for one- and two-body collisions (3.31) and (3.32). From the conservation of the total energy we have derived the equation of motion (4.5) for the collective variable  $q(t)$ . The master equation is coupled to the equation for  $q(t)$  by the dependence of the transition probabilities on  $q$ . The equation of motion for the collective variable is coupled to the master equation by the dependence of the dynamical force, the mass parameter and the friction coefficient on the occupation probabilities.

The application of the theory to the initial energy dissipation has some interesting features. The initial stage of a heavy-ion collision is characterized by diabatic single-particle motion. In this limit the ordinary friction coefficient becomes negligible and energy dissipation results only from the time dependence of the potential energy. This dynamical behaviour (dissipative diabatic dynamics) has been introduced and discussed within schematic models earlier [3,19-21]. This mechanism is expected to be effective for collective kinetic energies per nucleon in the range  $0.04 \text{ MeV} \ll \epsilon_{\text{coll}} \ll 40 \text{ MeV}$  and hence, should be essential for the energy dissipation in heavy-ion collisions.

Our time-dependent shell-model theory with residual interactions can be regarded as a simplified version of extended TDHF theories. However, apart from two-body collisions, we also describe some couplings of the one-body type by irreversible collision terms. At the cost of selfconsistency and with the constraint of the collective motion to a single or a few degrees of freedom, the formulation looks more transparent and can easily supply transport coefficients which may be used in transport equations. Thus this shell-model approach to the transport theory of large amplitude collective motion of nuclei seems to be promising for future applications.

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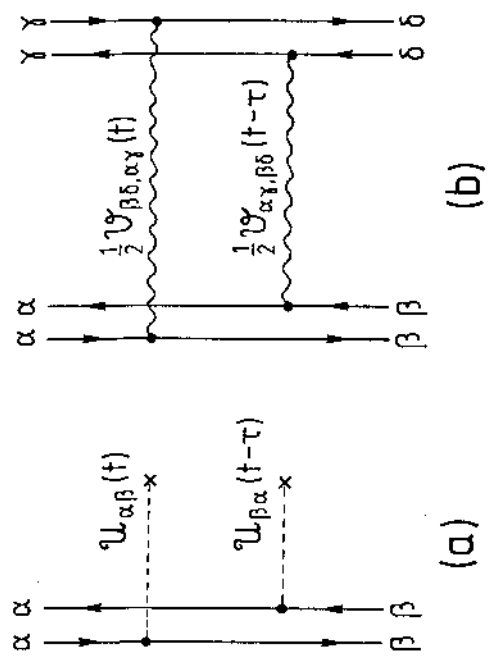


Fig. 1.: Graphs of the one- and two-body collision terms. The pair of lines denote a dynamical state (+) and a conjugate state (+). The time average allow significant contributions only from  $\tau$ -values not much larger than the correlation time of the matrix elements (cf. § 3.2).