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ON ENERGY CONSERVATION IN THE PRESENCE OF COLLISION TERMS

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Abstract

In the derivation of dissipative equations of motion it is a necessity to incorporate the global conservation laws into the approximations. Among the constants of motion usually the Hamiltonian itself is the most intricate one. The main purpose of this paper is to show that in a quite general approximation scheme, which is based on a projection on macro-observables followed by a perturbation expansion, the quest for energy conservation dictates how to split the Hamiltonian into an unperturbed part and a perturbation. In this scheme energy is conserved to each order seperately if the unperturbed Hamiltonian is the projected part of the full Hamiltonian. The very general considerations are exemplified with Zwanzig's projection method and with the extended time dependent Hartree-Fock equations.

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Contents

1 Introduction

The dynamics of a system with a very large number of degrees of freedom can often be described with a restricted set of macroscopic observables. Examples can be found in many areas of physics, *e.g.* the movement of a Brownian particle in a suspension, collective degrees of freedom for solids or plasmas, fluid dynamics, or the one-body observables of a many-particle system. In any case the choice of the appropriate macroscopic observables, which we shall denote by A_k, is guided by experimental evidence and physical intuition. The observables A_k are of macroscopic nature in the sense that they are an average over the individual constituents of the system. Therefore we shall call them macro-observables and their expectation values $a_k(t)$ macro-variables. The remaining degrees of freedom we shall refer to as micro-variables. Their interaction with the macro-variables causes a non-unitary time evolution for the latter, and the equations of motion become dissipative if the micro-variables vary on a much faster time scale than the macro-variables.

The projection operator technique [1,2,3,4,5,6,7,8] provides the tools for a reduced description of the system in terms of the macro-variables $a_k(t)$. One first projects the statistical operator $\rho(t)$ (which is the exact solution of the von Neumann equation) onto a reduced statistical operator $R(t)$ which depends only on the reduced knowledge about the physical system as represented by the $a_k(t)$. $R(t)$ and $\rho(t)$ are related by the condition that they provide the same expectation values for the A_k, *i.e.* $a_k(t) = Tr(A_k\rho(t)) = Tr(A_kR(t))$. Then one rewrites the dynamical equation and obtains a formally closed equation of motion for the reduced statistical operator $R(t)$ or equivalently a set of equations for the macro-variables $a_k(t)$. These nonlinear integro-differential equations which are still exact are useful as a starting point for approximations. The variety of approximations in the collision term is confined by the conservation laws of the exact equation. Especially in the context of extended time-dependent Hartree-Fock theories [9,10,11,12,13,14,15,16,17,18,19,20,21,22] the conservation of total energy has to be proven for the approximation used [23,24,25]

In this paper we show under which conditions one ensures energy conservation if the collision term is treated perturbatively by partial summation. It turns out that the quest for energy conservation imposes severe restrictions on the choice of the perturbation expansion.

In section 2 we sketch the projection operator technique as far as necessary for the purpose of this paper. The perturbation expansion is defined in section 3, and in section 4 we discuss in which sense energy should be conserved and work out the consequences for the perturbation expansion. In section 5 the general considerations are applied to Zwanzig's projection and the connection with the Markov approximation is discussed. Finally in section 6 we carry out explicitly the calculation for a collisional time-dependent Hartree-Fock theory.

2 Projection Formalism

Let us denote the full statistical operator of the system by $\rho(t)$ and the (time independent) macro-observables by A_k, where the expectation values

$$a_k(t) = Tr(A_k\rho(t)), \qquad k = 0, 1, 2, ..., N \tag{2.1}$$

are presumed to be known at time t. The A_k are hermitian and have to form a set of linearly independent operators. The macro statistical operator R is then some coarse grained ρ, where all micro degrees of freedom are averaged over. One requires for R the following properties: First R shall reproduce the mean values a_k of the macro-observables

$$Tr(A_kR(t)) = Tr(A_k\rho(t)) = a_k(t), \tag{2.2}$$

second it shall be completely determined by these expectation values

$$R(t) = R(a_0(t), a_1(t), ..., a_N(t)), \tag{2.3}$$

and finally it shall be normalized to one

$$Tr(R(t)) = 1. \tag{2.4}$$

We deal with this last condition by always including the unit operator into the set of macro-observables, since eq. (2.4) is equivalent to $Tr(A_0R) = a_0$ with A_0 being the unit operator and its expectation value a_0 set equal to 1. For reasons which will be explained later we add a fourth condition on R by requiring homogeneity of degree one with respect to the a_k :

$$R = \sum_k \frac{\partial R}{\partial a_k}\, a_k \tag{2.5}$$

The mapping of ρ onto R which is supposed to be linear can formally be expressed as a projection: $R = \mathcal{P}\rho$. Note that $\mathcal{P}$ is not an operator in the Hilbertspace of quantum states but instead acts in the space of linear operators which in turn act in the ordinary Hilbertspace. So the usual operators of quantum mechanics are vectors of this higher space which is called superspace. The linear operators acting on superspace vectors consequently are superoperators. Throughout this work we use curled symbols for superoperators to distinguish them from the ordinary Hilbertspace operators.

For any two vectors X and Y in superspace we define a scalar product by

$$(X, Y) := Tr(X^\dagger Y). \tag{2.6}$$

This enables us to define the operator $\mathcal{P}^\dagger$ conjugate to $\mathcal{P}$:

$$(\mathcal{P}^\dagger X, Y) := (X, \mathcal{P}Y). \tag{2.7}$$

Whereas $\mathcal{P}$ is supposed to act on a statistical operator (*cf.* eq. (2.10)), $\mathcal{P}^\dagger$ should be applied to the dual space of linear operators.
One requires the following plausible properties for $\mathcal{P}$ or $\mathcal{P}^\dagger$, respectively:
a) Linearity:

$$\mathcal{P}^\dagger(\alpha X + \beta Y) = \alpha \mathcal{P}^\dagger X + \beta \mathcal{P}^\dagger Y \tag{2.8}$$

b) Idempotency:

$$\mathcal{P}\mathcal{P} = \mathcal{P}. \tag{2.9}$$

One calls $\mathcal{P}$ a projector even if it is not hermitian.
c) Projection on R:

$$R = \mathcal{P}\rho \tag{2.10}$$

d) Since $\mathcal{P}$ projects on the macro statistical operator one demands that $\mathcal{P}^\dagger$ projects on the macro-operators:

$$\mathcal{P}^\dagger X = X \Longleftrightarrow X = \sum_k c_k A_k. \tag{2.11}$$

This is still not enough to make $\mathcal{P}$ unique. Hence one adds a further condition which will prove very convenient in the following. Since ρ, a_k and R depend on time the projector $\mathcal{P}$ will also depend on time. Addition of requirement e) which concerns this time dependence will make $\mathcal{P}$ unique.
e) Projection of $d\rho/dt$ on dR/dt:

$$\mathcal{P}(t)\frac{d\rho(t)}{dt} = \frac{dR(t)}{dt} \tag{2.12}$$

In the appendix we show that this implies the homogeneity of R as stated in eq. (2.5). We listed the homogeneity separately as a requirement on R in order to distinguish between the properties of R and those of $\mathcal{P}$.

The properties (2.2) through (2.5) of R and (2.8) through (2.12) of $\mathcal{P}$ determine uniquely the form of $\mathcal{P}$ and $\mathcal{P}^\dagger$ as

$$\mathcal{P}X = \sum_k \frac{\partial R}{\partial a_k} Tr(A_k X) \tag{2.13}$$

$$\mathcal{P}^\dagger X = \sum_k Tr\left(\frac{\partial R}{\partial a_k} X\right) A_k \tag{2.14}$$

We give a proof for the uniqueness of $\mathcal{P}$ in the appendix. Note that $\mathcal{P}$ as well as $\mathcal{P}^\dagger$ are functionals of the macro-variables a_k only. Note further that $\mathcal{P}^\dagger$ transforms any operator into a linear combination of the macro-observables A_k. Eq.(2.13) allows for a generalization of the idempotency property (2.9): Twofold application of $\mathcal{P}$ at different times t and t' results in (see appendix)

$$\mathcal{P}(t)\mathcal{P}(t') = \mathcal{P}(t) \tag{2.15}$$

For convenience one finally introduces the complementary projectors $\mathcal{Q}$ and $\mathcal{Q}^\dagger$:

$$\mathcal{Q} := 1 - \mathcal{P} \tag{2.16}$$

$$\mathcal{Q}^\dagger := 1 - \mathcal{P}^\dagger \tag{2.17}$$

Let ρ depend on time according to the von Neumann equation

$$i\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t) \tag{2.18}$$

with the Liouvillian $\mathcal{L}$

$$\mathcal{L}X := [H, X], \qquad \hbar = 1. \tag{2.19}$$

With the projection defined above one is able to derive a closed equation of motion for the macro statistical operator $R(t)$ on the basis of the von Neumann equation (2.18)[6]. First introduce the Greenfunction $\mathcal{G}(t,t')$ by the equation

$$\frac{\partial}{\partial t'}\mathcal{G}(t,t') = \mathcal{G}(t,t')\mathcal{Q}(t')i\mathcal{L}, \qquad \mathcal{G}(t,t) = 1, \tag{2.20}$$

which is an operator equation in superspace. From this one gets with the von Neumann equation (2.18) and with eq. (2.12)

$$\frac{\partial}{\partial t'}\left\{\mathcal{G}(t,t')\left(\rho(t') - R(t')\right)\right\} = -i\mathcal{G}(t,t')\mathcal{Q}(t')\mathcal{L}R(t').$$

Integration over t' yields

$$\rho(t) = R(t) - \int_0^t dt'\,\mathcal{G}(t,t')\mathcal{Q}(t')i\mathcal{L}R(t') + \mathcal{G}(t,0)\mathcal{Q}(0)\rho(0). \tag{2.21}$$

Acting on this equation with $-i\mathcal{P}(t)\mathcal{L}$ from the left and using again eq. (2.18) and (2.12) finally gives the desired equation for $R(t)$:

$$\frac{d}{dt}R(t) = -i\mathcal{P}(t)\mathcal{L}R(t) - \int_0^t dt'\,\mathcal{P}(t)\mathcal{L}\mathcal{G}(t,t')\mathcal{Q}(t')\mathcal{L}R(t') - i\mathcal{P}(t)\mathcal{L}\mathcal{G}(t,0)\mathcal{Q}(0)\rho(0). \tag{2.22}$$

Note that eqs. (2.21) and (2.22) are still exact. In eq. (2.21) the statistical operator $\rho(t)$ is - except for the initial value $\rho(0)$ - expressed exclusively as a functional of the macro-expectation values, since this is true for R as well as for $\mathcal{P}$, $\mathcal{Q}$ and therefore also for $\mathcal{G}$ (*cf.* eq. (2.20)). Consequently eq. (2.22) is a (formally) closed exact equation of motion for $R(t)$. The price one has to pay is that the equation is highly nonlinear and in addition nonlocal in time.

Let us mention that in eq. (2.22) one can insert a $\mathcal{Q}(t)$ in front of $\mathcal{G}(t,t')\mathcal{Q}(t')$ which may sometimes be useful:

$$\mathcal{G}(t,t')\mathcal{Q}(t') = \mathcal{Q}(t)\mathcal{G}(t,t')\mathcal{Q}(t') \tag{2.23}$$

This is easily seen by iterating eq. (2.20) which gives immediately $\mathcal{P}\mathcal{G}\mathcal{Q} = 0$.

From eq. (2.22) one gets the equation of motion for the macro-variables a_k by multiplying with A_k and taking the trace according to eq. (2.2):

$$\frac{da_k}{dt} = iTr([H,A_k]R(t)) - \int_0^t dt' Tr(A_k \mathcal{L}\mathcal{G}(t,t')\mathcal{Q}(t')\mathcal{L}R(t')) - iTr(A_k \mathcal{L}\mathcal{G}(t,0)\mathcal{Q}(0)\rho(0)). \tag{2.24}$$

3 Perturbation Expansion in Superspace

Up to now eqs. (2.21), (2.22) and (2.22) are exact and of little practical use. The complicated quantum mechanical many-body problem which generally cannot be solved exactly is still present in eq. (2.20). The advantage of this equation together with eq. (2.22) or (2.24) lies in the fact that they are formally closed in R or in the macro-variables a_k, whereas the von Neumann equation explicitly carries along all the micro degrees of freedom. One way to approximate the Greenfunction $\mathcal{G}(t,t')$ is to perform a power expansion around some unperturbed Liouvillian $\mathcal{L}_0$ [26] which will be specified later. Let us split $\mathcal{L}$ into

$$\mathcal{L} = \mathcal{L}_0(t) + \mathcal{L}_1(t) \tag{3.1}$$

with

$$\mathcal{L}_0(t)X = [H_0(t), X] \quad \text{and} \quad \mathcal{L}_1(t)X = [H_1(t), X].$$

Next we transform to the interaction picture in superspace writing

$$\mathcal{G}(t,t') = \hat{\mathcal{G}}_1(t,t')\hat{\mathcal{G}}_0(t,t') \tag{3.2}$$

where $\hat{\mathcal{G}}_0$ describes the time evolution according to $\mathcal{Q}\mathcal{L}_0$ instead of $\mathcal{Q}\mathcal{L}$ in eq. (2.20):

$$\frac{\partial}{\partial t'}\hat{\mathcal{G}}_0(t,t') = \hat{\mathcal{G}}_0(t,t')\mathcal{Q}(t')i\mathcal{L}_0(t'), \qquad \hat{\mathcal{G}}_0(t,t) = 1. \tag{3.3}$$

Then $\hat{\mathcal{G}}_1$ obeys the differential equation

$$\frac{\partial}{\partial t'}\hat{\mathcal{G}}_1(t,t') = \hat{\mathcal{G}}_1(t,t')\left\{\hat{\mathcal{G}}_0(t,t')i\mathcal{Q}(t')\mathcal{L}_1(t')\hat{\mathcal{G}}_0^{-1}(t,t')\right\}, \qquad \hat{\mathcal{G}}_1(t,t) = 1. \tag{3.4}$$

Formal integration of eq. (3.4) gives a corresponding integral equation which, when inserted into eq. (3.2), leads to a perturbation series in $\mathcal{L}_1$ for $\mathcal{G}$:

$$\mathcal{G}(t,t') = \left(1 - \int_{t'}^{t} dt'' \hat{\mathcal{G}}_0(t,t'')\mathcal{Q}(t'')i\mathcal{L}_1(t'')\hat{\mathcal{G}}_0^{-1}(t,t'') + \ldots\right)\hat{\mathcal{G}}_0(t,t') \tag{3.5}$$

Lowest order means to replace $\mathcal{G}(t,t')$ by $\hat{\mathcal{G}}_0(t,t')$. This could still be unfeasible since $\hat{\mathcal{G}}_0$ evolves with $\mathcal{Q}\mathcal{L}_0$. Unless $\mathcal{L}_0$ has special properties which simplify the evolution the perturbation expansion is still too complicated. One reasonable requirement is that the macro-observables evolve among themselves under $\mathcal{L}_0$:

$$\mathcal{L}_0 A_k = \sum_l c_{kl} A_l, \tag{3.6}$$

i.e. the A_k form an algebra under $\mathcal{L}_0$. By virtue of eqs. (2.14) and (2.11) this is equivalent to

$$\mathcal{L}_0 P^\dagger = P^\dagger \mathcal{L}_0 P^\dagger.$$

Hermitian conjugation of this equation gives ($\mathcal{L}_0 = \mathcal{L}_0^\dagger$)

$$P\mathcal{L}_0 = P\mathcal{L}_0 P. \tag{3.7}$$

We observe that $\hat{\mathcal{G}}_0$ is needed in $\mathcal{Q}$-space only. Therefore we try to define a different superoperator $\mathcal{G}_0(t,t')$ which equals $\hat{\mathcal{G}}_0(t,t')$ in $\mathcal{Q}$-space but obeys a simpler differential equation than $\hat{\mathcal{G}}_0(t,t')$. Starting from the $\mathcal{Q}$-space part of eq. (3.3)

$$\frac{\partial}{\partial t'}\hat{\mathcal{G}}_0(t,t')\mathcal{Q}(t'') = \hat{\mathcal{G}}_0(t,t')\mathcal{Q}(t')i\mathcal{L}_0(t')\mathcal{Q}(t'')$$

we can move $\mathcal{Q}(t')$ to the right by virtue of eq. (3.7) to yield

$$\frac{\partial}{\partial t'}\hat{\mathcal{G}}_0(t,t')\mathcal{Q}(t'') = \hat{\mathcal{G}}_0(t,t')i\mathcal{L}_0(t')\mathcal{Q}(t'').$$

To get this last equation we also used the relation $\mathcal{Q}(t')\mathcal{Q}(t'') = \mathcal{Q}(t'')$ which follows immediately from eq. (2.15). We consequently define $\mathcal{G}_0$ by

$$\frac{\partial}{\partial t'}\mathcal{G}_0(t,t') = \mathcal{G}_0(t,t')i\mathcal{L}_0(t'), \qquad \mathcal{G}_0(t,t) = 1. \tag{3.8}$$

This equation is much simpler than eq. (3.3) since it does not contain a projection and further more lets the space of the macro-observables invariant because of eq. (3.6). Replacing $\hat{\mathcal{G}}_0(t,t')$ by $\mathcal{G}_0(t,t')$ in eqs. (3.4) and (3.5) and adding a $\mathcal{Q}(t')$ in the last equation (remember that only the $\mathcal{Q}$-space part counts) finally gives

$$\frac{\partial}{\partial t'}\mathcal{G}_1(t,t') = \mathcal{G}_1(t,t')\mathcal{G}_0(t,t')i\mathcal{Q}(t')\mathcal{L}_1(t')\mathcal{G}_0^{-1}(t,t'), \qquad \mathcal{G}_1(t,t) = 1 \tag{3.9}$$

(again $\mathcal{G}_1$ equals $\hat{\mathcal{G}}_1$ only in $\mathcal{Q}$-space) and

$$\mathcal{G}(t,t')\mathcal{Q}(t') = \left(1 - \int_{t'}^{t} dt'' \mathcal{G}_0(t,t'')\mathcal{Q}(t'')i\mathcal{L}_1(t'')\mathcal{G}_0^{-1}(t,t'') + \ldots\right)\mathcal{G}_0(t,t')\mathcal{Q}(t'). \tag{3.10}$$

A natural perturbation series for the $\mathcal{Q}$-space part of $\mathcal{G}$ is then defined by

$$\begin{aligned} \mathcal{G}^{(0)}(t,t')\mathcal{Q}(t') &= \mathcal{G}_0(t,t')\mathcal{Q}(t'), \qquad (3.11) \\ \mathcal{G}^{(n)}(t,t')\mathcal{Q}(t') &= \mathcal{G}_0(t,t')\mathcal{Q}(t') \\ &\quad - \int_{t'}^{t} dt'' \mathcal{G}^{(n-1)}(t,t'')\mathcal{Q}(t'')i\mathcal{L}_1(t'')\mathcal{G}_0(t'',t')\mathcal{Q}(t') \qquad (3.12) \end{aligned}$$

This expansion in superspace is somewhat different from a usual perturbation expansion: Since the resulting equation of motion for $R(t)$ is closed, every order contains implicitly a partial summation in all powers of $\mathcal{L}_1$. This is why the approximation in superspace should be better than an expansion in ordinary Hilbertspace. Our expansion means that we take all contributions up to a given power in $\mathcal{L}_1$ and a selected class of higher "order" terms. As can be read off from eq. (2.22) the nth order of $\mathcal{GQ}$ means the $(n+2)$nd order in the equation for R.

4 Energy Conservation

Every reasonable approximation should comply with the conservation laws; in particular the total energy should be conserved. We first explain in which sense a quantity is required to be conserved and then deduce a severe restriction on the choice of $\mathcal{L}_0(t)$. If X is a constant of motion and $x(t)$ its expectation value calculated with $\rho(t)$ we have

$$\frac{d}{dt}x(t) = \frac{d}{dt}Tr\left(X\rho(t)\right) = 0.$$

The exact statistical operator ρ divides into an uncorrelated part defined by $\mathcal{P}\rho = R$ and a correlated part R_c defined by $\mathcal{Q}\rho$. Generally both parts contribute to the expectation value and only together ensure the conservation law. In the case of energy *e.g.* the uncorrelated energy (*i.e.* the energy which is calculated with $R(t)$) may change in time, but this change is exactly compensated by the opposite change of the correlation energy (*i.e.* $Tr(HR_c(t))$. If we want the conservation law to hold also in our approximation we have to define it in the same manner. The approximated ρ also splits into an uncorrelated part and a correlated part:

$$\rho^{(n)}(t) = R^{(n)}(t) + R_c^{(n)}(t), \qquad (4.1)$$

where $R_c^{(n)}$ is defined as (*cf.* eq. (2.21))

$$R_c^{(n)}(t) = -i\int_0^t dt' \mathcal{G}^{(n)}(t,t')\mathcal{Q}(t')\mathcal{L}R(t') + \mathcal{G}^{(n)}(t,0)\mathcal{Q}(0)R(0) \qquad (4.2)$$

The superscript $^{(n)}$ denotes the nth order in the expansion of $\mathcal{GQ}$ according to eq. (3.12). It is important to apply the same approximation for the correlated part $R_c^{(n)}$ as for the time evolution (2.22) of the uncorrelated part $R^{(n)}$.

Let us first take the simple case that the conserved operator X is a linear combination of the macro-observables A_k [4,8]. Then the correlation part vanishes since

$$Tr(X\mathcal{Q}\rho) = Tr\left((\mathcal{Q}^\dagger X)\rho\right) = 0$$

due to eq. (2.11). Moreover the conservation holds irrespective of the approximation for $\mathcal{GQ}$. Eq. (2.22) gives

$$\begin{aligned} \frac{d}{dt}Tr(XR^{(n)}(t)) &= -iTr\left(X\mathcal{P}(t)\mathcal{L}\left(R^{(n)}(t) + \mathcal{G}^{(n)}(t,0)\mathcal{Q}(0)\rho(0)\right)\right) \\ &\quad - Tr\left(X\mathcal{P}(t)\mathcal{L}\int_0^t dt' \mathcal{G}^{(n)}(t,t')\mathcal{Q}(t')\mathcal{L}R^{(n)}(t')\right) \end{aligned}$$

Acting with $\mathcal{P}$ to the left reproduces X, again due to eq. (2.11). It remains a trace over $X\mathcal{L}...$ which vanishes, since X is a constant of motion and therefore commutes with H. Obviously the specific approximation for $\mathcal{G}^{(n)}(t,t')$ did not enter anywhere. As a result all conserved macro-observables are trivially conserved within the approximation scheme.

Let us now turn to the more interesting case of energy conservation. Usually the total Hamiltonian will not be a member of the set of macro-observables. Therefore energy conservation is not necessarily fulfilled. We will require

$$\frac{dE^{(n)}}{dt} = \frac{d}{dt}Tr(H\rho^{(n)}) = 0, \qquad (4.3)$$

and from that we will arrive at a condition for $\mathcal{L}_0(t)$. Again we split $\rho^{(n)}$ into a correlated and an uncorrelated part according to eqs. (4.1) and (4.2). The corresponding correlated and uncorrelated energies $E_c^{(n)}$ and $E_0^{(n)}$ are

$$\begin{aligned} E_c^{(n)}(t) &= Tr(HR_c^{(n)}(t)) \qquad (4.4) \\ \text{and } E_0^{(n)}(t) &= Tr(HR^{(n)}(t)). \qquad (4.5) \end{aligned}$$

For the time derivatives we get from eqs. (2.22) and (2.21)

$$\begin{aligned} \frac{dE_0^{(n)}(t)}{dt} &= -iTr\left(H\mathcal{P}(t)\mathcal{L}\left(R^{(n)}(t) + \mathcal{G}^{(n)}(t,0)\mathcal{Q}(0)\rho(0)\right)\right) \\ &\quad - Tr\left(H\mathcal{P}(t)\mathcal{L}\int_0^t dt' \mathcal{G}^{(n)}(t,t')\mathcal{Q}(t')\mathcal{L}R^{(n)}(t')\right) \qquad (4.6) \end{aligned}$$

and

$$\begin{aligned} \frac{dE_c^{(n)}(t)}{dt} &= -iTr\left(H\left\{\mathcal{Q}(t)\mathcal{L}R^{(n)}(t) + i\frac{\partial}{\partial t}\mathcal{G}^{(n)}(t,0)\mathcal{Q}(0)\rho(0)\right\}\right) \\ &\quad -iTr\left(H\int_0^t dt' \frac{\partial}{\partial t}\mathcal{G}^{(n)}(t,t')\mathcal{Q}(t')\mathcal{L}R(t')\right) \qquad (4.7) \end{aligned}$$

From eq. (3.12) and eq. (3.8) we find by induction

$$\frac{\partial}{\partial t}\mathcal{G}^{(n)}(t,t')\mathcal{Q}(t') = -i\mathcal{L}_0(t)\mathcal{G}^{(n)}(t,t')\mathcal{Q}(t')$$

Using this and adding eqs. (4.7) and (4.6) we arrive at

$$\begin{aligned}\frac{dE^{(n)}(t)}{dt} &= -iTr(H\mathcal{L}R^{(n)}(t)) - iTr\left(H\left[\mathcal{P}(t)\mathcal{L}+\mathcal{L}_0(t)\right]\mathcal{G}^{(n)}(t,0)\mathcal{Q}(0)\rho(0)\right)\\ &- Tr\left(H\left[\mathcal{P}(t)\mathcal{L}+\mathcal{L}_0(t)\right]\int_0^t dt'\mathcal{G}^{(n)}(t,t')\mathcal{Q}(t')\mathcal{L}R^{(n)}(t')\right) \qquad (4.8)\end{aligned}$$

The first term vanishes. For both other terms we have to require

$$Tr\left(H\left[\mathcal{P}(t)\mathcal{L}+\mathcal{L}_0(t)\right]\ \ldots\right) = 0$$

or

$$\left[\mathcal{P}^\dagger(t)H - H_0(t), H\right] = 0.$$

It is possible to generalize this condition somewhat. First we write with (3.1) $H = H_0(t) + H_1(t)$. Then we realize that due to eq. (2.23) we can always move a $\mathcal{Q}$ to the left of $\mathcal{G}^{(n)}$ in eq. (4.8) which actually gives the condition

$$\mathcal{Q}^\dagger(t)\left[\mathcal{P}^\dagger(t)H - H_0(t), H\right] = 0. \qquad (4.9)$$

Because of the algebra condition (3.6) and with eq. (2.11) this is equivalent to

$$\mathcal{Q}^\dagger(t)\left[\mathcal{P}^\dagger(t)H - H_0(t), H_1(t)\right] = 0. \qquad (4.10)$$

If and only if $H_0(t)$ fulfills this condition energy will be conserved to each order of the perturbation expansion. This is a severe restriction on the splitting of $\mathcal{L}$ and therewith on the perturbation series. In practice one will take the simplest solution of eq. (4.10) which is

$$H_0(t) = \mathcal{P}^\dagger(t)H. \qquad (4.11)$$

This means that once one decides on the macro-observables and on the corresponding statistical operator R the projection formalism tells what to take for the unperturbed Liouvillian and what for the perturbation. Except for the more or less academic freedom which eq. (4.10) still allows for there is no arbitrariness left.

We mention that the algebra condition (3.6) which restricts the choice of the macro-observables is actually not needed for our argumentation. Without (3.6) we use instead of $\mathcal{G}_0(t,t')$ the more unwieldy $\hat{\mathcal{G}}_0(t,t')$ which evolves in time according to $\mathcal{Q}(t')\mathcal{L}_0(t')$ as defined in eqs. (3.3) to (3.5). The result is again condition (4.10).

5 Energy Conservation and Zwanzig's Projection

In this section we exemplify the foregoing ideas with Zwanzig's projection method. Let us denote by P_k a complete set of projection operators, *i.e.*

$$\sum_k P_k = 1, \qquad P_kP_l = P_lP_k = \delta_{kl}P_k \qquad (5.1)$$

If we regard the P_k as the macro-observables we obtain the following macro statistical operator:

$$R(t) = \sum_k p_k(t)P_k \qquad (5.2)$$

with

$$p_k(t) = Tr(\rho(t)P_k) = Tr(R(t)P_k).$$

From eqs. (2.13) and (2.14) we get Zwanzig's projection operator [2] as

$$\mathcal{P}X = \mathcal{P}^\dagger X = \sum_k Tr(P_kX)P_k. \qquad (5.3)$$

It is time independent and hermitian with the scalar product (2.6). For the perturbation expansion we decompose the Hamiltonian into

$$H = H_0(t) + H_1(t) \qquad (5.4)$$

and demand for H_0 the algebra condition (3.6)

$$[H_0(t), P_k] = \sum_l c_{kl}P_l. \qquad (5.5)$$

Using the orthogonality of the P_k (eq. (5.1)) we get

$$[H_0(t), P_k] = 0 \qquad (5.6)$$

and hence

$$H_0(t) = \sum_k h_k(t)P_k. \qquad (5.7)$$

If we insert this general form into the condition (4.9) for the energy conservation we obtain

$$\begin{aligned}0 &= \mathcal{Q}\left[\mathcal{P}H - H_0(t), H\right] = \left[\mathcal{P}H - H_0(t), H\right]\\ &= \sum_k\{\epsilon_k - h_k(t)\}\left[P_k, H\right], \qquad (5.8)\end{aligned}$$

where we introduced the eigenvalues ϵ_k of $\mathcal{P}H$,

$$\mathcal{P}H = \sum_k Tr(P_kH)P_k = \sum_k \epsilon_kP_k. \qquad (5.9)$$

In general H does not commute with P_k. Thus we demand (see (4.11))

$$\epsilon_k = h_k(t)$$

or

$$H_0(t) = H_0 = \mathcal{P}H \tag{5.10}$$

This is exactly Zwanzig's choice of a time independent unperturbed Hamiltonian, where the macro-observables are the projection operators onto its eigenspaces. Herewith also the perturbation $H_1 = H - \mathcal{P}H$ is uniquely given. There is still the nominal freedom of adding to $\mathcal{P}H$ a constant of motion δH

$$\delta H(t) := H_0(t) - \mathcal{P}H = \sum_k (h_k(t) - \epsilon_k) P_k, \tag{5.11}$$

but we shall see soon that this has no effect on the equations.

In second order perturbation and presuming that there are no initial correlations ($\mathcal{Q}\rho(0) = 0$) the equations of motion (2.24) for the macro-variables assume the form

$$\frac{d}{dt} p_l(t) = \sum_k Tr(HP_kHP_l) \int_0^t dt' \, 2\cos\left((\epsilon_k - \epsilon_l)(t-t')\right) [p_k(t') - p_l(t')]. \tag{5.12}$$

Here we used that $[H_0(t), P_k] = 0$ and thus $\mathcal{G}_0(t,t')P_k = P_k$. Let us now investigate explicitly the interplay between the energy residing in the macro degrees of freedom and the energy induced by the correlations. The correlation part of the statistical operator (c.f. (4.2)) is given by (in the following we suppress the superscript $^{(2)}$ which would stand for second order perturbation expansion)

$$R_c = -i \int_0^t dt' p_k(t') \left[\mathcal{G}_0(t,t')H, P_k\right]. \tag{5.13}$$

Even if $\mathcal{G}_0(t,t')$ is the time evolution according to $\mathcal{P}H + \delta H(t)$ we see immediately, since $[H, \delta H(t)] = 0$, that

$$\mathcal{G}_0(t,t')H = \sum_{lm} P_l H P_m exp\{-i(\epsilon_l - \epsilon_m)(t-t')\}, \tag{5.14}$$

and hence the effect of $\delta H(t)$ has disappeared. Thus the time evolution of $p_k(t)$ as well as the correlation energy which is given by

$$E_c(t) = Tr(R_c(t)H) = \sum_{kl} Tr(HP_kHP_l) \int_0^t dt' p_k(t') \, 2\sin\left((\epsilon_k - \epsilon_l)(t-t')\right), \tag{5.15}$$

does not depend on $\delta H(t)$. The uncorrelated energy is just

$$E_0(t) = Tr(R(t)H) = \sum_k p_k(t) Tr(P_k H) = \sum_k p_k(t)\epsilon_k. \tag{5.16}$$

One sees from the last two equations that in general both, E_0 and E_c, are time dependent, but due to the special choice of $H_0 = \mathcal{P}H$ their sum is not, as proven generally in eq. (4.8). It is now an easy task to show explicitly by differentiation of (5.15) and (5.16) that after reinsertion of the equations of motion for the probabilities $p_k(t)$ the energy $E_0(t) + E_c(t)$ is conserved.

If the spectrum of H_0 is dense a Marcov approximation is suited. Let us define energy bins $\{\lambda\}$ of width 2Δ by

$$\{\lambda\} = \{E_\lambda - \Delta < \epsilon_\lambda \leq E_\lambda + \Delta\} \quad \text{where} \quad E_{\lambda+1} = E_\lambda + 2\Delta. \tag{5.17}$$

We can now coarse grain the equation of motion (5.12) as

$$\frac{d}{dt} \sum_{l\in\{\lambda\}} p_l(t) = 2 \sum_\kappa \left\{ \sum_{k\in\{\kappa\}} \int_0^t dt' p_k(t') \left[\sum_{l\in\{\lambda\}} Tr(HP_kHP_l) \cos\left((\epsilon_k - \epsilon_l)(t-t')\right)\right] - \sum_{l\in\{\lambda\}} \int_0^t dt' p_l(t') \left[\sum_{k\in\{\kappa\}} Tr(HP_kHP_l) \cos\left((\epsilon_k - \epsilon_l)(t-t')\right)\right]\right\} \tag{5.18}$$

where $\sum_{l\in\{\lambda\}}$ is just a short hand notation for summation over l within the energy bin $\epsilon_l \in \{\lambda\}$. $Tr(HP_kHP_l) = |\langle k|H|l\rangle|^2$ is always a positive number. Let us assume that it changes only little with l if l belongs to the energy bin $\{\lambda\}$. Then we can replace it by an averaged matrix element and since the spectrum of H_0 is dense we may estimate

$$\begin{aligned} &\sum_{l\in\{\lambda\}} Tr(HP_kHP_l) \cos\left((\epsilon_k - \epsilon_l)(t-t')\right) \\ &\approx \left(\frac{1}{d_\lambda} \sum_{l\in\{\lambda\}} Tr(HP_kHP_l)\right) \frac{d_\lambda}{2\Delta} \int_{E_\lambda - \Delta}^{E_\lambda + \Delta} d\epsilon \cos\left((\epsilon_k - \epsilon_l)(t-t')\right) \\ &= \left(\frac{1}{d_\lambda} \sum_{l\in\{\lambda\}} Tr(HP_kHP_l)\right) \rho(E_\lambda) \, 2 \frac{\sin(\Delta(t-t'))}{t-t'} \cos\left((\epsilon_k - E_\lambda)(t-t')\right) \end{aligned} \tag{5.19}$$

Here d_λ denotes the number of states in bin $\{\lambda\}$, and $\rho(E_\lambda) = d_\lambda/(2\Delta)$ is the level density at energy E_λ. An analogue expression holds for the loss term in eq. (5.18). One sees that the superposition of many cosine functions results in an integrand which is localized in time around $t - t' \approx 0$ with a memory time of the order $\tau_{mem} \approx 1/(2\Delta) = \rho(E_\lambda)/d_\lambda$. If the probabilities vary slowly on a time scale set by τ_{mem} one can therefore replace $p_k(t')$ and $p_l(t')$ by $p_k(t)$ and $p_l(t)$, respectively, and eq. (5.18) is approximated by

$$\frac{d}{dt} \sum_{l\in\{\lambda\}} p_l(t) \approx 2 \sum_\kappa \sum_{\substack{k\in\{\kappa\} \\ l\in\{\lambda\}}} Tr(HP_kHP_l) \frac{\sin(\epsilon_k - \epsilon_l)t}{\epsilon_k - \epsilon_l} [p_k(t) - p_l(t)] \tag{5.20}$$

For times $t > \Delta^{-1}$ the peaked function $(\sin(\epsilon_k - \epsilon_l)t)/(\epsilon_k - \epsilon_l)$ allows only transitions for $\epsilon_k - \epsilon_l < \Delta$ or in other words ϵ_k and ϵ_l have to be in the same energy bin $\{\lambda\}$. Thus we replace

$$\frac{\sin(\epsilon_k - \epsilon_l)t}{\epsilon_k - \epsilon_l} \longrightarrow \pi\delta_{\kappa\lambda}\rho(E_\lambda) \quad \text{for} \quad t \gg \Delta^{-1}, \quad \epsilon_k \in \{\kappa\}, \quad \epsilon_l \in \{\lambda\}, \tag{5.21}$$

and eq. (5.20) becomes

$$\frac{d}{dt}\sum_{l\in\{\lambda\}} p_l(t) \approx 2\pi\rho(E_\lambda) \sum_{\substack{k\in\{\kappa\}\\ l\in\{\lambda\}}} Tr(HP_kHP_l)\,[p_k(t) - p_l(t)] = 0 \tag{5.22}$$

This tells us that the total occupation probability of bin $\{\lambda\}$ does not change in time if we assume a dense spectrum and weak coupling. The uncorrelated energy is therefore approximately conserved

$$\frac{d}{dt}E_0(t) = \sum_\lambda \sum_{l\in\{\lambda\}} \epsilon_l \frac{dp_l}{dt} \approx \sum_\lambda E_\lambda \sum_{l\in\{\lambda\}} \frac{dp_l}{dt} \approx 0. \tag{5.23}$$

For the correlation energy we cannot perform a Markov approximation, since the sine function in eq. (5.15) does not lead to a peaked function as the cosine did in eq. (5.12) under coarse graining (*cf.* (5.19)). But the time derivative of E_c

$$\frac{d}{dt}E_c(t) = \sum_{kl} Tr(HP_kHP_l)(\epsilon_k - \epsilon_l)\int_0^t dt' p_k(t')2\cos\left((\epsilon_k - \epsilon_l)(t - t')\right) \tag{5.24}$$

is of similar structure as eq. (5.12) and therefore well suited for the same approximation. Performing the Markov approximation on (5.24) will lead again to energy conservation. This means that both the correlated and the uncorrelated energy are only approximately conserved, but in such a way that their sum is time independent if the Markov approximation is done at the proper places.

6 Energy Conservation in Mean Field Theories with Collision Terms

Let us suppose that the dynamical evolution of a fermion system is following mainly a one-body Hamiltonian, and that residual two-body interactions only randomize the motion. For such a situation an appropriate choice of the macro-observables is the set of all one-body operators

$$\{a^\dagger_\alpha a_\beta;\ \ \alpha,\beta = 1,2,3,...\} \quad \text{with} \quad [a_\alpha, a^\dagger_\beta]_+ = \delta_{\alpha\beta}. \tag{6.1}$$

The matrix elements of the one-body density

$$\rho^{(1)}_{\alpha\beta}(t) := Tr(\rho(t)a^\dagger_\beta a_\alpha) = Tr(R(t)a^\dagger_\beta a_\alpha) \tag{6.2}$$

play the role of the macro-variables (see (2.1) and (2.2)). The corresponding macro statistical operator takes the form [16,27]

$$\begin{aligned} R(t) &= \frac{1}{Z(t)} exp\left\{-\sum_{\alpha\beta}\lambda_{\alpha\beta}(t)a^\dagger_\alpha a_\beta\right\} \\ &= \prod_\alpha \left\{(1 - n_\alpha(t))c_\alpha(t)c^\dagger_\alpha(t) + n_\alpha(t)c^\dagger_\alpha(t)c_\alpha(t)\right\} \end{aligned} \tag{6.3}$$

where $Z(t)$ is the partition sum. The second line represents the statistical operator in terms of eigenstates $c^\dagger_\alpha(t)|0\rangle$ and eigenvalues $n_\alpha(t)$ (mean occupation numbers) of the one-body density

$$\rho^{(1)}(t) = \sum_{\alpha\beta} a^\dagger_\alpha|0\rangle\rho^{(1)}_{\alpha\beta}(t)\langle 0|a_\beta = \sum_\alpha c^\dagger_\alpha(t)|0\rangle n_\alpha(t)\langle 0|c_\alpha(t). \tag{6.4}$$

The corresponding projector (as defined in (2.13) is most conveniently expressed in terms of $c^\dagger_\alpha(t)$ and $n_\alpha(t)$ as [18,16]

$$\begin{aligned} \mathcal{P}(t)X &= \left[1 - \sum_\alpha \frac{c^\dagger_\alpha(t)c_\alpha(t) - n_\alpha(t)}{1 - n_\alpha(t)}\right] Tr(X)R(t) \\ &+ \sum_{\alpha\beta} \frac{c^\dagger_\alpha(t)c_\beta(t) - \delta_{\alpha\beta}n_\beta(t)}{(1 - n_\alpha(t))n_\beta(t)} Tr(c^\dagger_\beta(t)c_\alpha(t)X)R(t) \end{aligned} \tag{6.5}$$

The adjoint $\mathcal{P}^\dagger(t)$ is given by

$$\begin{aligned} \mathcal{P}^\dagger(t)X &= \left[\langle X\rangle - \sum_\alpha \frac{\langle X(c^\dagger_\alpha(t)c_\alpha(t) - n_\alpha(t))\rangle}{1 - n_\alpha(t)}\right] \\ &+ \sum_{\alpha\beta} \frac{\langle X(c^\dagger_\alpha(t)c_\beta(t) - \delta_{\alpha\beta}n_\alpha(t))\rangle}{(1 - n_\alpha(t))n_\beta(t)} c^\dagger_\beta(t)c_\alpha(t) \end{aligned} \tag{6.6}$$

where the averages $\langle\ \rangle$ denote the mean values:

$$\langle X\rangle := Tr(R(t)X) \tag{6.7}$$

The Hamiltonian consists of a one-body and a two-body part

$$H = \sum_{\alpha\beta} T_{\alpha\beta}a^\dagger_\alpha a_\beta + \frac{1}{4}\sum_{\alpha\gamma\beta\delta} V_{\alpha\gamma,\beta\delta}a^\dagger_\alpha a^\dagger_\gamma a_\delta a_\beta \tag{6.8}$$

where $V_{\alpha\gamma,\beta\delta}$ are antisymmetrized matrix elements. As discussed in section 4 we choose for the unperturbed Hamiltonian $H_0(t) = \mathcal{P}^\dagger(t)H$ (see eq. (4.9)). Application of $\mathcal{P}^\dagger(t)$ as given in (6.6) results in

$$H_0(t) = \mathcal{P}^\dagger(t)H = \sum_{\alpha\beta} h^{MF}_{\alpha\beta}(t)a^\dagger_\alpha a_\beta - \frac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\gamma,\beta\delta}\rho^{(1)}_{\delta\gamma}(t)\rho^{(1)}_{\beta\alpha}(t) \tag{6.9}$$

with

$$h^{MF}_{\alpha\beta}(t) = T_{\alpha\beta} + \sum_{\gamma\delta} V_{\alpha\gamma,\beta\delta}\rho^{(1)}_{\delta\gamma}(t) \tag{6.10}$$

It is interesting to note that $P^\dagger(t)H$ turns out to be the time-dependent Hartree-Fock Hamiltonian $h^{MF}(t)$ minus a real number which takes care of the fact that the expectation value of the Hartree-Fock Hamiltonian contains the interaction energy twice [28]. Thus, we get the proper relation for the uncorrelated energy

$$\begin{aligned} E_0(t) &= Tr(HR(t)) = Tr(HP(t)\rho(t)) = Tr(H_0(t)\rho(t)) = Tr(H_0(t)R(t)) \\ &= \sum_{\alpha\beta} T_{\alpha\beta}\rho^{(1)}_{\beta\alpha}(t) + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} V_{\alpha\gamma,\beta\delta}\rho^{(1)}_{\delta\gamma}(t)\rho^{(1)}_{\beta\alpha}(t) \end{aligned} \tag{6.11}$$

In absence of initial correlations the general equations of motion (2.24) assume the form

$$\frac{d}{dt}\rho^{(1)}_{\beta\alpha}(t) = -iTr\left(a^\dagger_\alpha a_\beta \mathcal{L}R(t)\right) - \int_0^t dt' Tr\left(a^\dagger_\alpha a_\beta \mathcal{L}\mathcal{G}(t,t')Q(t')\mathcal{L}R(t')\right) \tag{6.12}$$

where the Liouvillian corresponds to the Hamiltonian given in (6.8). If we keep only terms up to second order in the perturbation expansion, $\mathcal{G}(t,t')$ in eq. (6.11) has to be replaced by $\mathcal{G}_0(t,t')$ (see eq. (3.11)). Although the evaluation of the integral kernel is done most efficiently in the $c^\dagger_\alpha(t)$ representation [15,18,16] we formulate the result again in the time independent $a^\dagger_\alpha$ representation

$$\frac{d}{dt}\rho^{(1)}_{\beta\alpha}(t) = -i\left[H_0(t),\rho^{(1)}(t)\right]_{\beta\alpha} + \int_0^t dt'\left\{C_{\beta\alpha}(t,t') + C_{\alpha\beta}(t,t')^*\right\} \tag{6.13}$$

where

$$C_{\beta\alpha}(t,t') = \frac{1}{2}\sum_{klm}\tilde{V}_{\beta k,lm}(t,t')X_{lm,\alpha k}(t'), \tag{6.14}$$

$$\begin{aligned} X_{lm,\alpha k}(t') = \sum_{\alpha' k' l' m'} V_{l'm',\alpha' k'}\Big\{ &\rho^{(1)}_{ll'}(t')\rho^{(1)}_{mm'}(t')\overline{\rho^{(1)}_{\alpha'\alpha}(t')}\;\overline{\rho^{(1)}_{k'k}(t')} \\ - &\overline{\rho^{(1)}_{ll'}(t')}\;\overline{\rho^{(1)}_{mm'}(t')}\rho^{(1)}_{\alpha'\alpha}(t')\rho^{(1)}_{k'k}(t')\Big\}, \end{aligned} \tag{6.15}$$

$$\overline{\rho^{(1)}_{\alpha\beta}(t')} = \delta_{\alpha\beta} - \rho^{(1)}_{\alpha\beta}(t') \tag{6.16}$$

and

$$\tilde{V}(t,t') = \mathcal{G}_0(t,t')^{-1}V. \tag{6.17}$$

Eq.(6.17) means that the matrix elements $\tilde{V}_{\alpha\beta,\gamma\delta}(t,t')$ of the two-body interaction V have to be calculated with time-dependent single-particle states which are evolved backwards in time from t to t' according to the mean-field Hamiltonian $H_0(t)$ given in eq.(6.9).

$$\tilde{V}_{\alpha\beta,\gamma\delta}(t,t') = \sum_{\alpha'\beta'\gamma'\delta'} U(t,t')_{\alpha\alpha'}U(t,t')_{\beta\beta'}V_{\alpha'\beta',\gamma'\delta'}U(t,t')^*_{\gamma\gamma'}U(t,t')^*_{\delta\delta'} \tag{6.18}$$

where

$$i\frac{d}{dt}U(t,t')_{\alpha\beta} = \{H_0(t)U(t,t')\}_{\alpha\beta},\quad U(t,t)_{\alpha,\beta} = \delta_{\alpha\beta}. \tag{6.19}$$

In a perturbation expansion one would be tempted to expect the residual interaction $(V - H_0(t))$ in the collision term. However, due to the presence of $\mathcal{Q}(t')$ (see eq. (6.12)) all one-body parts of $\mathcal{L}$ disappear and the two-body interaction V itself enters $C_{\alpha\beta}$ in eqs. (6.14) and (6.15).

Next we calculate explicitly in second order pertubation expansion the time derivatives of the uncorrelated energy and the correlation energy. For the uncorrelated energy follows immediately from eq. (6.11) and the eqs. of motion (6.13)

$$\begin{aligned} \frac{d}{dt}E_0(t) &= \sum_{\alpha\beta}\left(T_{\alpha\beta} + \sum_{\gamma\delta}V_{\alpha\gamma,\beta\delta}\,\rho^{(1)}_{\delta\gamma}(t)\right)\frac{d}{dt}\rho^{(1)}_{\beta\alpha}(t) = \sum_{\alpha\beta}h^{MF}_{\alpha\beta}(t)\frac{d}{dt}\rho^{(1)}_{\beta\alpha}(t) \\ &= \sum_{\alpha\beta}h^{MF}_{\alpha\beta}(t)\int_0^t dt'\{C_{\beta\alpha}(t,t') + C_{\alpha\beta}(t,t')^*\} \end{aligned} \tag{6.20}$$

According to eqs. (4.2) and (4.4) the correlation energy is given by

$$E_c(t) = -iTr\left(H\int_0^t dt'\,\mathcal{G}_0(t,t')\mathcal{Q}(t')\mathcal{L}R(t')\right) \tag{6.21}$$

and can be expressed in terms of $C_{\alpha\alpha}(t,t')$ given in eq. (6.14) as

$$E_c(t) = -\frac{i}{2}\int_0^t dt'\sum_\alpha C_{\alpha\alpha}(t,t') \tag{6.22}$$

(Note that the superscripts $^{(2)}$ which denote second order pertubation have been dropped again.) In the time derivative

$$\frac{d}{dt}E_c(t) = -\frac{i}{2}\int_0^t dt'\sum_\alpha\frac{\partial}{\partial t}C_{\alpha\alpha}(t,t') - \frac{i}{2}\sum_\alpha C_{\alpha\alpha}(t,t) \tag{6.23}$$

the last term vanishes which can be verified with eqs. (6.14), (6.15) and $\bar{V}(t,t) = V$. With help of eqs. (6.15) through (6.19) we obtain the time derivative for $\sum_\alpha C'_{\alpha\alpha}(t,t')$ as

$$\begin{aligned} \sum_\alpha\frac{\partial}{\partial t}C_{\alpha\alpha}(t,t') &= -\frac{i}{2}\sum_{\alpha klm}\left[H_0(t),\bar{V}(t,t')\right]_{\alpha k,lm}X_{lm,\alpha k}(t') \\ &= -i\sum_{\alpha\beta klm}\left(h^{MF}_{\alpha\beta}(t)\tilde{V}_{\beta k,lm}(t,t') - \bar{V}_{\alpha k,l\beta}(t,t')h^{MF}_{\beta m}(t)\right)X_{lm,\alpha k}(t') \\ &= -2i\sum_{\alpha\beta}h^{MF}_{\alpha\beta}(t)\left\{C_{\beta\alpha}(t,t') + C_{\alpha\beta}(t,t')^*\right\}. \end{aligned} \tag{6.24}$$

In order to get from the second to the third line we rename indices and use the anti-hermeticity of the two-body operator $\boldsymbol{X}(t')$ (see eq. (6.15)).
Thus, the change in the correlation energy

$$\frac{d}{dt}E_c(t) = -\sum_{\alpha\beta} h^{MF}_{\alpha\beta}(t) \int_0^t dt' \left\{ C_{\beta\alpha}(t,t') + C_{\alpha\beta}(t,t')^* \right\} \qquad (6.25)$$

balances exactly the opposite change in the uncorrelated energy $E_0(t)$ given in eq. (6.20). The action of two-body collisions transfers occupation probability to single particle states displaced in energy which may alter $E_0(t)$ but at the same time correlations are being built up which compensate for the change in $E_0(t)$.

7 Summary

Based on the projection formalism, which may serve as the the starting point for any derivation of dissipative equations of motion, we have investigated the consequences of conservation laws. In this context a conservation law is presumed to be fulfilled if the expectation value of the corresponding constant of motion is time independent during the dissipative evolution of the system. The easiest way to incorporate a conservation law is to include the constant of motion explicitly as a member into the set of macro-observables on which the projection is based. In that case almost any approximation of the memory kernel can be accepted and furthermore correlations in the system do not contribute to the mean value. Examples are the total particle number, total momentum or total angular momentum.

The total energy is usually not a member of the macro-observables because the Hamiltonian has to couple macro-variables with the remaining degrees of freedom in order to achieve randomization and equilibration. Therefore, only part of the Hamiltonian can be a macro-observable while the remaining part acts as a perturbation. In a very general derivation we showed under which conditions energy is conserved. First, the correlations (difference between the projected statistical operator and the exact one) carry part of the energy so that only the sum of the macro and the correlation energy is time independent. Second, in a properly defined perturbation expansion the time derivative of the correlation energy has to be calculated with the same approximations as the time derivative of the projected statistical operator. With these suppositions the quest for energy conservation determines how the Hamiltonian has to be split into an unperturbed part and a perturbation. This strong restriction in the choice of the perturbation allows a control on the strength of the perturbation only via the selection of the relevant macro-observables (thermodynamic variables).

We used two examples, Zwanzig's projection method (master equation) and time-dependent mean field theory extended by collision terms, to illustrate explicitly and in a less abstract way the implications of energy conservation. We want to emphasize, however, that the ideas worked out in the general derivation apply

to any treatment utilizing the projection formalism in conjunction with the weak coupling limit.

A Appendix

In the following we prove the uniqueness of the projector (2.13) under the given conditions and derive some consequences.
To simplify the calculations let us introduce a bra-ket notation in superspace: If $|X)$ is a vector in superspace, the dual vector $(Y|$ is defined via the scalar product (2.6)

$$(Y|X) = Tr(Y^\dagger X).$$

The macro-operators A_k correspond to the vectors $|A_k)$ in superspace. They are linearly independent but generally not orthogonal to each other. Let $|B_k)$ be a set of biorthogonal vectors to the A_k, *i.e.*

$$(B_k|A_l) = \delta_{kl}. \qquad (A.1)$$

Linearity, idempotency and the condition that $\mathcal{P}^\dagger$ projects onto the macro-observables (2.11) lead to

$$\mathcal{P} = \sum_k |B_k)(A_k| \qquad (A.2)$$

$$\mathcal{P}^\dagger = \sum_k |A_k)(B_k|. \qquad (A.3)$$

The appropriate $|B_k)$ are readily found. Since R depends only implicitly on time and with eq. (2.12) one sees

$$|\frac{dR}{dt}) = \sum_k \frac{da_k}{dt} |\frac{\partial R}{\partial a_k}) = \sum_k |B_k)(A_k|\frac{d\rho}{dt}) = \sum_k |B_k)\frac{da_k}{dt}. \qquad (A.4)$$

Due to the independence of $\partial R/\partial a_k$ and $|B_k)$ from da_k/dt (A.4) results in

$$|B_k) = |\frac{\partial R}{\partial a_k}). \qquad (A.5)$$

Together with (A.2) and (A.3) this is equivalent to eqs. (2.13) and (2.14), which closes the proof.

It is easy to see that condition (2.11) implies that R is homogenous of degree one in the a_k. We have only to insert eq. (A.5) into eq. (2.10):

$$|R) = \sum_k |B_k)(A_k|R) = \sum_k a_k |\frac{\partial R}{\partial a_k}).$$

With the above notation it is also easy to prove eq. (2.15):

$$\mathcal{P}(t)\mathcal{P}(t')|X) = \sum_{kl} |B_k(t))(A_k|B_l(t'))(A_l|X) = \sum_k |B_k(t))(A_k|X) = \mathcal{P}(t)|X),$$

since $(A_k|B_l(t')) = Tr(A_k \partial R(t')/\partial a_l(t')) = \partial a_k(t')/\partial a_l(t') = \delta_{kl}$.

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