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LETTER TO THE EDITOR

An algebraic approach to irreversible dynamical descriptions

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Abstract. We establish a connection between the non-unitary transformation scheme which breaks the time reversibility at the microscopical level and an algebraic deformation scheme which generalises the Lie product. This formal approach is further supported by an explicit construction of the various operators involved. The compatibility conditions are considered for this case and are found to be automatically satisfied by the algebraic deformation scheme in the particular case of the Fokker–Planck equation. In this way, a particular model of the non-unitary transformation scheme is given constructively.

In this note we present a construction of the Φ operator, which results formally in the Λ-transformation scheme of Prigogine and coworkers (Misra and Prigogine 1983, Prigogine 1979, 1981, Prigogine *et al* 1973), through an algebraic deformation approach (Fronteau *et al* 1979). Furthermore we shall demonstrate the intimate connection between the two aforementioned approaches and in particular, how the algebraic deformation scheme can be regarded as the case of what Prigogine *et al* call intrinsically random systems. We recall that the physically relevant distribution function ρ is defined in Prigogine (1981) by $\tilde{\rho} = \Lambda^{-1}\rho$, where Λ is a non-unitary transformation, and satisfies the modified Liouville equation

$$\mathrm{i}\partial_t\tilde{\rho} = \Phi\tilde{\rho} \tag{1}$$

where $\Phi(L) = \Lambda^{-1}L\Lambda$. Here L denotes the formal Liouville operator for a Hamiltonian system which is Hermitian and which can be easily adapted either to the classical (Poisson brackets) or to the quantum mechanical (commutator) case (Prigogine *et al* 1973). Now the requirement for the existence of a Lyapounov function implies the *star Hermiticity condition* on Φ, namely

$$\mathrm{i}\Phi(L) = [\mathrm{i}\Phi(L)]^* \tag{2}$$

where by definition

$$\Phi^*(L) = \Phi(-L)^\dagger \tag{2a}$$

and where the dagger denotes Hermitian conjugation. The above condition is a necessary ingredient for establishing an H-theorem (Prigogine 1981). In addition the star Hermiticity condition guarantees that in general the operator Φ can be divided into an even and an odd part. In other words instead of (1) we may write

$$\mathrm{i}\partial_t\tilde{\rho} = (\Phi^{\mathrm{odd}} + \Phi^{\mathrm{ev}})\tilde{\rho} \tag{1a}$$

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having so transformed the macroscopic thermodynamics distinction between reversible (Φ^{ev}) and irreversible (Φ^{odd}) processes into the microscopic description.

At this point, it is worth noticing that Grmela and Iscoe (1978) have also considered a *unique* decomposition of the general kinetic equation by writing

$$\partial_t \tilde{\rho} = R_-(\tilde{\rho}) + R_+(\tilde{\rho}) \tag{3}$$

where $R_-(\tilde{\rho})$ stands for the time reversible part of the right-hand side and $R_+(\tilde{\rho})$ incorporates the irreversible behaviour which according to the previous considerations may be thought of as brought about by the non-unitary mapping Λ.

It is important to notice the difference between ($1a$) and (3). As noted already, ($1a$) is a 'generalised' Liouville equation which transcribes to the microscopic domain the thermodynamical distinction between reversible and irreversible processes. Equation (3), on the other hand, is a genuine macroscopic equation. Attributing the latter equation to the microscopic domain, Fronteau (1981 and references therein) has reached an interesting new interpretation. According to Fronteau (1981) the non-equilibrium statistical mechanical equation (3) leads to a quasiparticle concept. This new concept corresponds to a 'total' picture emerging for a particle when the interaction with all other particles is taken into account. Here, there occurs an interesting analogy with quantum field theory where one considers a bare and dressed particle, the latter being conceived of as a 'final' entity emerging once microscopic interactions have been taken into account.

The question arises whether (3) can be cast in the operator form of ($1a$) and *vice versa*. We shall show that this can be naturally achieved within the Lie admissible deformation scheme which generalises the Lie algebraic structure of the Poisson bracket. We recall that according to Fronteau *et al* (1979) the classical Liouville equation can be generalised by replacing the Poisson bracket with a new one, namely

$$\partial_t \tilde{\rho} = (H, \tilde{\rho}) \tag{4}$$

where

$$(H, \tilde{\rho}) = HR\tilde{\rho} + \tilde{\rho}TH. \tag{4a}$$

In the above equations H is a 'Hamiltonian function' which describes only a part of the system. R and T are operators which in certain special cases reduce to functions on the phase space. We stress that (4) refers to the evolution of the physically relevant distribution function in phase space. It is for this reason that we have denoted the density in (4) by $\tilde{\rho}$.

Operators R and T describe the deformation content of the theory. According to our point of view these operators are capable of incorporating the dynamical content which leads to the quasiparticle picture.

We are now in position to relate, at least formally, the non-unitary transformation $\rho \to \tilde{\rho} = \Lambda^{-1}\rho$ with the aforementioned deformation scheme. In particular, if we start with the full Liouville equation and act by Λ^{-1} from the left we get

$$\mathrm{i}\partial_t \tilde{\rho} = \Lambda^{-1} H \Lambda \tilde{\rho} - \tilde{\rho} H. \tag{5}$$

Comparing with (4) and ($4a$) we notice that the operation by Λ^{-1} amounts to the identification

$$\Lambda^{-1} H \Lambda = HR, \qquad T = -I, \tag{6a, b}$$

where I is the identity operator.

Clearly, equations (6*a*) and (6*b*) relate (formally) the two aforementioned schemes. In particular, they provide a prescription for the specification of the non-unitary operator Λ provided that the deformation operator R is known. Conversely, if Λ is known a corresponding deformation operator can, in principle, be introduced via (6*a*).

In the bridging equations (6) appears only the Hamiltonian H and not the operator Φ. To proceed in this direction we construct the formal Liouville operator via the identification

$$L = \mathrm{i}\mathscr{H} \tag{7}$$

where

$$\mathscr{H} = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \right)$$

when the Hamiltonian H is known. In exactly the same way we may explicitly construct the operator Φ directly from (4) by taking into account the form of the generalised product (,) in the classical case (Fronteau *et al* 1979), namely

$$\Phi = \mathrm{i}\tilde{\mathscr{H}} \tag{8}$$

where

$$\tilde{\mathscr{H}} = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \right) + \sum_{i,j=1}^{n} \frac{\partial H}{\partial p_i} s_{ij} \frac{\partial}{\partial p_j}. \tag{8a}$$

Here s_{ij} is a well defined $n \times n$ matrix which expresses the content of the algebraic deformation in a precise form. We stress that the term $(\partial H/\partial p_i) s_{ij} \partial/\partial p_j$ should not be interpreted strictly as a friction term. This less interesting instance is also included in the formalism, but we are mostly interested in the case when s_{ij} includes the effective interaction of the whole with the individual. This is the case which leads to the quasiparticle concept.

Equations (7) and (8) split naturally in two parts. In particular we may write

$$\tilde{\mathscr{H}}^1 = \mathscr{H}^1 + \mathscr{S}, \qquad \tilde{\mathscr{H}}^2 = \mathscr{H}^2, \tag{9a, b}$$

where

$$\mathscr{H}^1 \equiv \sum_{i=1}^{n} \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i}, \qquad \mathscr{H}^2 \equiv -\sum_{i=1}^{n} \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i}, \qquad \mathscr{S} = \sum_{i,j=1}^{n} \frac{\partial H}{\partial p_i} s_{ij} \frac{\partial}{\partial p_j}.$$

Thus, given the Hamiltonian of the system and the algebraic deformation matrix s_{ij}, the formal operator Φ can be explicitly constructed through (9*a*), (9*b*) and (8). Clearly this is not enough. The star Hermiticity condition of Φ, or its counterpart on $\mathscr{S}$, has to be checked. In fact we have

$$\Phi(L) = \mathrm{i}\tilde{\mathscr{H}} = \mathrm{i}(-\mathrm{i}L + \mathscr{S}) = L + \mathrm{i}\mathscr{S}. \tag{10}$$

Now the star Hermiticity condition (2) imposed on (10) gives

$$-\tilde{\mathscr{H}} = (-\tilde{\mathscr{H}}(-L))^{\dagger} = -(\mathrm{i}L + \mathscr{S})^{\dagger} = \mathrm{i}L - \mathscr{S}^{\dagger} \tag{11}$$

which implies

$$\mathscr{S} = \mathscr{S}^{\dagger} \tag{12}$$

which means that the operator $\mathscr{S}$ is necessarily Hermitian.

As a particular example of the above analysis we consider the Fokker–Planck equation for one particle in three dimensions. In this case we have the decomposition (Grmela *et al* 1980)

$$\Phi^{\mathrm{ev}}\tilde{\rho}=\mathrm{i}R-\tilde{\rho}=\sum_{i=1}^{3} v_i\frac{\partial}{\partial r_i}\tilde{\rho}(\boldsymbol{r},\boldsymbol{v},t), \tag{13a}$$

$$\Phi^{\mathrm{odd}}\tilde{\rho}\equiv\mathrm{i}R+\tilde{\rho}=\sum_{i=1}^{3}\left(C\frac{\partial}{\partial v_i}(v_i\tilde{\rho}(\boldsymbol{r},\boldsymbol{v},t))+A\frac{\partial}{\partial v_i}\frac{\partial}{\partial v_i}\tilde{\rho}(\boldsymbol{r},\boldsymbol{v},t)\right) \tag{13b}$$

where C and A are the coefficients of dissipation and diffusion.

From (13a) the relevant Hamiltonian can be identified as $H=\frac{1}{2}mv_i^2$. On the other hand, from (13b) we have

$$\mathscr{S}=\sum_{i,j=1}^{3}\frac{\partial H}{\partial v_i}s_{ij}\frac{\partial}{\partial v_j}=C+\sum_{i=1}^{3}Cv_i\frac{\partial}{\partial v_i}+\sum_{i=1}^{3}A\frac{\partial}{\partial v_i}\frac{\partial}{\partial v_i}=\sum_{i,j=1}^{3}v_is_{ij}\frac{\partial}{\partial p_j}. \tag{14}$$

Condition (12) is automatically fulfilled for $\mathscr{S}$ by construction. The above is a particular instance of a more general situation. In fact, whenever the algebraic deformation scheme yields real and symmetric matrices s_{ij}, (12) will be automatically guaranteed by construction.

Concluding this note it is worth noticing that the alternative procedure for breaking time reversibility, namely via a projection operator P which acting on ρ eliminates unphysical effects, does not seem to have a deformation counterpart, in general. In order to study this situation, first we notice that P cannot commute with the Hamiltonian entering the Liouville equation (1).

In fact if it did we would have

$$\tilde{\rho}=P\rho=P\mathrm{e}^{-\mathrm{i}Ht}\rho(0)\mathrm{e}^{\mathrm{i}Ht}=\mathrm{e}^{-\mathrm{i}Ht}\tilde{\rho}(0)\mathrm{e}^{\mathrm{i}Ht}, \tag{15}$$

i.e. the evolution of $\tilde{\rho}$ would be determined by the original Hamiltonian which is undesirable.

Given that the commutator $[P,H]$ does not vanish we notice that the algebraic deformation scheme becomes effective only under special conditions. Specifically one must show the existence of an operator S which satisfies the relation

$$[P,H]=HSP. \tag{16}$$

If this happens to be the case we find

$$\mathrm{i}\partial_t\tilde{\rho}=PH\rho-\tilde{\rho}H=H(I+S)\tilde{\rho}-\tilde{\rho}H \tag{17}$$

where the natural identifications follow

$$R=I+S,\qquad T=-I. \tag{17a}$$

Clearly the conditions for the existence of an operator S satisfying (16) constitute an open question even in the formal case.

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