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LETTER TO THE EDITOR

Subdynamics approach to irreversibility in open systems

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Abstract. A new, explicitly time-dependent formulation of subdynamics is presented for the treatment of irreversible processes in non-equilibrium statistical mechanics. The theory generalises the subdynamics concept from the case where the Liouville superoperator is time independent to include the situation in which it may possess an explicit time dependence. The scope of the approach is considerably broadened thereby; as one particular consequence, the non-unitary ('star-unitary') transformation theory of the Brussels school may be extended to deal with large systems interacting with time-dependent external fields. Hence a unified description of irreversibility in both isolated and open systems begins to emerge.

The problem of explaining the irreversible evolution of macroscopic systems—as required by the second law of thermodynamics—on the basis of the microscopic dynamical equations has exercised the minds of many of the most eminent theoretical physicists of modern times. Two diametrically opposed schools of thought prevail: one maintains that irreversibility is actually an illusion, being brought about by our ignorance of the details of a purely reversible, dynamical description; the other asserts that irreversibility must be placed on an equally objective footing with reversibility [1, 2].

Over the past few years, important research in support of the latter viewpoint has been performed by the Brussels group; this has clearly shown how irreversibility can arise as an intrinsic property of isolated dynamical systems possessing sufficient complexity [1]. It should be pointed out that this work differs from other objective approaches, which tend to derive kinetic equations rigorously in certain mathematical limits; their validity is generally restricted to finite times only [3-5]. In complete contrast, much work in non-equilibrium statistical mechanics has sought to describe irreversibility by means of coarse graining [6, 7].

One particularly favoured area concerns the study of the irreversible evolution of open systems, by which we mean systems interacting with the external world. Here one must be careful not to confuse rigour with fundamentality of description: even the most mathematically rigorous approaches [8, 9] start from the assumption that irreversibility only arises by virtue of the coupling between system and environment—in flagrant contradiction with the second law.

Recent research by members of the Brussels group has led to a clear understanding of the relation between reversible unitary-group dynamics and irreversible semigroup

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evolution for certain isolated classical dynamical systems. This has been achieved by means of a non-unitary transformation theory tied to appropriate ergodic properties [10]. These results, while of considerable theoretical interest and importance, are too formal to be of value in applications to real systems (one has only to recall the difficulty in demonstrating that such systems possess the required properties).

Another approach, which should be more fruitful from this standpoint (although surprisingly little by way of applications has hitherto been undertaken), is based on the concept of subdynamics [1, 11, 12]. Originally introduced by Prigogine *et al* [13], it has played a central role in clarifying the relationship between dynamical and thermodynamic descriptions of large many-body systems [13, 14]. It has, moreover, proved to be a very powerful method for deriving kinetic equations in non-equilibrium statistical mechanics [15].

It will be helpful to recall that the subdynamics approach to irreversible processes in large isolated systems starts from the Liouville-von Neumann equation for the density matrix $\rho(t)$:

$$\mathrm{i}\,\partial\rho/\partial t = L\rho(t) \tag{1}$$

where L is written in perturbative form as $L_0 + \delta L$, L_0 being the Liouville superoperator for some solvable problem, and δL representing the interactions between the units defined thereby.

On the basis of the dynamics-of-correlations description of the time evolution of a many-body system [16, 17], one introduces a complete set of correlation states $\{|\nu\rangle\}$, which are eigenstates of L_0, and to which correspond spectral projections $P^{(\nu)} = |\nu\rangle\langle\nu|$ with the property

$$[L_0, P^{(\nu)}] = 0. \tag{2}$$

In the case of dissipative systems, for which L_0 possesses a continuous spectrum and the collision operator is non-vanishing [18], it is no longer possible to diagonalise the complete Liouvillian L [18, 19]. Nevertheless, one may demonstrate that, in the thermodynamic limit, a new complete set of non-Hermitian projectors $\{\boldsymbol{\Pi}^{(\nu)}\}$ exists, all of which commute with L itself:

$$[L, \boldsymbol{\Pi}^{(\nu)}] = 0 \tag{3}$$

as well as satisfying the projection properties of idempotency and orthogonality

$$\boldsymbol{\Pi}^{(\mu)}\boldsymbol{\Pi}^{(\nu)} = \delta_{\mu\nu}\boldsymbol{\Pi}^{(\nu)} \tag{4}$$

together with the completeness relation

$$\sum_{\nu} \boldsymbol{\Pi}^{(\nu)} = 1. \tag{5}$$

$\boldsymbol{\Pi}^{(\nu)}$ is therefore the generalisation of $P^{(\nu)}$ for the case of an interacting dissipative system. Using equation (2) in equation (1), it is easy to see that the projections $\rho^{(\nu)} = \boldsymbol{\Pi}^{(\nu)}\rho$ all evolve independently according to the Liouville-von Neumann equation:

$$\mathrm{i}\frac{\partial\rho^{(\nu)}}{\partial t} = L(t)\rho^{(\nu)}(t). \tag{6}$$

It is for this reason that one uses the term subdynamics.

A non-unitary ('star-unitary') transformation theory, which generalises for dissipative systems the unitary transformation theory of conventional quantum mechanics

[20], can then be framed in terms of the $\{\Pi^{(\nu)}\}$ [1, 11, 12, 19]. Briefly, the Λ transformation converts the density matrix to the physical representation ${}^{p}\rho$:

$$ {}^{p}\rho(t)=\Lambda^{-1}(t)\rho(t). \tag{7}$$

While ρ evolves according to a unitary group law

$$\rho(t)=U(t-t_0)\rho(t_0) \tag{8}$$

where $U(t)=\exp(-\mathrm{i}Lt)$, ${}^{p}\rho$ has an irreversible evolution described by a contractive semigroup [18]

$$ {}^{p}\rho(t)=W^*(t-t_0){}^{p}\rho(t_0) \tag{9}$$

for $t\geqslant t_0$, where

$$W^*(t-t_0)=\Lambda^{-1}U(t-t_0)\Lambda \tag{10}$$

(note that $\Lambda^{+}\neq\Lambda^{-1}$). A Lyapunov functional constructed in the physical representation would behave as a dynamical analogue of the generally non-equilibrium entropy [1, 12, 21].

Until now, the approach to the construction of these operators has been based on the so-called resolvent formalism [11, 19], which employs the Laplace transform method to write the solution of equation (1) in terms of a contour integral involving the resolvent $(z-L)^{-1}$. The $\{\Pi^{(\nu)}\}$ are then defined from the singularities of this operator, through the introduction of a mathematically well defined regularisation procedure known as the iε rule, when the limit of a continuous spectrum is taken [22]. In the thermodynamic limit, this rule is rendered complete by the additional intervention of a general theorem in the dynamics of correlations [23-25] which indicates the terms to be retained in this limit.

All these considerations hold for isolated dissipative systems, for which L is time independent. However, the resolvent formalism cannot handle the important case when L has an explicit time dependence. Thus, the vast range of irreversible phenomena involving the influence of the external world on a system has hitherto remained outside the scope of this approach.

We have now generalised the entire theory by developing an explicitly time-dependent formalism which extends directly to the case when L depends on the time. This is done by writing the solution to equation (1) in terms of the evolution operator $U(t)$ of equation (8), whose perturbation expansion is

$$U(t)=\sum_{n=0}^{\infty}(-\mathrm{i})^n U^0(*\delta L U^0)^n \tag{11}$$

where $U^0=\exp(-\mathrm{i}L_0t)$, and the symbol $A*B$ denotes the convolution of A and B. The general term in equation (11) may be written explicitly as

$$\begin{aligned}U_n(t)=&\int_0^t \mathrm{d}\tau_1\int_0^{t-\tau_1}\mathrm{d}\tau_2\int_0^{t-\tau_1-\tau_2}\mathrm{d}\tau_3\ldots\\ &\times\int_0^{t-\tau_1-\tau_2-\ldots-\tau_{n-1}}\mathrm{d}\tau_n\, U^0(\tau_1)\delta L U^0(\tau_2)\delta L U^0(\tau_3)\ldots\\ &\times\ldots\delta L U^0(\tau_n)\delta L U^0(t-\tau_1-\tau_2-\ldots-\tau_n).\end{aligned}\tag{12}$$

By means of a recently formulated regularisation (analytical continuation) procedure [26] (which is the analogue of the iε rule in the resolvent approach) we can extract, from any particular term (or, equivalently, diagram [16, 17]) in equation (12), the corresponding contribution to any given correlation component of the density matrix $\rho(t)$ in the thermodynamic limit in which the spectrum of L_0 becomes continuous.

Using this procedure, together with the general theorem referred to above [23, 24], one of us (PVC) has shown that the complete correlation subdynamics of a large dynamical system may be obtained within an explicitly time-dependent formalism [27]. Thus, with the proviso that the interactions are sufficiently regular for the integrals to exist and converge, one may define a complete set of projectors $\{\mathbf{\Pi}^{(\nu)}\}$, which obey exactly the same relations as those stated earlier, namely equations (3)-(5).

If the system interacts with a generally time-dependent external field, the Liouville-von Neumann equation becomes

$$\mathrm{i}\,\partial\rho/\partial t = L^{\mathrm{F}}(t)\rho(t) \tag{13}$$

with $L^{\mathrm{F}}(t) = L + \delta L^{\mathrm{F}}(t)$, L being as previously defined and $\delta L^{\mathrm{F}}(t)$ representing the system-surroundings interaction. Under these circumstances, the $\mathbf{\Pi}^{(\nu)}$ subspaces are themselves coupled in a fashion similar to that of the correlation states, $P^{(\nu)}$. Utilising all the results described thus far, and employing the subdynamics methodology a second time, one of us (PVC) has also shown that a new complete set of time-dependent non-Hermitian projectors $\{\boldsymbol{P}^{(\nu)}(t)\}$ exists [28]. These are an extension of the $\{\mathbf{\Pi}^{(\nu)}\}$, in the same sense that the latter are an extension of the $\{P^{(\nu)}\}$; they satisfy similar relations, although the generalisation is non-trivial:

$$\boldsymbol{P}^{(\mu)}(t)\boldsymbol{P}^{(\nu)}(t) = \delta_{\mu\nu}\boldsymbol{P}^{(\nu)}(t) \tag{14}$$

and

$$\sum_{\nu} \boldsymbol{P}^{(\nu)}(t) = 1. \tag{15}$$

In addition, the $\boldsymbol{P}^{(\nu)}(t)$ obey an intertwining (or pseudocommutation) relation with the exact evolution operator associated with equation (13)

$$\boldsymbol{P}^{(\nu)}(t)U^{\mathrm{F}}(t, t_0) = U^{\mathrm{F}}(t, t_0)\boldsymbol{P}^{(\nu)}(t_0). \tag{16}$$

These three relations ensure that the projections $\boldsymbol{P}^{(\nu)}(t)\rho(t) \equiv {}^{(\nu)}\rho(t)$ satisfy a generalised subdynamics, in the sense that

$$\mathrm{i}\frac{\partial^{(\nu)}\rho}{\partial t} = L^{\mathrm{F}}(t)^{(\nu)}\rho(t). \tag{17}$$

The results summarised here—full proofs and details of which have now appeared elsewhere [26-29]—represent a major generalisation of earlier work by Balescu and Misguich, who established the existence of a superkinetic projector $\boldsymbol{P}^{(0)}(t)$ [30]. This operator enabled them to write down an exact kinetic equation in the presence of arbitrary external fields, from which many special cases can be deduced [31]. A remarkable additional feature is that the entire evolution of the system is confined wholly within this instantaneous subspace, provided that the initial condition is such that the field is switched on after the system has reached a steady or equilibrium state (i.e. provided that $\rho(t_0) = \mathbf{\Pi}^{(0)}\rho(t_0)$).

It is important to grasp the repetitive nature of the approach we have employed. In the time-dependent perturbative formalism, the theory is developed in terms of convolution series in a hierarchical manner (one has to deal with convolutions within convolutions). It should therefore be clear that all kinds of situations can now be brought within the ambit of the subdynamics method. For example, in principle one can treat time-independent Liouvillians with several kinds of interactions present (e.g. $L = L_0 + \delta L_1 + \delta L_2$), and systems interacting simultaneously with more than one external field (e.g. $L^F(t) = L + \delta L_1^F(t) + \delta L_2^F(t)$). The latter situation is of obvious significance in the context of laser-plasma interactions.

Note that we have placed no restriction on the nature of the external field, which can in principle be of arbitrary spatial inhomogeneity and time dependence. Indeed, all the results quoted here are algebraically exact in the thermodynamic limit, and do not involve any dynamical approximations. However, we have implicitly assumed that the various interactions (within the system and with the surroundings) are sufficiently regular to ensure existence and convergence of the various integrals which arise in the formalism. A set of mathematically rigorous necessary and sufficient conditions on the Liouvillian is still required which would guarantee the existence of subdynamics. Until such conditions are formulated, it is necessary to check for existence in each particular case under study.

An important property of the projectors $\boldsymbol{P}^{(\nu)}(t)$ is that, like $\boldsymbol{\Pi}^{(\nu)}$, they are no longer time-reversal invariant (as a result of the analytical continuation used to define them): this is why they are non-Hermitian (actually 'star-Hermitian' [19]). Hence we are led to an extension of the non-unitary transformation theory [1, 11, 19] for open systems, through the relation

$$\boldsymbol{P}^{(\nu)}(t) = \Lambda(t) P^{(\nu)} \Lambda^{-1}(t). \tag{18}$$

Thus the physical representation ${}^p\rho$ is obtained from

$${}^p\rho(t) = \Lambda^{-1}(t)\rho(t). \tag{19}$$

${}^p\rho$ evolves irreversibly according to the generalised version of equations (9) and (10):

$${}^p\rho(t) = W^*(t, t_0)\,{}^p\rho(t_0) \tag{20}$$

with

$$W^*(t, t_0) = \Lambda^{-1}(t) U^F(t, t_0) \Lambda(t_0) \tag{21}$$

and $t \geqslant t_0$; a suitable candidate for the microscopic entropy operator would be

$$M(t) = \Lambda^+(t)\Lambda(t). \tag{22}$$

Hence a microscopic description of irreversibility and entropy in such open systems can begin to be forged. One should note, however, that there is a certain indeterminacy associated with the definition of Λ, the complete eradication of which remains as an open problem [12].

From a fundamental point of view, the existence of the Λ transformation has important consequences for the quantum theory of measurement. One can show that Λ is a non-factorisable superoperator [21]; as a result, it transforms pure states into mixtures. In this way, one achieves in principle a resolution of the measurement problem by incorporating the irreversible act of measurement within the macroscopic aspect of the measuring apparatus.

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