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On the extension of the general theorem in the dynamics of correlations to the statistical mechanics of large systems evolving in time dependent external fields

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Abstract. The formal subdynamics approach to irreversibility in non-equilibrium statistical mechanics is cursorily reviewed, emphasis being placed on a recently developed time dependent formalism which generalises naturally from isolated systems to systems open to external influence. By means of a diagrammatic approach, we apply this theoretical framework to begin the study of gases and plasmas evolving in the presence of time dependent external fields. The general theorem in the dynamics of correlations is extended to include these cases and a corollary is deduced which enables one to eliminate from consideration a large class of diagrams in the thermodynamic limit. Finally, we discuss briefly some consequences of the formalism which may serve as avenues for the investigation of problems of physical interest.

1. Introduction

Within the past two decades considerable progress has been made toward a fundamental theory of irreversible processes, notably by the Brussels group whose work has recently been reviewed in summary fashion (Coveney 1988). This research has shown how irreversibility can indeed arise as an intrinsic property of isolated dynamical systems, without the need for invoking 'anthropic arguments or unphysical assumptions' (Barrow and Tipler 1986).

From the point of view of applications to real systems, the subdynamics theory developed by the Brussels group (Prigogine *et al* 1973) seems to offer considerable possibilities. The concept of subdynamics, originally introduced by Prigogine *et al* (1973) for large isolated systems, has played a central role in clarifying the relation between dynamical and thermodynamic descriptions (George *et al* 1972); it has also provided a powerful method for the derivation of kinetic equations in non-equilibrium statistical mechanics (Balescu 1975).

A major problem in non-equilibrium statistical mechanics concerns the time evolution of a large dynamical system interacting with a time dependent external field. By generalising the subdynamics concept from that appropriate to isolated systems, Balescu

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and Misguich (1974a, b, 1975a, b) were able to provide a rigorous justification for the use of kinetic equations for plasmas evolving in time dependent external fields under well defined initial conditions. This equation contains, as approximations valid under differing circumstances, a whole host of special cases: the weak coupling Landau and Vlasov equations to *all* orders in the external field and, for strongly turbulent plasmas, the quasilinear stochastic approximations of Kraichnan (1972), Weinstock (1969) and Dupree (1966), as well as the Balescu-Lenard equation (Balescu 1975). A subsequent development along similar lines was made by Vstovskii (1977). In an unpublished thesis, Jowett (1982) continued the investigation of such kinetic equations.

In this paper, we build on more recent developments in the subdynamics theory of 'open' systems (where, in the spirit of Penrose (1979), we mean large systems evolving in external fields) due to Coveney and George (Coveney and George 1987, 1988, Coveney 1986, 1987a, b), in order to begin consideration of real physical problems. The paper is divided as follows. In § 2, we review some aspects of the subdynamics theory, with particular emphasis on those elements of importance to the present work. Section 3 makes use of a diagrammatic approach to the dynamics of correlations, which is cast into the new time dependent formalism. After a statement of the general theorem in correlation dynamics for isolated systems in § 4, we show in § 5 how these techniques may be applied to treat gases and plasmas evolving in inhomogeneous time dependent external fields, and we demonstrate that the general theorem in the dynamics of correlations may be extended to these cases (§ 5.3). The validity of this theorem is important not only in providing a justification for the formal theory, but also from a computational standpoint in eliminating a large class of diagrams which are negligible in the thermodynamic limit (§ 5.4). Finally, in § 6 we briefly discuss the utility of these results for future applications of the theory to concrete physical problems.

2. The subdynamics approach in non-equilibrium statistical mechanics

The starting point for non-equilibrium statistical mechanics is the Liouville equation for the phase space distribution function $\rho(q_1, v_1, \dots, q_N, v_N; t) \equiv \rho(t)$ (or the density operator in the quantal case) for an isolated system

$$i\frac{\partial\rho}{\partial t}(t) = L\rho(t) \tag{1}$$

which is to be considered in the thermodynamic limit. This is the limit in which the number of particles of any species present (N) and the volume (Ω) both tend to infinity in such a way that the density or concentration $(C = N/\Omega)$ remains finite. We shall sidestep the formidable mathematical difficulties associated with taking this limit by assuming that the pathological initial conditions leading to singular behaviour in ρ are in some sense of zero measure (physically speaking, all intensive properties of the system, such as the pressure, reduced distribution functions, etc, are assumed to be finite).

We shall consider a classical gas or plasma consisting of N structureless particles in a volume Ω (although the theory carries over directly to the quantal case at the price of increased complexity arising from quantum statistics). Each particle is characterised by a mass m_i and possibly a charge e_i , its coordinates are q_i and its velocity v_i . Introducing the following notation:

$$\partial_{t} \equiv \partial/\partial t \qquad \nabla_{i} \equiv \partial/\partial q_{i}$$

$$\partial_{i} \equiv \frac{1}{m_{i}} \frac{\partial}{\partial v_{i}} \qquad \partial_{ij} \equiv \partial_{i} - \partial_{j}$$
(2)

we may write the total Liouvillian operator of an isolated system in the perturbative form

$$L = L_0 + \lambda \delta L \tag{3}$$

where L_0 represents the free motion of the N particles,

$$\delta L = i \sum_{i=1}^{N} \boldsymbol{v}_i \cdot \boldsymbol{v}_i \tag{4}$$

and δL the interactions between them

$$\delta L = i \sum_{i < j} \left(\boldsymbol{\nabla}_i \boldsymbol{V}_{ij} \right) \cdot \boldsymbol{\partial}_{ij}$$
⁽⁵⁾

 λ being the coupling constant. The particles are supposed to interact through potentials $V_{ij} = V(|\mathbf{q}_i - \mathbf{q}_j|)$ which are binary, central and of finite range. As is well known, the Coulomb interaction between charged particles in a plasma is effectively rendered of finite range due to the collective screening effect. Although out of equilibrium the screening mechanism is much more complex than for equilibrium, the dominant contributions still come from the many-body ring diagrams (Balescu 1975).

For a system open to influence from a time dependent external field, the Liouville equation becomes

$$i\partial_t \rho(t) = L^F(t)\rho(t). \tag{6}$$

The total Liouvillian

$$L^{F}(t) = L + \xi \delta L^{F}(t) \tag{7}$$

where L is the system Liouvillian of (3), has now acquired an explicit time dependence by virtue of the external field: the second term represents the system-external field interaction

$$\delta L^{F}(t) = \sum_{i=1}^{N} \delta L_{i}^{F}(t) = i \sum_{i=1}^{N} F_{i}(\boldsymbol{q}_{i}, \boldsymbol{v}_{i}; t) \cdot \boldsymbol{\partial}_{i}$$

$$\tag{8}$$

and ξ is a coupling constant. In general the external field will be spatially inhomogeneous. As an example, for the case of a plasma evolving in an external electromagnetic field, F_i is the Lorentz force acting on the *i*th particle:

$$\mathbf{F}_i(\mathbf{q}_i, \mathbf{v}_i; t) = -\mathbf{e}_i \{ \mathbf{E}(\mathbf{q}_i; t) + \mathbf{v}_i \wedge \mathbf{B}(\mathbf{q}_i; t) \}.$$
(9)

These equations represent the same model as that of Balescu and Misguich (1974a).

2.1. Dynamics of correlations: the ground level

Now the time evolution of a many-body system can be described very conveniently in terms of a dynamics of correlations (Prigogine 1962, Balescu 1963). This description of dynamics is the point of departure for the subdynamics approach which is employed here. It is the ground level underpinning all of the subsequent theory that we shall develop. There are, however, two slightly different methods used by members of the Brussels group. On the one hand, Balescu (1963, 1975) works with a distribution vector, the components of which are the reduced distribution functions $f_s(q_1, v_1, \ldots, q_s, v_s; t)$, with $1 \le s \le N$. On the other hand, in contradistinction to Balescu, the approach that we shall adopt, which follows that of Prigogine, George and others, is to work directly with the full N-particle distribution function $\rho(t)$ and only to go over to the reduced distribution functions f_s at a later stage of the calculation. Further discussion of this version of the dynamics of correlations, laying emphasis on the important associated diagrammatic techniques, can be found in § 3.

However, at this point it will be useful to introduce the complete set of Hermitian projection operators $\{\stackrel{\nu}{P}\}$ which project out of $\rho(t)$ the ν th correlated components $\rho_{\nu}(t)$ in the Fourier representation of the distribution function. The projectors $\stackrel{\nu}{P}$ commute with the evolution operator or propagator for the unperturbed motion

$$U^{0}(t-t_{0}) = e^{-i(t-t_{0})L_{0}}$$
(10)

and hence also with L_0 :

$$[\stackrel{(\nu)}{P}, U^0] = 0 \qquad [\stackrel{(\nu)}{P}, L_0] = 0.$$
 (11)

2.2. Subdynamics description of isolated systems: the first level

A remarkable result, originally demonstrated by George (1973) for homogeneous isolated systems, and later extended to inhomogeneous systems by Škarka and George (Škarka 1981, Škarka and George 1983), is that, in the presence of interactions (δL),

one can define a new complete set of non-Hermitian projectors $\{\stackrel{\nu}{\Pi}\}$ which decompose the distribution function into a set of orthogonal subspaces that are invariant under the motion.

Introducing the evolution operator for the system

$$U(t - t_0) = \exp[-i(t - t_0)L]$$
(12)

such that the formal solution to equation (1), subject to the initial condition $\rho(t_0)$, is

$$\rho(t) = U(t - t_0)\rho(t_0)$$
(13)

one may show that $\prod_{\nu=1}^{(\nu)}$ satisfies the following commutation relations:

$$[\overset{(\nu)}{\Pi}, U] = 0 \qquad [\overset{(\nu)}{\Pi}, L] = 0 \tag{14}$$

for all ν (cf equation (11)). Thus each component of the distribution function

$$\stackrel{(\nu)}{\rho}(t) \equiv \stackrel{(\nu)}{\Pi} \rho(t) \tag{15}$$

evolves independently of the others according to the Liouville equation, and is said to obey its own subdynamics. We shall refer to this as the first level of subdynamics.

If the interactions δL within the system are extinguished, the $\Pi^{(\nu)}$ projectors reduce to the corresponding $P^{(\nu)}$:

$$\lim_{\delta L \to 0} \prod^{(\nu)} = \stackrel{(\nu)}{P}.$$
 (16)

The $\{\Pi\}$ exist, provided that certain regularity conditions are satisfied by the potential (Balescu 1972, 1975).

For the construction of the $\{\Pi\}$ one needs, however, to make use of two elements additional to the dynamics of correlations. The first is a general theorem in the dynamics of correlations, applicable to both homogeneous and inhomogeneous systems, which indicates what contributions to the ν -correlation state of interest are negligible in the thermodynamic limit (Henin 1971, Škarka 1978a, b). The second is a suitable analytical continuation procedure for this limit, which enables one to handle the remaining contributions in a mathematically well defined way when the spectrum of L_0 becomes continuous.

In fact, the aforementioned general theorem, which immediately enables one to exclude from consideration a large class of diagrams (see §§ 3 and 4), is a prerequisite for the application of the latter procedure.

The original approach to the subdynamics decomposition of $\rho(t)$ was based on the contour integral solution to the Laplace transform of the Liouville equation (1), in which the resolvent $(z - L)^{-1}$ plays a central role. However, since we are concerned here with extending the theory to open systems—for which L is time dependent (equation (6)) and the resolvent formalism is then inapplicable (see § 2.3)—it is of much greater interest to work with an explicitly time dependent formalism. Such a formalism has recently been constructed (Coveney 1986, 1987a): it is based on a time dependent analytical continuation procedure due to Coveney and George (1987), coupled with the general theorem in the dynamics of correlations. We shall not discuss the details here, although we shall refer to this procedure repeatedly in the remainder of the paper: the reader is therefore urged to consult the references for further information.

2.3. Time dependent subdynamics description of open systems: the second level

Turning to the case of systems interacting with external fields, it has recently been shown by using the time dependent formulation of the first level (§ 2.2) that the $\{ \stackrel{(\nu)}{\Pi} \}$ projectors can be further generalised to define another complete set of non-Hermitian time dependent projectors $\{ \stackrel{(\nu)}{P}(t) \}$ (Coveney 1987b).

Introducing the evolution operator $U^{F}(t, t_{0})$, in terms of which the formal solution to equation (6) is written

$$\rho(t) = U^{F}(t, t_{0})\rho(t_{0})$$
(17)

one may show that the $\{\stackrel{\nu}{P}(t)\}$ obey an intertwining relation with U^F :

$$\overset{(\nu)}{P}(t) U^{F}(t, t_{0}) = U^{F}(t, t_{0}) \overset{(\nu)}{P}(t_{0})$$
(18)

but they do not commute with $L^{F}(t)$ since

$$i\partial_t \mathbf{P}^{(\nu)}(t) = L^F(t) \mathbf{P}^{(\nu)}(t) - \mathbf{P}^{(\nu)}(t) L^F(t).$$
(19)

It follows from equation (18) that the components

$$\rho^{\nu}(t) \equiv \stackrel{(\nu)}{P}(t)\rho(t) \tag{20}$$

all independently satisfy the Liouville equation (6) and constitute a generalised (super-) subdynamics. We shall refer to this as the second level of subdynamics.

The $\{ \overset{(\nu)}{P}(t) \}$ exist, subject to the convergence of the time integrals involved, and with the proviso that the general theorem in the dynamics of correlations carries over to the present case. This latter result is proved for plasmas and gases in § 5. It is clear that the general theorem must be considered here (rather than simply Henin's theorem for homogeneous systems (Henin 1971)) since the external field can itself induce inhomogeneities within the system.

3. Dynamics of correlations and inhomogeneities: the diagrammatic approach

3.1. Isolated systems

As outlined in § 2, within the framework of the dynamics of correlations (Prigogine 1962, Balescu 1963), the evolution of an isolated system is described in terms of the change of correlations due to the interactions, with the Liouville equation written in the representation of the eigenfunctions of the Liouvillian without interactions, L_0 . This corresponds to the Fourier expansion of the N-particle distribution function. The inhomogeneities as well as the correlations between the particles are associated with the wavevectors $\{k_i\}$ in the Fourier coefficients and in the free propagators. In the notation of Prigogine (1962), the formal solution of the Liouville equation in the interaction representation, written in terms of its convolution form, corresponds to a perturbation series with respect to the interactions:

$$\rho_{\{k\}}(\{v\}; t) = \sum_{\{k'\}} \langle \{k\} | U(t) | \{k'\} \rangle \rho_{\{k'\}}(\{v\}; 0)$$

$$= \sum_{n=0}^{\infty} \sum_{\{k'\}} \langle \{k\} | U_n(t) | \{k'\} \rangle \rho_{\{k'\}}(\{v\}; 0)$$

$$= \sum_{n=0}^{\infty} \sum_{\{k'\}} (-i)^n \langle \{k\} | U^0(*\lambda \delta L U^0)^n\} | \{k'\} \rangle \rho_{\{k'\}}(\{v\}; 0)$$
(21)

where A^*B denotes the convolution of A with B, and the general term is given explicitly by

$$U_{n}(t) = (-i)^{n} \lambda^{n} \int_{0}^{t} d\tau_{1} \int_{0}^{t-\tau_{1}} d\tau_{2} \int_{0}^{t-\tau_{1}-\tau_{2}} d\tau_{3} \dots \int_{0}^{t-(\tau_{1}+\tau_{2}+\tau_{3}+\dots+\tau_{n-1})} d\tau_{n}$$

$$\times U^{0}(\tau_{1}) \delta L U^{0}(\tau_{2}) \delta L U^{0}(\tau_{3}) \dots \delta L U^{0}(\tau_{n})$$

$$\times \delta L U^{0}(t - [\tau_{1}+\tau_{2}+\tau_{3}+\dots+\tau_{n}]).$$
(22)

By $\{k\}$ we mean $\{k_1, k_2, \ldots, k_N\}$ and similarly for $\{v\}$, i.e. the set of wavevectors and velocities of the N particles comprising the system.

Any term arising in the expansion of equation (21) may be evaluated explicitly using the following matrix elements (Balescu 1963):

$$\langle \{\boldsymbol{k}\} | \boldsymbol{U}^{0}(\tau_{i}) | \{\boldsymbol{k}'\} \rangle = \exp\left(-i\tau_{i}\sum_{j}\boldsymbol{k}_{j}\cdot\boldsymbol{v}_{j}\right) \prod_{s=1}^{N} \delta(\boldsymbol{k}_{s}-\boldsymbol{k}_{s'})\delta(\boldsymbol{v}_{s}-\boldsymbol{v}_{s'})$$
(23*a*)

$$\langle \{\boldsymbol{k}\}|\delta L|\{\boldsymbol{k}'\}\rangle = -\frac{8\pi^3}{\Omega} V_{|\boldsymbol{k}'-\boldsymbol{k}|}(\boldsymbol{k}'_j-\boldsymbol{k}_j) \cdot \boldsymbol{\partial}_{jn} \delta(\boldsymbol{k}'_j+\boldsymbol{k}'_n-\boldsymbol{k}_j-\boldsymbol{k}_n) \prod_{(r\neq j,n)} \delta(\boldsymbol{k}'_r-\boldsymbol{k}_r)$$
(23b)

which may be readily deduced from equations (4) and (5) together with the fact that the particles interact through binary, central potentials. In addition, it should be noted that the interaction potential has been transformed to the Fourier representation

$$V_{jn}(|\mathbf{x}_j - \mathbf{x}_n|) = \frac{8\pi^3}{\Omega} \sum_{l} V_l \exp[i\mathbf{l} \cdot (\mathbf{x}_j - \mathbf{x}_n)]$$
(24)

(which is the origin of the factor $(1/\Omega)$ in equation (23b)).

For inhomogeneous systems the non-vanishing total wavevector $\mathbf{K} = \sum_i \mathbf{k}_i$ is conserved. The system follows what has been called the \mathbf{K} dynamics (Škarka and George 1983). The vacuum of correlations is then defined by the set of Fourier coefficients ρ_{K_α} , with only one vector different from zero and thus equal to \mathbf{K} . In the diagrammatic formulation of the dynamics of correlations (Škarka 1974), the propagator for the vacuum of correlations appears as a single line (figure 1).

Now a correlation of degree *n* can be created from the vacuum of correlations by means of at least *n* interactions $(\lambda \delta L)$. An interaction can be represented diagrammatically by any one of six different elementary vertices (A-F in figure 2).

There is a one-to-one correspondence between the terms in the perturbative expansion (21) and the diagrams (Balescu 1963). For example, the important case known as the cycle shown in figure 3 corresponds to the following algebraic expression:

$$\rho_{\{0\}}(\{\boldsymbol{v}\}; t) = -\lambda^2 \left(\frac{8\pi^3}{\Omega}\right)^2 \sum_j \int_0^t \mathrm{d}\tau_1 \int_0^{t-\tau_1} \mathrm{d}\tau_2 \sum_l V_l \boldsymbol{l} \cdot \boldsymbol{\partial}_{\alpha j} \exp[-\mathrm{i}\tau_2 \boldsymbol{l} \cdot (\boldsymbol{v}_\alpha - \boldsymbol{v}_j)] \times V_l(-\boldsymbol{l}) \cdot \boldsymbol{\partial}_{\alpha j} \rho_{\{0\}}(\{\boldsymbol{v}\}; 0).$$
(25)

Κα

Figure 1. The inhomogeneous vacuum of correlations; the label α refers to the particle carrying momentum (wavevector) K.



Figure 2. The six elementary vertices for internal interactions.



Figure 3. The cycle.

As discussed in § 2.2, with each correlation we may associate a corresponding subdynamics in the thermodynamic limit (T limit). Coveney and George (1987) have given a prescription for doing this, which essentially consists of retaining a convolution series for the propagators of the correlation state whose subdynamics is sought, while extending the domain of integration of the time intervals associated with all remaining propagators to $\pm \infty$ in a systematic way.

It is important that care be taken not to confuse either the terminology or the diagrams with similar ones arising in the quantum field theory of many-particle systems. Despite a superficial similarity, the entire philosophy of approach as well as the details are quite distinct in the two cases. For example, whereas in quantum field theory the term 'vacuum' denotes a state without particles, in the present context it means a state without correlations.

3.2. Formalism in the presence of a time dependent field

For a system evolving under the influence of an external time dependent field, the formal solution of the Liouville-von Neumann equation (6) is given by a double perturbation expansion with respect to both the internal interactions $(\lambda \delta L)$ and the external field $(\xi \delta L^F)$ (Coveney 1987b),

$$\rho_{\{k\}}(\{v\}; t) = \sum_{n=0}^{\infty} \sum_{\{k'\}} (-i)^n \langle \{k\} | (U\xi \delta L^{F*})^n U | \{k'\} \rangle \rho_{\{k\}}(\{v\}; 0).$$
(26)

Each of the evolution operators U(t) given by equations (12) and (21) may be decomposed into a complete set of independent subdynamics components (Coveney 1987a, § 2.2). Therefore, the dynamics of the system in the second subdynamics level (§ 2.3) consists of a series of first-level subdynamics evolutions, which are now, however, coupled together by virtue of the external field (the so-called dynamics of kinetic and non-kinetic states).

In the ground level of the dynamics of correlations (§ 2.1) the evolution appears as a series of external field terms $(\xi \delta L^F)$ and particle interactions $(\lambda \delta L)$ separated by free evolution propagators. As Balescu and Misguich (1974a) pointed out, in contradistinction to the internal interaction potential $(\lambda \delta L)$ the external field $(\xi \delta L^F)$ acts on the particles individually in the same way as the free Liouvillian L_0 (both being sums of single-particle operators, equations (4) and (8)). Therefore, this field cannot modify the correlations between particles without internal structure. However, a spatially dependent field (e.g. equation (9)) influences the spatial distribution of all particles. Hence each term $\xi \delta L^F$ in the expansion with respect to the external field, equation (26), modifies the inhomogeneity of the system, as represented by the total wavevector **K**. Consequently the total wavevector **K** is no longer conserved. The action of the external field modifies the total vector **K** by an amount **K'**, i.e. it changes the **K** dynamics into the $(\mathbf{K} - \mathbf{K}')$ dynamics. In the diagrammatic representation, this corresponds to the introduction of a new kind of vertex affecting only single lines. The vertices are given in figure 4 where, by analogy with the Feynman diagrams of quantum field theory, we use a full circle from which a zig-zag tail emanates.

The vertex G corresponds to a change of inhomogeneity in the system. The special cases are the transitions from a non-zero wavevector (inhomogeneous state) to the zero wavevector (homogeneous state) and vice versa (vertices H and I in figure 4). Following the perhaps unfortunate yet established convention (Balescu 1963), we read the diagrams from left to right; thus, in what follows, the final and initial states will often be called the 'starting' and 'ending' states respectively (remember that time is taken to increase from right to left in the diagrams).

3.3. Classification of states with respect to their overall degree

For later convenience, we now introduce the degree of inhomogeneity I. The homogeneous vacuum of correlations, represented by an absence of lines (zero wavevector), corresponds to an inhomogeneity of zero degree. The inhomogeneous vacuum of correlations (a single line carrying a non-zero wavevector as in figure 1) has degree of inhomogeneity one. Every new line labelled by an independent wavevector K', corresponding to the introduction of a new inhomogeneity by the external field vertex H, increases the degree of inhomogeneity by one. In order to obtain the overall degree D of a state in a diagram both the degree of inhomogeneity I and the degree of correlation n (see § 3.1) have to be taken into account. In the Fourier representation, a state of overall degree D contains D independent wavevectors labelling D lines. A state of degree D can have more than D lines if the extra lines are labelled by dependent vectors (carrying the same labels as the independent vectors). For instance, in figure 9 (see later) the third and the fifth states have the same overall combined degree D=3but different numbers of lines. (Notice that an independent vector labelling a line can contain several dependent vectorial indices on condition that at least one index is independent (e.g. index m in the fifth state of figure 9).) The magnitude of each independent vector in a state of overall degree D is proportional to the inverse volume of the system Ω^{-D} , since it takes at least D vertices to reach this state from the homogeneous vacuum (corresponding to either the internal interaction δL or the action of the external field δL^F , both being proportional to Ω^{-1}).

3.4. Negligible diagrams: a general criterion

In order to discover which contributions to the evolution of the various components are negligible in the thermodynamic limit, it is necessary to investigate their dependence on the volume and the number of particles in the system, i.e. to determine the order of magnitude of the corresponding diagram in the form





(see Škarka (1974, 1978a, b) for the case without an external field). Therefore, since C is finite in this limit, the value of M has to be determined in order to decide whether the contribution of a given diagram is negligible or not. This contribution is obtained by summation over all diagrams leading to the final state $\rho_{\{k\}}(t)$ from any initial state. Hence, for each type of diagram we sum over all independent wavevectors (such as l, m and K' in figures 2 and 4) and particles (such as a in the same figures) which do not appear in the final state. These are called 'integrating vectors', since the summation over them becomes an integration in the T limit

$$\sum_{k} \rightarrow (\Omega/8\pi^{3}) \int \mathrm{d}\mathbf{k}.$$
 (28)

Each summation thus brings a factor Ω into the expression (26).

Now our final concern lies in the reduced distribution functions involving a finite set $\{\sigma\}$ of particles. As a consequence, in a vertex one does not sum over 'named' particles (particles which belong either to $\{\sigma\}$ (Greek label) or which are present on both sides of the vertex). The summation is performed only over the remaining 'field' particles (Roman label); each of them introduces a factor N into the formula (27). Furthermore, each vertex also introduces a factor $1/\Omega$, since it corresponds to the Fourier transform of either the internal or the external field interaction energy, as in equation (24). Therefore, the value of M in the ratio (27) is determined by the following four terms:

(i) the difference in overall degree (ΔD) between the initial (D_0) and the final state (D_t), $\Delta D = D_0 - D_t$;

- (ii) the number of vertices (V);
- (iii) the number of integrating wavevectors (α) ;
- (iv) the number of field particles (β) .

It follows that

$$M = \Delta D + V - \alpha - \beta. \tag{29}$$

Thus from (27) an important criterion is obtained concerning the order of magnitude of the diagrams (which we shall soon apply to systems evolving in the presence of external fields): in the thermodynamic limit, a diagram is negligible if M > 0 and is finite if M = 0.

This criterion involves global counting of the additive variables which determine M, and can be applied to any diagram. Values of M are given for the diagrams in figures 2, 4-8 and 14-16 of this paper. (It has previously been shown in the case of an isolated system that M cannot be negative (Škarka 1974), a result which remains valid in the present context.)

Now, in the absence of an external field, for a well defined class of diagrams, a general theorem in the dynamics of correlations has been established using this criterion, which makes it possible to decide whether or not a diagram is negligible in the T limit on the basis of its 'topological' properties alone (Škarka 1978a, b). By the topological properties of a diagram, we mean those properties relating to the lines (labelled by wavevectors) without taking into account their particle labels. The theorem is summarised in § 4. In order to avoid having again to construct and evaluate negligible diagrams, we shall proceed in § 5 to extend the general theorem to systems evolving in external fields.

4. The general theorem in the dynamics of correlations

The general theorem concerns that class of diagrams in which a wavevector appears twice. Reading the diagram from left to right, such a repeating vector is, after its first appearance, modified by a vertex denoted V_1 and then, after an arbitrary number of dynamical steps, it reappears by means of the vertex V_2 , possibly to be modified once again by the vertex V_3 . By definition, a vector is modified when some of its vectorial indices are removed, when other indices are brought in, as well as when, in a single dynamical step, some indices vanish while others are added.

The theorem states (Škarka 1978a, b) that a diagram with a repeating wavevector is negligible in the thermodynamic limit if the following two conditions are fulfilled:

(i) the repeating wavevector appears together with some other wavevector to the immediate left of the vertex V_1 ;

(ii) these vectors are connected in the 'domain' between the vertices V_1 and V_3 .

The so-called 'domain' is demarcated by two vertical lines dividing up the diagram in such a way that V_1 stays within it but V_3 does not. By definition, two wavevectors are connected if, starting from the line which is labelled by one vector and following the lines in a continuous manner through the diagram, we can reach the line labelled by the second vector. An example of such a negligible diagram is given in figure 9 below, where the vectors $(\mathbf{K} - \mathbf{l})$ and \mathbf{l} are connected at the vertex V_c .

The theorem has previously been proved in the case of isolated systems by demonstrating that any diagram in the above-mentioned class necessarily contains at least one of the four types of negligible fragments shown in figure 5 (Škarka 1978a, b). A fragment of a diagram is defined as a domain containing only one vertex. However, in order to determine which of the fragments is negligible the diagram has to be considered in its totality; whether the summation over a particle label or the integration over a wavevector in a fragment is allowed (or forbidden) depends on its absence (or presence respectively) on the left-hand side of the fragment considered (see the full and the broken line fragments in figures 5 and 7).

5. Extension of the general theorem in the dynamics of correlations to include time dependent external fields

In this section we proceed to generalise the theorem by first classifying, in §§ 5.1 and 5.2, the negligible fragments which arise from the internal and external field interactions respectively. As is often the case with rules derived from diagrammatic perturbation theory, the proof in § 5.3 proceeds via consideration of the various generic properties of the diagrams. It will be most comprehensible to the reader who has already developed a general familiarity with the rules for evaluation of the orders of magnitude of diagrams in correlation dynamics, which are given in their most lucid form by Balescu (1963).

5.1. Classification of the negligible internal interaction fragments

The only vertices which introduce a field particle are of the type C, D or E (figure 2). These vertices may also reintroduce a lost field particle (see figure 5). Such a particle, having already appeared in that part of the diagram to the left of the vertex under consideration, reappears as a named particle and we cannot sum over it. Consequently the corresponding value of M will be increased (see equation (28)). Such vertices belong to the first group of negligible fragments shown in figure 5.



Figure 5. The four groups of negligible internal interaction fragments which arise in the general theorem. Group IV contains 'mixing on the left' fragments where vertices are labelled by triangles (∇) .

Similarly, a new integrating wavevector is introduced to the right of vertices C, D and F only (see vectors l and m in figure 2). In order to satisfy the requirement imposed by momentum conservation (§ 3.1), a new vector always appears together with its complement at each interaction vertex. If the vector introduced thereby is not new but has been lost somewhere to the left of such a vertex, an integration cannot be performed over it. Therefore, the fragments containing such non-integrating vectors are negligible (group II in figure 5).

Likewise, we cannot integrate over a vector to the right of a vertex if its index remains present on the left of the same vertex, as for m and l respectively in the negligible fragments D'_3 , F'_3 of group III in figure 5.

A third reason for neglecting a fragment occurs when, to the left of the vertex, a dependent integrating vector of the irreducible subcorrelation replaces an independent integrating vector in the corresponding non-negligible reference fragment. (An irreducible subcorrelation is a homogeneous correlation such that all partial summations of its vectors are non-zero (e.g. -I and I of B'_4 in figure 5).) The vector becomes dependent since its complementary vector in the irreducible subcorrelation is always independent when it labels a propagation line. This happens when, to the left of the vertex in a fragment, a line of an irreducible subcorrelation is connected at the vertex with one of the remaining lines (Henin 1971). Such a mixing on the left corresponds to the fourth group of negligible fragments (vertices labelled with a triangle; group IV in figure 5).

Conversely, however, when a line of an irreducible subcorrelation on the right of the vertex joins a remaining line at the vertex, the corresponding mixing on the right does not make the fragment negligible. Indeed, the missing integrating vector is compensated for by a decrease in the initial overall degree (the values of D_0 and α for the fragments in figure 6, depending upon the same vector, occur with opposite sign in equation (28)).



Figure 6. 'Mixing on the right' fragments; vertices are labelled by squares (\Box) .

5.2. Classification of the negligible external field fragments

In order to extend the general theorem, the new kind of vertices arising due to the external field (figure 4) must also be studied.

By analogy with the preceding section, four groups of negligible fragments containing external field vertices can be identified using the general criterion enunciated in § 3.4 (see figure 7). To the first group belong the fragments with the vertex H (see figure 4) in which a particle lost somewhere to the left of the vertex is reintroduced instead of a field particle as in figure 6.

The reappearance of a lost wavevector in place of an integrating one is the reason why the fragments in the second group are negligible. Notice that, in contradistinction with the interaction vertex, the external field vertex always introduces an inhomogeneity vector without its complement, thereby changing the total wavevector (momentum is no longer conserved within the system).

The third group of negligible fragments results from the fact that we cannot integrate over an inhomogeneity vector to the right of the vertex if its vectorial index is also present on the left.

The fragments of the fourth group do not participate in 'mixing' because the external field vertices never involve more than one particle and, therefore, never more than one line. However, as in the 'mixing on the left' fragments of figure 6, an irreducible subcorrelation on the left of the vertex disappears on its right. By virtue of the presence of the dependent vector in the subcorrelation, the value of D_t in (28) decreases, thereby increasing the value of M.

By contrast, note that the mirror image of a fragment from the fourth group in figure 7 is not negligible since the subcorrelation is on the right of the vertex, as in the 'mixing on the right' fragments of figure 6 (see figure 8).



Figure 7. The four groups of negligible external field interaction fragments which arise in the extension of the general theorem.



M = 1 + 1 - 0 - 0 = 0



5.3. Proof of the extended theorem

The theorem holds trivially when the repeating wavevector is modified by the elimination of some of its indices at the vertex V_1 , which can be either an interaction vertex (e.g. D'_3 and F'_3 in figure 5 and B in figure 2) or an external field vertex G (in figure 4). Special cases arise when the repeating vector is lost, as in the vertex I (figure 4), or eliminated, when its exact complement is introduced via the interaction vertex A. Consequently, the vertex V_2 , which in the former case reintroduces one index of the repeating vector and in the latter case the whole vector, necessarily belongs to the second group of negligible fragments (figures 5 and 7).

Hence, only the modification of the repeating vector by the addition of another, different, vectorial index needs further consideration. Moreover, the theorem manifestly holds if the starting fragment is already negligible since it then belongs to the fourth group.

To modify the repeating vector the vertex V_1 must be of the type G, B, D or F. (Indeed the vertices C and H introduce a new vector which alone labels its line, while the vertex E, which leaves the vector unchanged, may also be omitted from consideration.) The repeating vector is modified by adding either an inhomogeneity vector using external field vertex G or a correlation vector via one of the interaction vertices B, D or F. Since the repeating vector is modified by the addition of a different wavevector, it can reappear at the vertex V_2 only if the added vector is removed either by separation or by elimination. At an interaction vertex, a vector is either separated from the others or eliminated in conjunction with its complement. An added inhomogeneity vector can be eliminated by a field vertex (of type I in figure 4).

Our intention is to show that the connection of a repeating vector with another starting vector prohibits the subsequent reappearance of the repeating vector if the diagram is not to contain any negligible fragments.

With this in mind, let us consider first a starting fragment with a vertex V_1 of type D, followed by interaction fragments which merely serve to fix the topological properties of the diagram. The repeating vector is modified by adding a correlation vector (-m), which is introduced at V_1 together with its complement m (see figure 9).



Figure 9. Example of a diagram with two blocks in a domain.

Obviously, the D-type vertex cannot connect the repeating vector ((K - I)) in figure 9) with another vector (I) appearing on the left of V₁. As a consequence, each of them belongs to a separate block. A block is a part of a diagram disconnected from other parts in a given domain, and is delineated (as in figure 9) by broken horizontal lines (see Škarka 1985).

The repeating vector reappears at the vertex V_2 only if the added vector (-m) is either separated or eliminated. But the separation of a vector as well as its elimination without the simultaneous introduction of a novel vector both lead to the loss of one momentum integration (see, for example, the fragments D'_{3} and F'_{3} in figure 5). Therefore, such fragments belong to the third group of negligible fragments, except when an irreducible subcorrelation is created causing a 'mixing on the right' (figure 6). Such a mixing on the right appears when the separation occurs inside the block of the repeating vector (see figure 9). In this block the sum of vectors is equal to the repeating vector, provided that all other vectors are introduced together with their complements (their sum is zero). For the same reason, inside the block the complement m can be separated from the other vectorial indices via a 'mixing on the right' fragment and thus can be found labelling a line by itself. Only in conjunction with its complement m alone on a line can the added vector (-m) be eliminated in a non-negligible fragment V_2 of type B. Therefore, by this procedure of either separation or elimination of vectorial indices, the repeating vector may reappear in its block either alone or in the presence of an irreducible subcorrelation and in so doing it avoids giving rise to any negligible fragments.

Now, in order to satisfy the conditions stipulated by the theorem, let us suppose that the repeating vector $(\mathbf{K} - \mathbf{l})$ is connected with the starting vector (\mathbf{l}) originating from another block. When $(\mathbf{K} - \mathbf{l})$ reappears it cannot be connected by itself with a vector of the second block since it would be modified once again and the connection vertex V_c would then coincide with V₃. Such an occurrence is excluded from consideration by the theorem. Let us thus make the connection with the other block between V₂ and V₃, via a vector belonging to the remaining subcorrelation (figure 9). It then involves a 'mixing on the left' fragment which belongs to the fourth group of negligible fragments in figure 5. (Notice that the subcorrelation persists between the 'mixing on the right' and the 'mixing on the left' fragments, or their analogues for the external field vertex (V₂ and V_e in figure 9).)

In order to avoid a negligible 'mixing on the left' fragment, the subcorrelation can now be destroyed by an external field vertex, which introduces an inhomogeneity vector (as in figure 9). But the external field vertex does not change the topology of the diagram; rather it converts a dependent vector into an independent one and such a fragment also belongs to the fourth group of negligible fragments (in figure 7).

Let us now examine the possible connections which can be made between vertices V_1 and V_2 . In the first case, the separation of some vectorial indices is performed in a 'mixing on the right' fragment in order to prepare for the reappearance of the repeating vector before the connection (V_c) occurs (as in figure 10). Therefore, if one of the lines associated with the previously created subcorrelation participates at the vertex V_c it mixes with a vector of the second block, which renders the diagram negligible as in the preceding example. Otherwise, if one of the remaining vectors (e.g. the modified repeating vector (K - l - m) or the complement m of the added vector in figure 10) is connected with a vector of the second block, the effect of the previous separation is lost, and a 'parasite' vector has to be removed. Such a situation is then similar to the second case, discussed below, where the connection is performed without any preceding preparative separation.

In the second case, the starting fragments B and F can be treated together with the starting fragment D (e.g. as in figure 11). (Indeed, the vertices B and F not only modify the repeating vector but also connect it directly with some other vector of the starting state and the two blocks soon merge into one.) The repeating vector modified by





Figure 11. See text for discussion.

adding a vector (e.g. -m in figure 2) reappears at the vertex V₂ only if the added vector is either separated or eliminated. However, the separation of the added vector (e.g. see the fragment D'₃ in figure 5) and its elimination in conjunction with its complement *m* which is not alone on a line (e.g. in figure 11) both involve a negligible fragment of the third group.

As shown above, the vertex V_2 can escape negligibility either when, before its elimination, the complement *m* labels a line by itself, or when the separation is done through a 'mixing on the right' fragment (see D_5 in figure 6). However, both such variants demand as a prerequisite another separation, namely that of the complement *m* (in figure 12), but such a separation can only be made via a fragment of the third group which renders this contribution negligible.

In a previous case (see figure 9), any separation in the block of the repeating vector corresponded to mixing on the right, since a subcorrelation could be created. Here, in contradistinction, there is no block for the repeating vector by virtue of the connection; the parasite vectorial index originating in the other block prevents the appearance of a subcorrelation, leading to a fragment of the third group. Notice that with B as



Figure 12. See text for discussion.

the starting fragment (in figure 12), the starting vector (-m) has a dual role: it joins and modifies the repeating vector. Its complement m can be alone on a line, but then it forms with (-m) an irreducible subcorrelation and consequently the vertex V_1 is already mixing on the left. Hence, this particular situation is not considered from the outset.

In each separation or elimination, a new vector can be simultaneously added, which makes the fragment non-negligible. Nonetheless, in order to admit the reappearance of the repeating vector, this new vector has to be removed in one of the subsequent dynamical steps through a negligible fragment (as in figure 13).

Finally, let us consider the case where the field vertex G modifies the repeating vector by adding an inhomogeneity vector \mathbf{K}' . The repeating vector can only reappear when this vector \mathbf{K}' is either eliminated using another field vertex G' (figure 14), or separated by means of an interaction vertex of type D (figure 15), both of which, however, belong to the third group of negligible fragments. It has already been noted that the fragment D can remain finite in two different circumstances. The first one is when D becomes a 'mixing on the right' fragment, i.e. when on its left the exact complement \mathbf{K}' of the added vector $(-\mathbf{K}')$ is introduced by a vertex H (as in figure 15). However, now the latter vertex belongs to the second group of negligible fragments, since \mathbf{K}' is not an integrating wavevector. A second circumstance in which the fragment D is non-negligible occurs when, in the separation, a new vector and its complement can be simultaneously added. However, once more the new wavevector has to be removed subsequently, with the consequence that the contribution is again negligible.



Figure 13. See text for discussion.



M=0+2-1-0=1 Figure 14. See text for discussion.



Figure 15. See text for discussion.

All the diagrams of the above class remain negligible even when an arbitrary number of external field fragments are incorporated, since the change in the diagrams only involves vectorial indices on the lines: in short, the topology of the diagram remains unchanged.

We have thus shown that a connection between the repeating vector and another starting vector (i.e. between their respective blocks), in the domain between the vertices V_1 and V_3 , makes the diagram negligible even when external field fragments are included. Therefore, the general theorem holds for systems evolving in time-dependent external fields.

Only the topology of the wavevectors is relevant in the theorem. Therefore, the diagrams considered for the theorem all contain negligible external field and/or interaction fragments of the second, third or fourth group. Furthermore, since in a diagram a lost particle can be reintroduced through either an external field or an internal interaction fragment of the first group, the scope of the theorem may be enlarged by the following statement.

A diagram is negligible if a field particle is lost and afterwards reintroduced.

A further extension of the theorem is afforded by reconsideration of those cases involving external field vertices which have already been investigated for the purpose of demonstrating the theorem itself. Note that, when introduced into a diagram, the external field either modifies a vector on an existing line, thereby changing the total vector of the corresponding block (see figure 9), or creates a new line and hence a new block.

In the former case, even if the inhomogeneity vector introduced by the field does not modify the repeating vector but another one instead, it still has to be removed. Indeed, this vector prohibits the reappearance of the repeating vector via non-negligible fragments either directly (as in figure 16) or indirectly, by destroying an irreducible subcorrelation or preventing its creation. In fact, any external field vertex has the same effect as a connection vertex (V_c), since it introduces a parasite inhomogeneity vectorial index. This additional vectorial index has to be either eliminated, using a negligible fragment (as in figure 14), or separated. In both cases this can only be done via a negligible fragment.



M=1+3-1-1=1Figure 16. See text for discussion.

Therefore, the mere presence of a single external field fragment in the block of a repeating vector—even without any connection with other blocks—renders the diagram negligible.

The theorem can thus be extended by adding the following statement to the previous formulation.

A diagram without any connection is also negligible if at least one external field vertex appears in the block of a repeating vector in the domain between the vertices V_1 and V_2 .

5.4. Corollary of the theorem

The following corollary of the theorem may now be stated.

A diagram in which a state appears twice is negligible in the thermodynamic limit if any one of the following conditions is fulfilled.

(i) Two vectors of the repeating state are mutually connected in the domain between its first and second appearance.

 (ii) At least one external field vertex appears in the block associated with one vector of the repeating state.

(iii) A field particle is lost and afterwards reintroduced.

Using this corollary, one can immediately eliminate not only all diagrams involving diagonal transitions from a state (of given degree) to itself, provided at least one of the intermediate states is of equal or lower degree (a case which could be disregarded altogether for homogeneous systems using Henin's theorem (Henin 1971)), but also some diagrams with intermediate states of a higher degree (Škarka 1978a, b). In this way an important result is obtained.

In the thermodynamic limit, diagrams with a repeating state have to be retained if and only if, in the domain between the first and second appearance of a repeating state, they are split into at least as many blocks as there are lines in the repeating state—each block containing at most one of the lines belonging to the repeating state—and provided that, in the blocks containing a line of the repeating state, there is no external field vertex.

Therefore, in the domain between state repetition, particles of one block do not interact with particles of any other block. In addition, an external field vertex can only appear in a block with no line belonging to the repeating state. Considered



Figure 17. An example of a diagram whose contribution is finite in the thermodynamic limit.

separately such a block begins with the homogeneous vacuum of correlation states and ends in the same way (see figure 17).

6. Conclusion

The theorem which we have now established, on the basis of the topological properties of the diagrams, is of importance for a variety of interconnected reasons.

As noted in §§ 2.2 and 2.3, the theorem is a prerequisite for the application of the analytical continuation procedure of Coveney and George (1987), which in turn leads into the subdynamics decomposition for dissipative systems in the thermodynamic limit. It therefore completes the formal aspects of the subdynamics theory for systems of structureless particles evolving in spatially varying time dependent external fields (Coveney 1987).

In the case of (spatially) uniform external fields, it is obvious that Henin's theorem (Henin 1971) for homogeneous systems is sufficient, because then the system-field interaction $\xi \delta L^F$ is diagonal in the correlation states $\{|\nu\rangle\}$ (the eigenfunctions of L_0) and plays no role in the dynamics of correlations.

The situation is quite different when the field is inhomogeneous however, since then the interaction $\xi \delta L^F$ induces transitions between states of differing overall degree. For the successful application of the analytical continuation procedure, we require that all diagonal transitions involving intermediate states of equal overall degree be negligible in the T limit. The general theorem—and in particular its corollary (§ 5.4) guarantees that this condition is met. In addition, all diagrams containing intermediate states of a lower overall degree, as well as some with intermediate states of a higher degree, are also negligible.

Beyond completing the formal theoretical development outlined in § 2, it should be noted that the general theorem established herein is also a necessary condition for the so-called dynamical factorisation of the subdynamics evolution superoperators (Škarka 1985, 1987). This factorisation leads to a considerably simplified description of irreversible processes in gases and plasmas, which has already been exploited for the treatment of isolated inhomogeneous gases (Škarka 1985).

Furthermore, explicit formal solutions of the non-linear Vlasov equation describing inhomogeneous collisionless plasmas have been obtained using subdynamics (Škarka and George 1984). The method is effectively a generalisation of that due to van Kampen (1955, 1957) and Case (1959) for the linearised version of the Vlasov equation. We hope to return in the future with a consideration of the more complex situation which pertains in the presence of time dependent external fields, a problem of central interest in the context of plasma physics.

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