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Formal manipulations relating the *S*-matrix and density matrix formalisms

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Abstract. The present paper provides a formal derivation of a set of equations linking the *S*-matrix and density matrix methods. The formal manipulations involved permit a clear statement of the mathematical assumptions required in order to arrive at the associated set of time-irreversible equations. They should thus permit future investigations to put the whole theory on a more rigorous basis.

1. Introduction

For a system with a total Hamiltonian H of the form

$$H = H_0 + V \tag{1.1}$$

in which H_0 is the unperturbed Hamiltonian and V is the perturbation, the density matrix p of the system obeys the Liouville–von Neumann equation

$$\partial p/\partial t = -(\mathrm{i}/\hbar)[H, p] = -\mathrm{i}\mathscr{L}p = -\mathrm{i}\mathscr{L}_0 p - \mathrm{i}\mathscr{L}_1 p \tag{1.2}$$

where, in terms of commutator brackets,

$$\mathscr{L} = [H, \ ], \qquad \mathscr{L}_0 = [H_0, \ ], \qquad \mathscr{L}_1 = [V, \ ].$$

Equation (1.2) is exact and time reversible. Recently (Roberts and Hagston 1979a) we proposed in place of equation (1.2) the following irreversible equation for the diagonal part p_d of the density matrix:

$$\partial p_\mathrm{d}/\partial t = -(\mathrm{i}/\hbar)\Omega_-^+[V, p]\Omega_- \tag{1.3}$$

where the Møller operators $\Omega_\pm$ are defined by (Roman 1965)

$$\Omega_\pm = 1 + \operatorname*{Lim}_{\eta \to 0^+} \frac{1}{E_a - H_0 \pm \mathrm{i}\eta} T_\pm \tag{1.4}$$

and E_a refers to the energy eigenvalue of the (unperturbed) state upon which $\Omega_\pm$ acts, whilst T is the usual t-matrix of scattering theory. An appropriate generalisation of equation (1.3) for the case of open systems was postulated in a second paper (Roberts and Hagston 1979b). No attempt at a formal justification of equation (1.2) or its generalisation was attempted in either of these papers. However it was shown that, starting from these equations, various other well known equations of physics could be rapidly and easily derived. As a result it was argued that the postulated equations must have some range of validity.

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It is clear that, for example, equation (1.3) cannot be of universal validity since it is a Markoffian equation. Although the latter cover a large and important class of physical systems (van Kampen 1976) there are systems which cannot be described by Markoffian equations. In order to form an appraisal of the range of validity of equations such as (1.3) it is essential to have first some formal derivation (however approximate) of these equations. Concerning this point it is to be emphasised that *any* derivation of an *irreversible* equation from a reversible one must of necessity invoke some type of approximation. The basic aim of the present paper is to provide a formal derivation of equation (1.3) and its generalisation for open systems.

In the process of this derivation certain mathematical difficulties arise which, although far from trivial, are not peculiar to the present discussion but occur in a wide range of physical problems. One such example is the time development operator $U(t, t_0)$ defined below. It has long been known (see e.g. Jauch and Rohrlich 1955) that this operator becomes ill defined when one or more of its time arguments becomes infinite. Nonetheless the time development operator has, in exactly this context, played a major role in the evaluation of the Green functions of many-body systems by time-dependent perturbation theory (Abrikosov *et al* 1963, Fetter and Walecka 1971). Hence in what follows we tacitly assume that entities such as $U(t, t_0)$ exist in the appropriate limit. This is in accord with our main theme which is simply to provide a formal derivation of the basic equations of the theory, since this is regarded as being the problem of first importance. Once this has been achieved it is hoped that bringing this derivation to the attention of other workers in the field will result in a resolution of the various mathematical difficulties previously alluded to, and the placing of the theory on a much firmer foundation.

2. Formal manipulations involving a limit procedure

One characteristic feature of the present analysis is the use of a certain limit procedure (see below for details). Since the conditions for the validity of this procedure would require a long and detailed analysis which we are at present unable to give, we adopt the alternative of seeking a justification for its validity by employing it to establish certain formal results obtained previously by other authors using a different technique.

2.1. The density matrix and the Møller wave operators

The general solution of the Liouville–von Neumann equation is

$$p(t) = \exp\left[-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right] p(t_0) \exp\left[\frac{\mathrm{i}}{\hbar}H(t-t_0)\right]. \tag{2.1}$$

Employing the interaction picture (Roman 1965), this becomes

$$p^{\mathrm{I}}(t) = \exp\left(\frac{\mathrm{i}}{\hbar}H_0 t\right) \exp\left[-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right] \exp\left(-\frac{\mathrm{i}}{\hbar}H_0 t_0\right) p^{\mathrm{I}}(t_0) \exp\left(\frac{\mathrm{i}}{\hbar}H_0 t_0\right)$$
$$\times \exp\left[\frac{\mathrm{i}}{\hbar}H(t-t_0)\right] \exp\left(-\frac{\mathrm{i}}{\hbar}H_0 t\right) \tag{2.2}$$

which simplifies to

$$p^{\mathrm{I}}(t) = U(t, t_0) p^{\mathrm{I}}(t_0) U^{+}(t, t_0) \tag{2.3}$$

where $U(t, t_0)$ is the well known time development operator (Roman 1965) and is given by

$$U(t, t_0) = \exp\left(\frac{\mathrm{i}}{\hbar}H_0 t\right) \exp\left[-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right] \exp\left(-\frac{\mathrm{i}}{\hbar}H_0 t_0\right). \tag{2.4}$$

Naively taking the limits $t \to +\infty$ and $t_0 \to -\infty$ we obtain, assuming that the limit of the product on the right-hand side of equation (2.3) is the product of the limits taken separately,

$$p^{\mathrm{I}}(\infty) = Sp^{\mathrm{I}}(-\infty)S^{+} \tag{2.5}$$

where we have used the fact (Roman 1965) that the S-matrix is given by

$$S = \lim_{\substack{t \to +\infty \\ t_0 \to -\infty}} U(t, t_0). \tag{2.6}$$

On the other hand it follows from equation (2.3) that under the same type of limiting procedure

$$p^{\mathrm{I}}(0) = U(0, -\infty)p^{\mathrm{I}}(-\infty)U^{+}(0, -\infty) = \Omega_{+}p^{\mathrm{I}}(-\infty)\Omega_{+}^{+} \tag{2.7}$$

and

$$p^{\mathrm{I}}(0) = U(0, +\infty)p^{\mathrm{I}}(+\infty)U^{+}(0, +\infty) = \Omega_{-}p^{\mathrm{I}}(+\infty)\Omega_{-}^{+} \tag{2.8}$$

which follows from the fact (Roman 1965) that

$$\Omega_{\pm} = \lim_{t_0 \to \mp\infty} U(0, t_0) = \lim_{t_0 \to \mp\infty} \exp\left(\frac{\mathrm{i}}{\hbar}Ht_0\right) \exp\left(-\frac{\mathrm{i}}{\hbar}H_0 t_0\right). \tag{2.9}$$

The results expressed in equations (2.5), (2.7) and (2.8) are generalisations of the relations derived by Stanton (1971) for the case of pure states, and, as demonstrated by this author, they provide a useful alternative to that of formal scattering theory for calculating the T-matrix.

2.2. Analysis of the BBGKY hierarchy

The purpose of the present section is to describe a method of introducing the Møller wave operators into the derivation of the quantum Boltzmann equation. This problem was discussed initially by Snider (1960) with later formalistic interpretations by Snider and Sanctuary (1971).

The first two equations in the BBGKY hierarchy read as follows (Snider 1960):

$$\mathrm{i}\hbar\dot{p}(1, t) = L(1)p(1, t) + \phi \operatorname*{Tr}_{2} L'(1, 2)p(1, 2, t), \tag{2.10}$$

$$\mathrm{i}\hbar\dot{p}(1, 2, t) = L(1, 2)p(1, 2, t) + \phi \operatorname*{Tr}_{3} [(L'(1, 3) + L'(2, 3))p(1, 2, 3, t)]. \tag{2.11}$$

In an obvious notation, $p(1, t)$ is the one-particle density matrix of particle 1 with Liouvillian $L(1)$, $p(1, 2, t)$ is the two-particle density matrix with Liouvillian $L(1, 2)$ whilst $L'(1, 3)$ is the interaction Liouvillian for particles 1 and 3 etc. The constant ϕ is simply the (number) density of particles. For a dilute gas the probability of a triple collision between particles 1, 2 and 3 is very small, hence, for the purposes of calculating

$p(1, 2, t)$, we ignore the second term on the RHS of equation (2.11). As a result this equation simplifies to

$$i\hbar\dot{p}(1, 2, t) = L(1, 2)p(1, 2, t) \tag{2.12}$$

which has the formal solution

$$p(1, 2, t) = \exp\left[-\frac{i}{\hbar}H(1, 2)(t-t_0)\right] p(1, 2, t_0) \exp\left[+\frac{i}{\hbar}H(1, 2)(t-t_0)\right]. \tag{2.13}$$

From the definition of $U(t, t_0)$ in equation (2.4) we obtain

$$\begin{aligned} &U(0, t_0) = \exp\left(\frac{i}{\hbar}Ht_0\right) \exp\left(-\frac{i}{\hbar}H_0t_0\right), \\ &\therefore \qquad U(0, t_0-t) = \exp\left[\frac{i}{\hbar}H(t_0-t)\right] \exp\left[-\frac{i}{\hbar}H_0(t_0-t)\right]; \end{aligned} \tag{2.14}$$

hence

$$\exp\left[-\frac{i}{\hbar}H(t-t_0)\right] = U(0, t_0-t) \exp\left[-\frac{i}{\hbar}H_0(t-t_0)\right]. \tag{2.15}$$

For the two-particle system which occurs in equation (2.13), $H_0(1, 2)$ is the kinetic energy and internal state energy operator referring to particles 1 and 2. These considerations enable us to rewrite equation (2.13) in the form

$$\begin{aligned} p(1, 2, t) = U(0, t_0-t) &\exp\left[-\frac{i}{\hbar}H_0(1, 2)(t-t_0)\right] \\ &\times p(1, 2, t_0) \exp\left[+\frac{i}{\hbar}H_0(1, 2)(t-t_0)\right] U(0, t_0-t). \end{aligned} \tag{2.16}$$

At time t it is argued (Snider 1960) that the particles are colliding, whereas t_0 is an earlier time prior to the collision commencing and where the Boltzmann property is assumed to hold, namely

$$p(1, 2, t_0) = p(1, t_0)p(2, t_0). \tag{2.17}$$

The effect of $\exp[-(i/\hbar)H_0(1, 2)(t-t_0)]$ is to take a wavefunction at a time t_0 to a time t under the action of a Hamiltonian which contains no interaction. From equation (2.16) and the commutative properties of $H_0(1)$ and $H_0(2)$ we find that

$$\exp\left[-\frac{i}{\hbar}H_0(1, 2)(t-t_0)\right] p(1, 2, t_0) \exp\left[+\frac{i}{\hbar}H_0(1, 2)(t-t_0)\right] = p(1, t)p(2, t). \tag{2.18}$$

If we choose $t_0 \to -\infty$, so that $t_0 - t \to -\infty$, we find, by invoking equations (2.15) and (2.9) and assuming the validity of the limiting procedure employed earlier, that equation (2.16) becomes

$$p(1, 2, t) = \Omega_+(1, 2)p(1, t)p(2, t)\Omega_+^+(1, 2). \tag{2.19}$$

With this result the 'closed' equation of motion for the single-particle density matrix is, from (2.10),

$$i\hbar\dot{p}(1, t) = L(1)p(1, t) + \phi \operatorname*{Tr}_2 L'(1, 2)\Omega_+(1, 2)p(1, t)p(2, t)\Omega_+^+(1, 2).$$

Expanding this expression and employing the well known result (Roman 1965)

$$H^1(1,2)\Omega_+(1,2) = T_+(1,2) = T(1,2)$$

together with its Hermitian conjugate, where T is the transition matrix related to the S-matrix by

$$S = 1 + T,$$

we have

$$i\hbar\dot{p}(1,t) = L(1)p(1,t) + \phi \operatorname*{Tr}_2 [T(1,2)p(1,t)p(2,t)\Omega_+^+(1,2)$$
$$- \Omega_+(1,2)p(1,t)p(2,t)T^+(1,2)].$$

If we now employ the expression for Ω_+ given in equation (1.4) and take arbitrary matrix elements, we readily obtain (Snider 1960)

$$i\hbar\frac{\partial}{\partial t}p(1,t)_{a_1b_1}$$
$$= H_0(1)_{a_1}p(1,t)_{a_1b_1} - p(1,t)_{a_1b_1}H_0(1)_{b_1}$$
$$+ 2\pi i\phi \sum_{cc'a_2b_2} T_{ac}p(1,t)_{c_1c_1'}p(2,t)_{c_2c_2'}T_{c'b}\delta_{a_2b_2}\delta(E_b - E_c)$$
$$+ \phi \sum_{ca_2b_2} [T_{ac}p(1,t)_{c_1b_1}p(2,t)_{c_2b_2} - p(1,t)_{a_1c_1}p(2,t)_{a_2c_2}T^+_{cb}] \qquad (2.20)$$

where a_1 is the eigenvalue of $H_0(1)$ for particle 1, a_2 that for particle 2 and a is the comprehensive eigenvalue denoting a_1, a_2. This holds for b, c and c' as well.

Starting from equation (2.20) we can obtain (see Snider 1960) the usual Boltzmann equation for a dilute gas and the modified Boltzmann equation for the corresponding Wigner distribution function. Snider and Sanctuary (1971) argue that the replacement of $p(1,2,t)$ by $\Omega_+p(1,t)p(2,t)\Omega_+^+$ (see equation (2.19)) is a natural approximation in accordance with the 'philosophy' of the Boltzmann equation. We note that it is a simple consequence of the presumed validity of the limiting procedure we have employed.

3. Derivation of the 'asymptotic' equations of motion

3.1. Closed systems

In the present section we will invoke the same type of limiting procedure as that described above in order to derive the equation of motion for a closed system in a form identical with that postulated in an earlier paper (Roberts and Hagston 1979a, b). The complete time behaviour of any closed system is, in the interaction picture, governed by the Liouville–von Neumann equation (Roman 1965):

$$\frac{\partial p^{\mathrm{I}}}{\partial t} = -\frac{i}{\hbar}\exp\left(\frac{i}{\hbar}\mathscr{L}_0 t\right)[V, p(t)], \qquad (3.1)$$

where

$$p^{\mathrm{I}}(t) = \exp[(i/\hbar)\mathscr{L}_0 t]p(t).$$

Introduce an entity D which acts on operators only according to the prescription

$$DA = \sum_{\alpha} \langle\alpha|A|\alpha\rangle|\alpha\rangle\langle\alpha| \tag{3.2}$$

where A is an arbitrary operator, and where the $|\alpha\rangle$ are eigenkets of the unperturbed Hamiltonian H_0. For any well behaved observable operator B that does not possess pathological properties, we clearly have

$$\langle\alpha|[H_0, B]|\alpha\rangle = 0.$$

From this and the definition of D it follows that we have the identities

$$D\mathscr{L}_0 = \mathscr{L}_0 D \equiv 0. \tag{3.3}$$

The result expressed in equation (3.3) is the operator analogue of the well known Zwanzig identities (Zwanzig 1960). Applying D to both sides of equation (3.1) and employing equation (3.3) on the LHS shows that

$$D\frac{\partial p^{\mathrm{I}}(t)}{\partial t} = D\frac{\partial p}{\partial t} = \dot{p}_{\mathrm{d}}(t) = -\frac{\mathrm{i}}{\hbar} D \exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}_0 t\right)[V, p(t)]. \tag{3.4}$$

If we now employ equation (3.3) on the RHS of equation (3.4) it is clear that we can replace the time variable t in the exponential operator by any arbitrary time variable τ (say), thus giving

$$\dot{p}_{\mathrm{d}}(t) = -(\mathrm{i}/\hbar) D \exp[(\mathrm{i}/\hbar)\mathscr{L}_0\tau][V, p(t)]. \tag{3.5}$$

Inserting the unit operator in the form $\exp[-(\mathrm{i}/\hbar)\mathscr{L}\tau]\exp[(\mathrm{i}/\hbar)\mathscr{L}\tau]$ into equation (3.5) gives

$$\begin{aligned}\dot{p}_{\mathrm{d}}(t) &= -\frac{\mathrm{i}}{\hbar} D \exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}_0\tau\right)\exp\left(-\frac{\mathrm{i}}{\hbar}\mathscr{L}\tau\right)\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}\tau\right)[V, p(t)] \\ &= -\frac{\mathrm{i}}{\hbar} DU^{+}(0,\tau)\exp\left(\frac{\mathrm{i}}{\hbar}H\tau\right)[V, p(t)]\exp\left(-\frac{\mathrm{i}}{\hbar}H\tau\right)U(0,\tau)\end{aligned} \tag{3.6}$$

where we have employed equation (2.14). Taking the limit $\tau \to \infty$ and assuming validity of the limit procedure gives

$$\begin{aligned}\dot{p}_{\mathrm{d}}(t) &= -\frac{\mathrm{i}}{\hbar}\operatorname*{Lim}_{\tau\to\infty} D\Omega_{-}^{+}\exp\left(\frac{\mathrm{i}}{\hbar}H\tau\right)[V, p(t)]\exp\left(-\frac{\mathrm{i}}{\hbar}H\tau\right)\Omega_{-} \\ &= -\frac{\mathrm{i}}{\hbar}\operatorname*{Lim}_{\tau\to\infty} D\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}_0\tau\right)\Omega_{-}^{+}[V, p(t)]\Omega_{-} \\ &= -\frac{\mathrm{i}}{\hbar} D\Omega_{-}^{+}[V, p(t)]\Omega_{-}\end{aligned} \tag{3.7}$$

where in the first step we have employed equation (2.9), in the second we have used the intertwining relation (Roman 1965)

$$H_0\Omega_{\pm} = \Omega_I H$$

and in the final step we have utilised equation (3.3). Hence what we have shown is that the equation of motion is

$$\dot{p}(t) = -(\mathrm{i}/\hbar)\Omega_{-}^{+}[V, p(t)]\Omega_{-} \tag{3.8}$$

as long as it is understood that we take diagonal elements *only*. It is seen that equation (3.8) is identical with that proposed earlier (Roberts and Hagston 1979a, b) and since the manipulations in this paper involved diagonal elements only, we have thus obtained a formal justification for the validity of the procedures employed there.

3.2. Open systems

The extension of the above derivation to the case of an open system is straightforward. Thus we consider a closed system composed of two subsystems B and C which interact with one another. The total system is completely described by the density operator p which, in the interaction picture, obeys the Liouville–von Neumann equation

$$\frac{\partial p^{\mathrm{I}}}{\partial t} = -\frac{\mathrm{i}}{\hbar}\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}^0 t\right)[V, p] \tag{3.9}$$

where

$$\mathscr{L}^0 = [H^0, \ ], \qquad H^0 = H_{\mathrm{B}}^0 + H_{\mathrm{C}}^0, \qquad V = V_{\mathrm{B}} + V_{\mathrm{C}} + V_{\mathrm{BC}}.$$

In this notation, H_{B}^0, for example, is the unperturbed Hamiltonian associated with system B, V_{B} is its internal perturbation whilst V_{BC} is the coupling of system B to system C. Application of the total diagonalising projection operator $D = D_{\mathrm{B}}D_{\mathrm{C}}$ (where D_{B} is the diagonalising projection operator for system B, etc) to equation (3.9) gives

$$\begin{aligned} D\frac{\partial p^{\mathrm{I}}(t)}{\partial t} &= \dot{p}_{\mathrm{d}}(t) \\ &= -\frac{\mathrm{i}}{\hbar}D\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}^0 t\right)[V_{\mathrm{B}}, p(t)] - \frac{\mathrm{i}}{\hbar}D\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}^0 t\right)[V_{\mathrm{C}}, p(t)] \\ &\quad -\frac{\mathrm{i}}{\hbar}D\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}^0 t\right)[V_{\mathrm{BC}}, p(t)]. \end{aligned} \tag{3.10}$$

Again utilising the relations $D_{\mathrm{B}}\mathscr{L}_{\mathrm{B}}^0 = D_{\mathrm{C}}\mathscr{L}_{\mathrm{C}}^0 = D\mathscr{L}^0 \equiv 0$, we have

$$\begin{aligned} \dot{p}_{\mathrm{d}} &= -\frac{\mathrm{i}}{\hbar}D_{\mathrm{C}}D_{\mathrm{B}}\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}_{\mathrm{B}}^0\tau\right)[V_{\mathrm{B}}, p] - \frac{\mathrm{i}}{\hbar}D_{\mathrm{B}}D_{\mathrm{C}}\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}_{\mathrm{C}}^0\tau\right)[V_{\mathrm{C}}, p] \\ &\quad -\frac{\mathrm{i}}{\hbar}D\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}^0\tau\right)[V_{\mathrm{BC}}, p]. \end{aligned}$$

Inserting the identities

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\mathscr{L}_{\mathrm{B}}\tau\right)\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}_{\mathrm{B}}\tau\right) = \exp\left(-\frac{\mathrm{i}}{\hbar}\mathscr{L}_{\mathrm{C}}\tau\right)\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}_{\mathrm{C}}\tau\right) = \exp\left(-\frac{\mathrm{i}}{\hbar}\mathscr{L}^1\tau\right)\exp\left(\frac{\mathrm{i}}{\hbar}\mathscr{L}^1\tau\right) \equiv 1$$

where

$$\mathscr{L}_{\mathrm{B}} = [H_{\mathrm{B}}^0 + V_{\mathrm{B}}, \ ], \qquad \mathscr{L}_{\mathrm{C}} = [H_{\mathrm{C}}^0 + V_{\mathrm{C}}, \ ], \qquad \mathscr{L}^1 = [H_{\mathrm{B}}^0 + H_{\mathrm{C}}^0 + V_{\mathrm{BC}}, \ ],$$

and taking the limit $\tau \to \infty$ we obtain, in the same manner as before, after making use of the corresponding intertwining relations,

$$\begin{aligned} \dot{p}_{\mathrm{d}}(t) &= -(\mathrm{i}/\hbar)D\Omega_-^+(\mathrm{B})[V_{\mathrm{B}}, p]\Omega_-(\mathrm{B}) - (\mathrm{i}/\hbar)D\Omega_-^+(\mathrm{C})[V_{\mathrm{C}}, p]\Omega_-(\mathrm{C}) \\ &\quad -(\mathrm{i}/\hbar)D\Omega_-^+(\mathrm{BC})[V_{\mathrm{BC}}, p]\Omega_-(\mathrm{BC}) \end{aligned} \tag{3.11}$$

where

$$\Omega_-(\mathrm{B}) = \operatorname*{Lim}_{\tau\to\infty} \exp\left(\frac{\mathrm{i}}{\hbar}H_{\mathrm{B}}\tau\right)\exp\left(-\frac{\mathrm{i}}{\hbar}H_{\mathrm{B}}^0\tau\right),$$

$$\Omega_-(\mathrm{C}) = \operatorname*{Lim}_{\tau\to\infty} \exp\left(\frac{\mathrm{i}}{\hbar}H_{\mathrm{C}}\tau\right)\exp\left(-\frac{\mathrm{i}}{\hbar}H_{\mathrm{C}}^0\tau\right), \tag{3.12}$$

$$\Omega_-(\mathrm{BC}) = \operatorname*{Lim}_{\tau\to\infty} \exp\left[\frac{\mathrm{i}}{\hbar}(H^0 + V_{\mathrm{BC}})\tau\right]\exp\left(-\frac{\mathrm{i}}{\hbar}H^0\tau\right),$$

with

$$H_{\mathrm{B}} = H_{\mathrm{B}}^0 + V_{\mathrm{B}}, \qquad H_{\mathrm{C}} = H_{\mathrm{C}}^0 + V_{\mathrm{C}}. \tag{3.13}$$

Again the results expressed in equations (3.11) to (3.13) provide a formal justification for the equations of motion for an open system postulated in an earlier paper (Roberts and Hagston 1979a, b).

4. Discussion and conclusion

In the above we have shown that the assumption of the validity of a certain limiting procedure, when coupled with the presumed existence of the limits of the various entities taken separately, leads to certain formal results relating the S-matrix and density matrix formalisms obtained by other authors using a different approach (Snider 1960, Stanton 1971). Employing the same technique has enabled us to obtain a formal justification for the equations we postulated earlier relating the S-matrix and density matrix methods (Roberts and Hagston 1979a, b). In this sense the main aim of the paper has been realised. It is to be emphasised however that the manipulations themselves raise many difficult mathematical points and only when these have been clearly resolved will the theory be placed on a sound footing. It is hoped that by drawing the attention of other workers to the points of principle involved, the present paper will be instrumental in this purpose.

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