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Determinantal solution of density matrix equations in time-dependent quantum mechanics: I. Constant perturbation

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Abstract. The determinantal formalism previously built up in the evolution operator problem is extended to the density matrix equation in the case, here, of a Heaviside step external perturbation, and in the presence of internal collision potential. Reduced determinantal forms, matched to those first derived for the evolution operator, are obtained and compared with both the iterative expansion and the initial Fredholm–Laplace solution. They not only exhibit the multiple transition structure of the physical response, along with the associated transition width upon expansion, but also the trace conservation requirement is shown to be satisfied at any order and all times. An illustration is given in a simplified physical system.

1. Introduction

A determinantal method derived from a so called ‘Fredholm–Laplace formalism’ has been worked out, in previous papers (Fortini 1979, 1981), for solving the Schrödinger equation of the evolution operator in the widespread practical cases of an harmonic or constant external perturbation.

The purpose of the present paper is to extend the same mathematical method to the density matrix problem. The interest of such a task lies first in the setting up of sufficiently general but tractable approximate formulae for the density matrix elements, commonly required in a large number of applications, such as semi-classical interaction of matter with radiation and transport phenomena. Particularly important in applications are resonance problems, in which usual methods often fail, so that for the purpose of comparison with experiment, important quantities such as linewidth, damping, energy shift are introduced *a posteriori* in an *ad hoc* manner. It will be shown that the determinantal formalism is able to yield convergent results in resonance cases. Connection with the perturbation iterative expansion is brought out at any important stage.

The density matrix response to a given time-dependent external field is much more interesting information than the evolution operator, for calculating quantum and statistical mean values of observables. Moreover, damping effects which do not require a quantum mechanical treatment can easily be incorporated in a phenomenological manner. The counterpart of these advantages lies in that the mathematics is rather more involved.

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Another fundamental interest of extending the method to the density matrix problem is to take advantage of the inherent unitarity of the determinantal solution. It has been pointed out (Fortini 1981) that the determinantal solution of the evolution operator does not yield secular terms which are known to be responsible for the lack of unitarity in the usual iterative approach. In fact, the unitary requirement of the determinantal solution is satisfied at any order, but the demonstration of this important property was delayed because it requires the calculation of a convolution integral which is nothing other than the density matrix Laplace transformed. Verification of the trace conservation theorem at any order is straightforward on a definite reduced determinantal expression of the density matrix solution.

Methods capable of yielding tractable expansions of the time-dependent density matrix (Golden 1977, Roberts and Hagston 1979) have been much less investigated than for time-dependent wavefunctions or evolution operators. Owing to the above mentioned advantages of the knowledge of the density matrix in applications, this may appear rather surprising, but there are, strictly speaking, no extra formal difficulties in mathematical treatments.

For the sake of simplicity, we will again restrict ourselves to the often encountered cases of static and harmonic external perturbation. The present paper (I) is devoted to the static case, in which the essentials of the method can be made explicit in the simplest scheme. The harmonic case which, in fact, can be regarded as a simple extension of the static one, will be separately treated in a subsequent paper (II).

2. Fredholm-Laplace solution for the density matrix

We will again start with the same typical Hamiltonian of the physical system as in Fortini (1981)

$$H = H_0 + V + AY(t), \quad (2.1)$$

where H_0 is an unperturbed Hamiltonian whose eigenstates $|k\rangle$ and the related eigenvalues $E_k = \hbar\omega_k$ are assumed to be known. V represents a collisional potential and $AY(t)$ the interaction with a constant external field, assumed to be applied from $t = 0$, as expressed by the Heaviside step function $Y(t)$. Although in the present case the applied external field and the collisional potential are both constant in time, for $t > 0$, their matrix elements and associated selection rules are generally quite different for each of them. The notational distinction will, therefore, be maintained throughout. In practice the state basis of $H_0 + V$ is unknown, and the physical response will be formulated with the help of expansions on the unperturbed basis of H_0 . This proves quite valid as long as collision events are sufficiently rare and of moderate strength, and will give rise to collision broadening of transitions which differ markedly from the natural broadening associated with the external field A . In particular applications, the distinction between the V and A contributions to the result will be further enhanced if the initial state is specified to be, as often occurs, a mixing of $H_0 + V$ eigenstates.

The density matrix $\rho(t)$ is connected with the evolution operator $U(t)$ by the well known equation

$$\rho(t) = U(t)\rho(0)U^+(t) \quad (2.2)$$

and satisfies the following equation of motion, directly derived from the time-dependent Schrödinger equation for $U(t)$

$$d\rho/dt = (i\hbar)^{-1}[H, \rho(t)]. \quad (2.3)$$

We will introduce the Laplace transform of $\rho(t)$ defined as

$$R(\nu) = \int_0^\infty e^{-\nu t} \rho(t) dt \quad \text{or } R(\nu) \subset \rho(t). \tag{2.4}$$

Since

$$d\rho/dt \supset \nu R(\nu) - \rho(0),$$

the Laplace transform of equation (2.3) is given by

$$\nu R(\nu) = \rho(0) + (i\hbar)^{-1} [H_0 + V + A, R(\nu)]. \tag{2.5}$$

Taking this equation between the states b and c

$$\nu R_b^c(\nu) = \rho_b^c(0) - i\omega_{cb} R_b^c(\nu) + i\hbar^{-1} [V_k^c R_b^k(\nu) - R_k^c(\nu) V_b^k] + i\hbar^{-1} [A_k^c R_b^k(\nu) - R_k^c(\nu) A_b^k], \tag{2.6}$$

where $R_b^c(\nu) = \langle c | R(\nu) | b \rangle$, $\omega_{cb} = \omega_c - \omega_b$. Summation over repeated indices is, as usual, implicit. In the following, $\rho_b^c(0)$ will be written as ρ_b^c , as long as no confusion may occur with $\rho_b^c(t)$.

In Fortini (1981) we have constructed the linear system whose complete solution is represented by the ‘column-vector’ defined by the $F_a^b(\nu)$ b -components of the Laplace transformed $F(\nu) \subset U(t)$ of the evolution operator. The row index is the superscript b , whereas the subscript a only refers to the initial pure state in which the system is assumed to be confined at $t = 0$. In other words, $F(\nu)$ is a vector belonging to the Hilbert space \mathcal{E}_{H_0} sustained by the eigenstates of H_0 .

Analogously, $R(\nu)$ will be regarded as a vector belonging to the tensorial product of \mathcal{E}_{H_0} by its own dual $\mathcal{E}_{H_0}^*$

$$\mathcal{E}_{H_0 H_0} = \mathcal{E}_{H_0} \otimes \mathcal{E}_{H_0}^*,$$

and $R_b^c(\nu)$ will denote the cb component of this column-vector. Equation (2.6) defines a linear system obeyed by the R_b^c .

In order to rewrite this equation in a much more convenient form, we will define the kernel K operating in the $\mathcal{E}_{H_0 H_0}$ space by

$$\langle c_1 b_1 | K | c_2 b_2 \rangle = K_{c_2 b_1}^{c_1 b_2} = K_{c_2}^{c_1} \delta_{b_1}^{b_2} - \delta_{c_2}^{c_1} K_{b_1}^{b_2}, \tag{2.7}$$

where

$$K_{c_2}^{c_1} = i\hbar^{-1} (V_{c_2}^{c_1} + A_{c_2}^{c_1}) \tag{2.8}$$

is the kernel previously defined in the \mathcal{E}_{H_0} space, in which we will still make the assumption that the diagonal elements of the perturbation are zero, i.e.

$$V_k^k = 0, \quad A_k^k = 0.$$

The adopted indices in the kernel (2.7) are such as to preserve the convenient notation K_b^c of the cb matrix elements, together with the subscript–superscript position of adjacent repeated indices in implicit summations. Regarded as a column-vector of the $\mathcal{E}_{H_0 H_0}$ space, R will be denoted \mathbf{R} , and the R_b^c component as

$$R_b^c = \mathbf{R}_b^c \equiv \langle c b | \mathbf{R} \rangle.$$

Since cb refers to a row index, the kernel matrix element (2.7) must be read as

$$K_{c_1}^{c_2} \rangle_{b_2}^{b_1} \begin{cases} \text{column index} \\ \text{row index} \end{cases} \tag{2.9}$$

It must be outlined that, in (2.7) $K\delta$ (or δK) is not the product of two operators belonging to \mathcal{E}_{H_0} , but a convenient symbol for denoting a specific operator of $\mathcal{E}_{H_0H_0}$.

Let us now examine conjugation relations. Owing to the hermiticity of iK , we have

$$(K_{c_2}^{c_1})^* = -i\hbar^{-1}(V_{c_1}^{c_2} + A_{c_1}^{c_2}) = -K_{c_1}^{c_2}.$$

Then

$$(K\delta)^+ = -K\delta, \quad (\delta K)^+ = -\delta K, \tag{2.10}$$

since

$$\begin{aligned} \langle c_2b_2|(K\delta)^+|c_1b_1\rangle &= \langle\langle c_1b_1|K\delta|c_2b_2\rangle\rangle^* \\ &= (K_{c_2}^{c_1}\delta_{b_1}^{b_2})^* = -K_{c_1}^{c_2}\delta_{b_2}^{b_1} = -\langle c_2b_2|K\delta|c_1b_1\rangle. \end{aligned}$$

The hermiticity of K follows as

$$K^+ = -K, \tag{2.11a}$$

i.e.

$$(K_{c_1}^{c_2b_1})^* = -K_{c_2b_1}^{c_1} = K_{b_1c_2}^{b_2c_1} \tag{2.11b}$$

on account of definition (2.7). Besides the introduction of the kernel K , we shall put

$$d_{cb} = \nu + i\omega_{cb}.$$

This quantity is a particular eigenvalue of the operator

$$d = \nu\mathbf{1} + i\hbar^{-1}H_0, \tag{2.12}$$

where $\mathbf{1}$ denotes the identity operator in $\mathcal{E}_{H_0H_0}$ and

$$H_0 = H_0\delta - \delta H_0 \tag{2.13}$$

is defined in the same manner as K .

With the help of these definitions, (2.6) can be rewritten in the compact form

$$d_{cb}R_b^c + K_{c_1}^c{}_{b_1} R_{b_1}^{c_1} = \rho_b^c,$$

equivalent to

$$(d + K)|R\rangle = |\rho\rangle, \quad \text{or} \quad (\mathbf{1} + d^{-1}K)|R\rangle = d^{-1}|\rho\rangle. \tag{2.14a, b}$$

The kernel K is analogous to the ‘superoperator’ introduced by Barker (1973) in transport problems and the tensorial device $\mathbf{K} = K\delta - \delta K$ provides a convenient means of calculating its repeated action on vectors of the $\mathcal{E}_{H_0H_0}$ space. Operators in \mathcal{E}_{H_0} become vectors in $\mathcal{E}_{H_0H_0}$ and superoperators become operators. The \mathbf{K} action on any O could as well be written

$$K|O\rangle = |[K, 0]\rangle, \tag{2.15}$$

with the evident trace property

$$\text{Tr}[K, 0] = \sum_{bb} \langle bb|K|O\rangle = 0. \tag{2.16}$$

We now write out the general solution of the linear system defined by (2.14b). Current matrix elements of R are given by

$$R_b^c = (D_{c_1b}^{cb_1}/d_{c_1b_1})\rho_{b_1}^{c_1}, \tag{2.17}$$

where D denotes the determinant of the system, i.e.

$$D = \det(\mathbf{1} + \mathbf{d}^{-1}\mathbf{K}), \tag{2.18}$$

and $D_{c_1b}^{cb_1}$ the algebraic minor at the crossing of the c_1b_1 row and the cb column

$$D_{c_1b}^{cb_1} \begin{cases} \text{row index} \\ \text{column index} \end{cases} \tag{2.19}$$

Notice the inversion of the meaning of the indices relative to the kernel (2.9).

The mathematical tools used in Fortini (1981) to derive reliable expansions of determinants in increasing orders of the kernel can be used without any extra formal difficulty. Assuming the system is, initially, in a state distribution defined as

$$|\rho\rangle = \sum_{a'a} \rho_a^{a'} |a'a\rangle, \tag{2.20}$$

the Fredholm expanded form of the solution (2.17) is written as

$$\mathbf{R}_b^c = \frac{-\mathbf{K}_{a'b}^{ca} + (\mathbf{K}_{c_1b}^{cb_1} \mathbf{K}_{a'b_1}^{c_1a} / d_{c_1b_1}) - \dots}{d_{cb} d_{a'a} [1 - (\mathbf{K}_{c_2b_1}^{c_1b_2} \mathbf{K}_{c_1b_2}^{c_2b_1} / 2! d_{c_1b_1} d_{c_2b_2}) + \dots]} \rho_a^{a'} \tag{2.21}$$

with $c_1b_1, c_2b_2, \dots \neq a'a$ in the numerator, and $c \neq b$. In diagonal bb elements (they are diagonal in the \mathcal{E}_{H_0} space), the ρ_b^b contribution must be written separately,

$$\begin{aligned} \mathbf{R}_b^b &= \frac{1 - (\mathbf{K}_{c_2b_1}^{c_1b_2} \mathbf{K}_{c_1b_2}^{c_2b_1} / 2! d_{c_1b_1} d_{c_2b_2}) + \dots}{d_{bb} [1 - (\mathbf{K}_{c_2b_1}^{c_1b_2} \mathbf{K}_{c_1b_2}^{c_2b_1} / 2! d_{c_1b_1} d_{c_2b_2}) + \dots]} \rho_b^b \\ &+ \frac{-\mathbf{K}_{a'b}^{ba} + (\mathbf{K}_{c_1b}^{bb_1} \mathbf{K}_{a'b_1}^{c_1a} / d_{c_1b_1}) - \dots}{d_{a'a} d_{bb} [1 - (\mathbf{K}_{c_2b_1}^{c_1b_2} \mathbf{K}_{c_1b_2}^{c_2b_1} / 2! d_{c_1b_1} d_{c_2b_2}) + \dots]} \rho_a^{a'} \end{aligned} \tag{2.22}$$

where $c_1b_1, c_2b_2, \dots \neq bb$ (or $a'a$) in the numerators. The successive terms can easily be written, for instance, by using the exponential or operational expression of D and non-diagonal minors (equations (A6), (20) and (A12) in Fortini (1981)).

Complete division in (2.21) and (2.22) yields the iterative expansion for the density matrix elements. Thus

$$\mathbf{R}_b^c = \left(-\frac{\mathbf{K}_{a'b}^{ca}}{d_{cb} d_{a'a}} + \frac{\mathbf{K}_{c_1b}^{cb_1} \mathbf{K}_{a'b_1}^{c_1a}}{d_{cb} d_{c_1b_1} d_{a'a}} - \dots \right) \rho_a^{a'}, \tag{2.23}$$

where index restrictions have now vanished. Using the operational form of determinant quotients (see (A15) in Fortini (1981)), this can be written

$$\mathbf{R}_b^c = d_{a'a}^{-1} \langle cb | (\mathbf{1} + \mathbf{d}^{-1}\mathbf{K})^{-1} | a'a \rangle \rho_a^{a'}.$$

In this form the result can be directly derived from (2.14b). Similar expressions can be written for the iterative expansion of the diagonal element \mathbf{R}_b^b .

Expressions (2.21), (2.22) and (2.23) represent the convolution integration of the analogous expressions of the related $F(\nu)$ matrix elements, according to the Laplace transform of (2.2)

$$R(\nu) = [F(\nu) * F^+(\nu)] \rho(0), \tag{2.24}$$

where the asterisk stands for convolution integration. We can verify that the hermiticity property (2.11b) of \mathbf{K} , and that of $\mathbf{d}(\mathbf{d}_{cb}^* = \mathbf{d}_{bc})$, when applied to (2.21), leads to the conjugate of $\mathbf{R}_b^c = (F_a^c * F_b^{+a}) \rho_a^{a'}$, which is given by $(\mathbf{R}_b^c)^* = (F_a^b * F_c^{+a'}) \rho_a^{a'} = \mathbf{R}_c^b$.

Since the above expressions represent the exact solution of the time-dependent Schrödinger equation of the density matrix, they are expected to satisfy the trace conservation theorem

$$\text{Tr } \rho(t) = 1$$

at all times, inasmuch as $\text{Tr } \rho(0) = 1$. This simply results from the hermiticity of the hamiltonian operator (2.1). However, in the iterative perturbation expansion as well as in the Fredholm form of the solution, this mathematical requirement arises in a form of little practical interest. Consider first the Fredholm form. Equation (2.17) can be rewritten as

$$\mathbf{R}^b_b = (\mathbf{D}^{bb}/\nu\mathbf{D})\rho_b^b + (\mathbf{D}^{ba}/\mathbf{d}_{a'a}\mathbf{D})\rho_a^a, \quad (2.25)$$

where the bb term is separated out in the right-hand side ($a'a \neq bb$). Expanding \mathbf{D} by the bb row then gives

$$\mathbf{D} = \mathbf{D}^{bb} + (1/\nu)\mathbf{K}_{c_1b}^{bb_1}\mathbf{D}_{bb_1}^{c_1b}. \quad (2.26)$$

On the other hand, rewrite the $a'a$ row in place of the bb row. The resulting determinant is zero, so that on expanding it by the $a'a$ row

$$\mathbf{D}_{a'b}^{ba} + (1/\nu)\mathbf{K}_{c_1b}^{bb_1}\mathbf{D}_{a'b_1}^{c_1a} = 0. \quad (2.27)$$

The substituting \mathbf{D}_{bb}^{bb} and $\mathbf{D}_{a'b}^{ba}$ in (2.25) from (2.26) and (2.27), we obtain

$$\mathbf{R}^b_b = (1 - \mathbf{K}_{c_1b}^{bb_1}\mathbf{D}_{bb_1}^{c_1b}/\nu\mathbf{D})\rho_b^b/\nu - (\mathbf{K}_{c_1b}^{bb_1}\mathbf{D}_{a'b_1}^{c_1a}/\nu\mathbf{d}_{a'a}\mathbf{D})\rho_a^a \quad (2.28)$$

($a'a \neq bb$). A similar expression, written in perturbation series, can be derived upon performing the divisions by \mathbf{D}

$$\mathbf{R}^b_b = [1 - \langle bb|\mathbf{K}(\mathbf{I} + \mathbf{d}^{-1}\mathbf{K})^{-1}\mathbf{d}^{-1}|bb\rangle]\rho_b^b/\nu - \langle bb|\mathbf{K}(\mathbf{I} + \mathbf{d}^{-1}\mathbf{K})^{-1}\mathbf{d}^{-1}|a'a\rangle\rho_a^a/\nu. \quad (2.29)$$

Owing to the property (2.16), in further summing over b , the second and the third term in the right-hand side of (2.28) and (2.29) cancel each other out, since

$$\sum_{bb} (\mathbf{K}_{c_1b}^{bb_1}\mathbf{D}_{c_2b_1}^{c_1b_2}/\nu\mathbf{d}_{c_2b_2}\mathbf{D})\rho_{b_2}^{c_2} = 0,$$

which results in the trace conservation as

$$\sum_{bb} \mathbf{R}^b_b = (1/\nu) \sum_b \rho_b^b = 1/\nu.$$

If the total number of states in the system is sufficiently large, the long time limit of the last term in (2.28) or (2.29) should sum up to 1 in the trace, whereas the remaining terms in ρ_b^b should decrease toward zero, in accordance with the physically expected population transfer from initial to final states. This is not clearly visible on the Fredholm form, but was established with some assumptions by Van Hove (1955) in the iterative expansion case. Furthermore, as discussed in Fortini (1981), Fredholm expressions cannot be used in applications for they involve spurious terms without physical meaning in both numerators and denominators. Iterative expansions, on the other hand, involve divergent secular contributions which finally cancel in the trace, but render partial summations of little practical interest. We are going to see, in the next section, that the solution $\mathbf{R}(\nu)$ can be given a considerably improved form through a suitable extension of the 'reduction' procedure elaborated in Fortini (1981)

3. Reduced determinantal expressions of the density matrix solution

3.1. Reduction of the Fredholm solution

From (2.14a), \mathbf{R} is formally given by

$$|\mathbf{R}\rangle = (\mathbf{d} + \mathbf{K})^{-1}|\rho\rangle. \tag{3.1}$$

Assume, for simplicity, the system initially in a pure a state

$$|\rho\rangle = |aa\rangle.$$

Bearing in mind that the spirit of the reduction procedure consists in a reformulation of determinant expansions so as to emphasise the starting state, expression (3.1) of the solution will first be identically rewritten as

$$|\mathbf{R}\rangle = (\mathbf{d} + \mathbf{K})^{-1}(\mathbf{d} + \mathbf{K}Q_{aa})\mathbf{d}^{-1}|aa\rangle. \tag{3.2}$$

P_{aa} and $Q_{aa} = \mathbf{1} - P_{aa}$ denote the projector on the aa state, and the complementary projector, respectively. We have, equivalently,

$$(\mathbf{1} + \mathbf{d}^{-1}\mathbf{K}Q_{aa})^{-1}(\mathbf{1} + \mathbf{d}^{-1}\mathbf{K})|\mathbf{R}\rangle = \mathbf{d}^{-1}|aa\rangle. \tag{3.3}$$

Making use of the splitting

$$\mathbf{d}^{-1}\mathbf{K} = \mathbf{d}^{-1}\mathbf{K}Q_{aa} + \mathbf{d}^{-1}\mathbf{K}P_{aa},$$

this equation can also be written as

$$[\mathbf{1} + (\mathbf{1} + \mathbf{d}^{-1}\mathbf{K}Q_{aa})^{-1}\mathbf{d}^{-1}\mathbf{K}P_{aa}]|\mathbf{R}\rangle = \mathbf{d}^{-1}|aa\rangle. \tag{3.4}$$

The vector $|\mathbf{R}\rangle$ can now be regarded as the solution of the linear system defined by the operator on the left-hand member. Calculation of the related determinant and minors is straightforward (see Fortini (1981) Appendix A). We thus have

$$\begin{aligned} D &= \det[\mathbf{1} + (\mathbf{1} + \mathbf{d}^{-1}\mathbf{K}Q_{aa})^{-1}\mathbf{d}^{-1}\mathbf{K}P_{aa}], \\ &= 1 + \langle aa | (\mathbf{1} + \mathbf{d}^{-1}\mathbf{K}Q_{aa})^{-1}\mathbf{d}^{-1}\mathbf{K} | aa \rangle, \\ &= 1 + \langle aa | \mathbf{d}^{-1}\mathbf{K}(\mathbf{1} + Q_{aa}\mathbf{d}^{-1}\mathbf{K})^{-1} | aa \rangle, \end{aligned} \tag{3.5}$$

and, similarly, for the cb - aa minor

$$\begin{aligned} D_{ab}^{ca} &= -\langle cb | (\mathbf{1} + \mathbf{d}^{-1}\mathbf{K}Q_{aa})^{-1}\mathbf{d}^{-1}\mathbf{K} | aa \rangle, \\ &= -\langle cb | \mathbf{d}^{-1}\mathbf{K}(\mathbf{1} + Q_{aa}\mathbf{d}^{-1}\mathbf{K})^{-1} | aa \rangle. \end{aligned} \tag{3.6}$$

These expressions suggest the introduction of the S_{aa} operator defined by

$$S_{aa} = \mathbf{1} + Q_{aa}\mathbf{d}^{-1}\mathbf{K} \tag{3.7}$$

which only differs from the initial one, (2.14b), by the presence of the complementary projector Q_{aa} . Returning then to a general initial distribution (restricted to diagonal elements for simplicity), the \mathbf{R} -components will be written in the form

$$R_b^c = -\frac{\langle cb | \mathbf{d}^{-1}\mathbf{K}S_{aa}^{-1} | aa \rangle}{\nu + \langle aa | \mathbf{K}S_{aa}^{-1} | aa \rangle} \rho_a^a \tag{3.8}$$

for $c \neq b$, and

$$\mathbf{R}^b_b = \frac{\rho_b^b}{\nu + \langle bb | \mathbf{K} \mathbf{S}_{bb}^{-1} | bb \rangle} - \frac{\langle bb | \mathbf{d}^{-1} \mathbf{K} \mathbf{S}_{aa}^{-1} | aa \rangle}{\nu + \langle aa | \mathbf{K} \mathbf{S}_{aa}^{-1} | aa \rangle} \rho_a^a, \quad (3.9)$$

for any diagonal component bb ($bb \neq aa$ in the second term). Use has been made of $\mathbf{d}_{bb} = \mathbf{d}_{aa} = \nu$.

It is readily realised that a systematic way of obtaining (3.8) and (3.9) may consist in using the reduction procedure introduced in Fortini (1981). A simple comparison of equations (3.3) and (2.14*b*), rewritten for the same initial condition as

$$(\mathbf{1} + \mathbf{d}^{-1} \mathbf{K}) | \mathbf{R} \rangle = \sum_{aa} \mathbf{d}^{-1} \rho_a^a | aa \rangle, \quad (3.10)$$

shows, indeed, since

$$\det(\mathbf{1} + \mathbf{d}^{-1} \mathbf{K} \mathbf{Q}_{aa})^{-1} = (\mathbf{D}_{aa}^{aa})^{-1},$$

that

$$\mathbf{R}^c_b = (\mathbf{D}_{ab}^{ca} (\mathbf{D}_{aa}^{aa})^{-1} / \nu \mathbf{D} (\mathbf{D}_{aa}^{aa})^{-1}) \rho_a^a \quad (c \neq b), \quad (3.11)$$

and

$$\mathbf{R}^b_b = \frac{\rho_b^b}{\nu \mathbf{D} (\mathbf{D}_{bb}^{bb})^{-1}} + \frac{\mathbf{D}^{ba} (\mathbf{D}_{aa}^{aa})^{-1}}{\nu \mathbf{D} (\mathbf{D}_{aa}^{aa})^{-1}} \rho_a^a \quad (a \neq b), \quad (3.12)$$

where the symbol \mathbf{D} refers, here, to determinant and minors pertaining to (3.10). Carrying through the determinant divisions in (3.11) and (3.12) again gives the results (3.8) and (3.9). These can be further detailed by means of expansions in $\mathbf{d}^{-1} \mathbf{K}$. The second-order expression of \mathbf{R}^c_b , for instance, is written as follows

$$\mathbf{R}^c_b = \frac{-\mathbf{K}_{ab}^{ca} + \mathbf{K}_{c_1 b}^{c b_1} \mathbf{K}_{a b_1}^{c_1 a} / \mathbf{d}_{c_1 b_1} - \dots}{\mathbf{d}_{cb} (\mathbf{d}_{aa} - \mathbf{K}_{c_1 a}^{a b_1} \mathbf{K}_{a b_1}^{c_1 a} / \mathbf{d}_{c_1 b_1} + \dots)} \rho_a^a \quad (3.13)$$

with $c_1 b_1, c_2 b_2, \dots \neq aa$ in both the upper and the lower series.

It must be emphasised that the strategy of the reduction, at this stage, lies in the elimination of broadening terms starting from states other than the proper initial state a . The Fredholm forms (2.21) and (2.22), instead, involve broadening contributions starting from any intermediate state in the evolution of the system. This elimination proves particularly useful when further summations on intermediate states are required by the particular structure of the system spectrum, e.g. in the continuum limit.

3.2. Trace conservation

Intimately connected with the elimination of 'intermediate' contributions to broadening, is the quite important property possessed by the foregoing expressions satisfying the trace conservation requirement in a much more tractable form than the Fredholm-type results do. Consider the second term in (3.9); making use of the property (2.16), we have

$$- \sum_{bb \neq aa} \langle bb | \mathbf{d}^{-1} \mathbf{K} \mathbf{S}_{aa}^{-1} | aa \rangle = \frac{1}{\nu} \langle aa | \mathbf{K} \mathbf{S}_{aa}^{-1} | aa \rangle.$$

Hence

$$\text{Tr } R = \sum_{bb} R^b_b = \sum_b \frac{\rho_b^b}{\nu + \langle bb | \mathbf{KS}_{bb}^{-1} | bb \rangle} + \sum_a \frac{\langle aa | \mathbf{KS}_{aa}^{-1} | aa \rangle}{\nu + \langle aa | \mathbf{KS}_{aa}^{-1} | aa \rangle} \rho_a^a$$

and, since b is now a dummy index,

$$\text{Tr } R = \sum_a \frac{1 + \langle aa | \mathbf{KS}_{aa}^{-1} | aa \rangle}{\nu + \langle aa | \mathbf{KS}_{aa}^{-1} | aa \rangle} \rho_a^a = \sum_a \frac{\rho_a^a}{\nu} = \frac{1}{\nu}. \tag{3.14}$$

Unlike what occurs in (2.28) or (2.29), the instantaneous occupation probability of any state, (3.9) or (3.12), now pictures much more clearly the actual physical situation. Upon simple examination of the above expressions, it is quite obvious that the initial population of any b state decreases toward zero in increasing time, whereas the transition induced population in the same state tends toward some definite value. The overall final occupation probability, at once, tends toward unity. It must be emphasised, furthermore, that these properties are satisfied at any order, as could be shown by replacing the formal operator with their equivalent expansions. This is of considerable importance in applications, particularly in resonance phenomena.

3.3. Further reduction of the solution

Long-term values of expressions (3.8) and (3.9) often reduce to their numerators in a wide class of applications (long lifetime of excited states with regard to the predominant collision relaxation time), so that the iterative expansion is recovered, avoiding broadening effects. Direct calculation of (2.24), on the other hand, using reduced quantities for F matrix elements (this is possible in some cases) leads to more detailed expressions than (3.8) and (3.9). To get formulae of practical interest, immediately satisfying trace conservation, we thus have to take the reduction process one step further, as follows.

The matrix elements appearing in (3.8) and (3.9) can, in turn, be considered as the components of vectors \mathbf{X} which are solutions of the following type of matrix equations in the $\mathcal{E}_{H_0H_0}$ space

$$(\mathbf{1} + \mathbf{d}^{-1} \mathbf{K} \mathbf{Q}_{aa}) | \mathbf{X} \rangle = \mathbf{d}^{-1} \mathbf{K} | aa \rangle = \mathbf{K}_a^k \mathbf{d}^{-1} | ka \rangle - \mathbf{K}_k^a \mathbf{d}^{-1} | ak \rangle, \tag{3.15}$$

for the system initially in the a state. Thus

$$\langle cd | \mathbf{d}^{-1} \mathbf{K} \mathbf{S}_{aa}^{-1} | aa \rangle = \langle cb | \mathbf{X} \rangle = \mathbf{X}^c_b, \text{ etc. } \dots$$

Separating out the initial state ka (or ak) in the solution of (3.15), in the same way as in (3.2), leads to expressions of the \mathbf{X}^c_b similar to (3.8) and (3.11)

$$\mathbf{X}^c_b = \frac{\mathbf{D}_{kb}^{ca} (\mathbf{D}_{ka}^{ka})^{-1}}{\mathbf{d}_{ka} \mathbf{D} (\mathbf{D}_{ka}^{ka})^{-1}} \mathbf{K}_a^k - \frac{\mathbf{D}_{ab}^{ck} (\mathbf{D}_{ak}^{ak})^{-1}}{\mathbf{d}_{ak} \mathbf{D} (\mathbf{D}_{ak}^{ak})^{-1}} \mathbf{K}_k^a, \tag{3.16}$$

where the \mathbf{D} now pertain to the system (3.15). In the operational form

$$\mathbf{X}^c_b = - \frac{\langle cb | \mathbf{d}^{-1} \mathbf{K} \mathbf{S}_{aaka}^{-1} | ka \rangle}{\mathbf{d}_{ka} + \langle ka | \mathbf{K} \mathbf{S}_{aaka}^{-1} | ka \rangle} \mathbf{K}_a^k + \frac{\langle cb | \mathbf{d}^{-1} \mathbf{K} \mathbf{S}_{aaak}^{-1} | ak \rangle}{\mathbf{d}_{ak} + \langle ak | \mathbf{K} \mathbf{S}_{aaak}^{-1} | ak \rangle} \mathbf{K}_k^a, \tag{3.17}$$

with

$$\mathbf{S}_{aaka} = \mathbf{1} + \mathbf{Q}_{aa} \mathbf{Q}_{ka} \mathbf{d}^{-1} \mathbf{K}, \text{ etc. } \dots$$

The expressions (3.11) and (3.12) of R^c_b and R^b_b will be finally written, in the second reduction stage, as

$$R^c_b = -\frac{X^c_b(aa)}{\nu + X^a_a(aa)} \rho^a_a \tag{3.18}$$

($c \neq b$) and

$$R^b_b = \frac{\rho^b_b}{\nu + X^b_b(bb)} - \frac{X^b_b(aa)}{\nu + X^a_a(aa)} \rho^a_a \tag{3.19}$$

($a \neq b$). X 's matrix elements are assumed to be given by the solutions (3.16) or (3.17) of (3.15), the relevant initial state of which is recalled in a bracket. Subsequent practical formulae will next be obtained through expansion of the operational forms, as in (3.13). Trace conservation is again satisfied at any time, and any order. Proceeding as in § 3.2, we first have $-\sum_{bb \neq aa} \langle bb | d^{-1} K S^{-1}_{aaka} | ka \rangle = (1/\nu) \langle aa | K S^{-1}_{aaka} | ka \rangle$, whence $-\sum_{bb} X^b_b(aa) = (1/\nu) X^a_a(aa)$, and from (3.19)

$$\sum_{bb} R^b_b = \sum_{bb} \frac{\rho^b_b}{\nu + X^b_b(bb)} + \sum_{aa} \frac{X^a_a(aa)}{\nu [\nu + X^a_a(aa)]} \rho^a_a = \frac{1}{\nu} \sum_{aa} \rho^a_a.$$

Finally, the above determinantal expressions remain valid in the continuum limit where summations over dummy indices are replaced by integrations. Care must be taken, however, in allowing the number of states to become arbitrarily high, because we are not sure that the limit of any particular subset of the discrete sums is the same as the subset of the limit, as has already been discovered for the Fredholm solution in Fortini (1981). It is recommended, therefore, to pass to the continuum limit only after having performed all intermediate calculations on discrete summations. It will be appreciated, for example, that replacing every term in (3.19) with its limiting value preserves trace conservation.

Of course, the continuum limit can be considered in the calculation of the original function as well. As discussed in Fortini (1981), continuous parts of the spectrum then give rise to cuts in the ν plane. In practical applications, however, it is often sufficient to retain the steady-state value of the density matrix, which is obtained as $t \rightarrow \infty$. The latter is directly derived from the Laplace transform $R(\nu)$, by using the well known rule

$$\rho(t \rightarrow \infty) = \lim_{\nu \rightarrow +0} [\nu R(\nu)].$$

4. Application to a simple model

We reconsider the simple physical system already dealt with in Fortini (1981). The constant perturbation A which is switched on at $t = 0$, induces transitions from the initial pure state a into any state b, c, \dots which belong to a quasi-continuum. The collision potential is zero (or included in the definition of H_0). The Hamiltonian is written as

$$H = H_0 + AY(t), \tag{4.1}$$

so that

$$K = i\hbar^{-1}A, \quad \mathbf{K} = i\hbar^{-1}(A\delta - \delta A). \tag{4.2}$$

It is easy to write down second-order expressions of the density matrix elements as a simple application of the above formulae. Let us first consider the reduced form (3.8) of any element $R^c_b (c \neq b)$

$$\begin{aligned}
 R^c_b &= \frac{\langle cb | d^{-1} K Q_{aa} d^{-1} K | aa \rangle}{\nu - \langle aa | K Q_{aa} d^{-1} K | aa \rangle} \\
 &= - \frac{d_{cb}^{-1} \hbar^{-2} (A_{c_1}^c \delta_b^{b_1} - \delta_{c_1}^c A_b^{b_1}) d_{c_1 b_1}^{-1} (A_a^{c_1} \delta_{b_1}^a - \delta_a^{c_1} A_{b_1}^a)}{\nu + \hbar^{-2} (A_{c_1}^a \delta_a^{b_1} - \delta_{c_1}^a A_a^{b_1}) d_{c_1 b_1}^{-1} (A_a^{c_1} \delta_{b_1}^a - \delta_a^{c_1} A_{b_1}^a)} \\
 &= \frac{\hbar^{-2} A_a^c A_b^a}{\nu + i\omega_{cb}} \frac{(\nu + i\omega_{ca})^{-1} + (\nu + i\omega_{ab})^{-1}}{\nu + (|A_a^k|^2 / \hbar^2) [(\nu + i\omega_{ka})^{-1} + (\nu + i\omega_{ak})^{-1}]} \tag{4.3}
 \end{aligned}$$

This expression also applies to the diagonal element $R^b_b (b \neq a)$, with $c = b$. As to the diagonal element R^a_a which represents the occupation probability of the initial state, we get from (3.9)

$$\begin{aligned}
 R^a_a &= (\nu - \langle aa | K Q_{aa} d^{-1} K | aa \rangle)^{-1} \\
 &= \left[\nu + \frac{|A_a^k|^2}{\hbar^2} \left(\frac{1}{\nu + i\omega_{ka}} + \frac{1}{\nu + i\omega_{ak}} \right) \right]^{-1} \tag{4.4}
 \end{aligned}$$

Equations (4.3) and (4.4) lead to the following second-order expression of the trace

$$\begin{aligned}
 \text{Tr } R &= \left[\nu + \frac{|A_a^k|^2}{\hbar^2} \left(\frac{1}{\nu + i\omega_{ka}} + \frac{1}{\nu + i\omega_{ak}} \right) \right]^{-1} \\
 &+ \sum_b \frac{(|A_a^b|^2 / \hbar^2) [(\nu + i\omega_{ba})^{-1} + (\nu + i\omega_{ab})^{-1}]}{\nu \{ \nu + (|A_a^k|^2 / \hbar^2) [(\nu + i\omega_{ka})^{-1} + (\nu + i\omega_{ak})^{-1}] \}} = \frac{1}{\nu} \tag{4.5}
 \end{aligned}$$

in accordance with the trace conservation requirement, (3.14).

Direct convolution of $F_a^c(\nu)$ and $F_b^{+a}(\nu)$, initially derived in Fortini (1981), leads to more involved expressions than (4.3) and (4.4). The latter will be recovered by using the reduced forms given in (3.18) and (3.19), with the help of the operational expression (3.17) of the relevant determinant ratios. From (3.18):

$$R^c_b = \frac{[i\hbar^{-1} \langle cb | d^{-1} K S_{aaka}^{-1} | ka \rangle A_a^k / (d_{ka} + \langle ka | K S_{aaka}^{-1} | ka \rangle)] - [i\hbar^{-1} \langle cb | d^{-1} K S_{aaak}^{-1} | ak \rangle A_a^k / (d_{ak} + \langle ak | K S_{aaak}^{-1} | ak \rangle)]}{\nu - [i\hbar^{-1} \langle aa | K S_{aala}^{-1} | la \rangle A_a^l / (d_{la} + \langle la | K S_{aala}^{-1} | la \rangle)] + [i\hbar^{-1} \langle aa | K S_{aaal}^{-1} | al \rangle A_a^l / (d_{al} + \langle al | K S_{aaal}^{-1} | al \rangle)]} \tag{4.6}$$

We then have to second order in A

$$\begin{aligned}
 i\hbar^{-1} \langle cb | d^{-1} K S_{aaka}^{-1} | ka \rangle A_a^k &= -\hbar^{-2} d_{cb}^{-1} (A_c^c \delta_b^a - \delta_c^c A_b^a) A_a^k \\
 &= (A_b^a A_a^c / \hbar^2 d_{cb}) \delta_c^c.
 \end{aligned}$$

Similarly

$$i\hbar^{-1} \langle cb | d^{-1} K S_{aaak}^{-1} | ak \rangle A_a^k = -(A_a^c A_b^a / \hbar^2 d_{cb}) \delta_b^k.$$

Consider, next, the bracket in ka

$$\begin{aligned}
 \langle ka | K S_{aaka}^{-1} | ka \rangle &= \hbar^{-2} (A_{c_1}^k \delta_a^{b_1} - \delta_{c_1}^k A_a^{b_1}) d_{c_1 b_1}^{-1} (A_{c_1}^{c_1} \delta_{b_1}^a - \delta_{c_1}^{c_1} A_{b_1}^a) \\
 &= |A_k^m|^2 / \hbar^2 d_{ma} + |A_a^m|^2 / \hbar^2 d_{km}.
 \end{aligned}$$

The first term on the right drops out since it is assumed that no transition can occur from any k state of the final continuum. The similar bracket in ak , in (4.6), is simply the conjugate of the previous one. In the denominator, we calculate one of the two conjugate terms

$$\begin{aligned} i\hbar^{-1}\langle aa|\mathbf{KS}_{aa}^{-1}|aa\rangle A_a^l &= -\hbar^{-2}(A_l^a\delta_a^a - \delta_l^a A_a^a)A_a^l \\ &= -|A_a^l|^2/\hbar^2. \end{aligned}$$

We finally obtain the second-order expression of \mathbf{R}^c_b as

$$\mathbf{R}^c_b = \frac{\hbar^{-2}A_a^c A_b^a}{\nu + i\omega_{cb}} \frac{[\nu + i\omega_{ca} + (\hbar^{-2}|A_a^m|^2/(\nu + i\omega_{cm}))]^{-1} + [\nu + i\omega_{ab} + (\hbar^{-2}|A_a^m|^2/(\nu + i\omega_{mb}))]^{-1}}{\nu + \hbar^{-2}|A_a^l|^2/[\nu + i\omega_{la} + (\hbar^{-2}|A_a^m|^2/(\nu + i\omega_{lm}))] + \hbar^{-2}|A_a^l|^2/[\nu + i\omega_{al} + (\hbar^{-2}|A_a^m|^2/(\nu + i\omega_{ml}))]}, \tag{4.7}$$

and for the initial state occupation

$$\mathbf{R}^a_a = \left(\nu + \frac{\hbar^{-2}|A_a^l|^2}{\nu + i\omega_{la} + \hbar^{-2}|A_a^m|^2/(\nu + i\omega_{lm})} + \frac{\hbar^{-2}|A_a^l|^2}{\nu + i\omega_{al} + \hbar^{-2}|A_a^m|^2/(\nu + i\omega_{ml})} \right)^{-1}. \tag{4.8}$$

Trace conservation is evident in equations (4.7) and (4.8)

$$\mathbf{R}^a_a + \sum_{b \neq a} \mathbf{R}^b_b = 1/\nu. \tag{4.9}$$

The calculation can be pushed further if we assume that the A matrix elements are constant in the relevant spectral range (ω_1, ω_2) which is, in fact, confined to final states of energy close to ω_a . We will take

$$\omega_b \approx \omega_c \approx \omega_a.$$

If, in addition, the density of states $\theta(\omega)$ is slowly varying in that range, the function $\theta(\omega)$ can be averaged to a constant value taken out of integrations. Consider, therefore, the second-order complex transition widths appearing in (4.7) and (4.8). A term such as $\hbar^{-2}|A_a^m|^2/(\nu + i\omega_{mb})$, where summation over m is implied, is approximately given by the following integral

$$\sum_m \frac{\hbar^{-2}|A_a^m|^2}{\nu + i\omega_{mb}} \cong \frac{|A|^2\theta_b}{\hbar^2} \int_{\omega_1}^{\omega_2} \frac{d\omega_m}{\nu + i\omega_{mb}} = -i \frac{|A|^2\theta_b}{\hbar^2} - \ln \frac{\nu + i\omega_{2b}}{\nu + i\omega_{1b}},$$

which takes the following value along each side of the cut ($-i\omega_2, -i\omega_1$) (see figure 1(a))

$$-i \frac{|A|^2\theta_b}{\hbar^2} \left(\ln \left| \frac{\eta + \omega_{2b}}{\eta + \omega_{1b}} \right| \pm i\pi \right) \cong -i\beta_b \pm \gamma_b,$$

where

$$\gamma_b = \pi|A|^2\theta_b/\hbar^2, \tag{4.10}$$

$$\beta_b = \frac{\gamma_b}{\pi} \ln \left| \frac{\eta + \omega_{2b}}{\eta + \omega_{1b}} \right|, \tag{4.11a}$$

and the sign before γ_b is + or - according to whether the cut is approached from the right- or left-hand side.

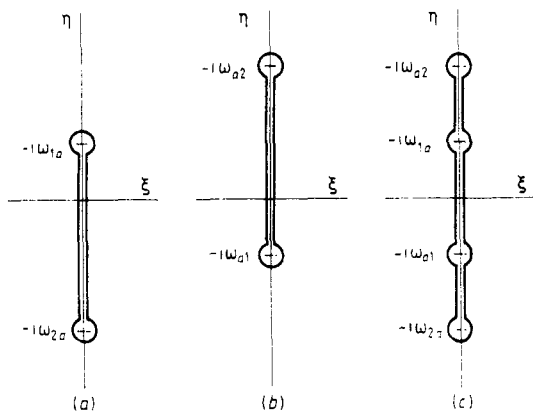


Figure 1. Cuts in the complex $\nu(\xi, \eta)$ plane used for calculating the complex transition width (a, b), and the original (c) of the density matrix Laplace transform in the simplified model.

As the natural logarithm in β_b is a smooth function of η , and, in addition, $\eta \approx 0$ owing to energy conservation, we will take β_b as a constant

$$\beta_b \cong (\gamma_b/\pi) \ln |\omega_{2b}/\omega_{1b}|. \tag{4.11b}$$

Proceeding the same way (figure 1(b)), we then have

$$\begin{aligned} \sum_c \frac{\hbar^{-2}|A_a^m|^2}{\nu + i\omega_{cm}} &= i \frac{|A|^2\theta_c}{\hbar^2} \ln \frac{\nu + i\omega_{c2}}{\nu + i\omega_{c1}} \\ &= i \frac{|A|^2\theta_c}{\hbar^2} \left(\ln \left| \frac{\eta + i\omega_{c2}}{\eta + i\omega_{c1}} \right| \mp i\pi \right) \cong i\beta_c \pm \gamma_c. \end{aligned}$$

Because the energy of the relevant c, b, l, m states is close to $\hbar\omega_a$, to within the transition width, the constants β and γ have nearly the same value in all complex linewidths appearing in (4.7) and (4.8). Moreover, inasmuch as the energy range of interest (ω_1, ω_2) is sufficiently larger than the β, γ , the remaining integrations over l in the denominator are given by

$$\int_{\omega_1}^{\omega_2} \frac{\hbar^{-2}|A_a^l|^2\theta_a d\omega_l}{\nu + i(\omega_{la} + \beta_l) \pm \gamma_l} \cong \frac{|A|^2\theta_a}{\hbar^2} \ln \frac{\nu + i(\omega_{2a} + \beta_l) \pm \gamma_l}{\nu + i(\omega_{1a} + \beta_l) \pm \gamma_l} \cong i\beta_a + \gamma_a$$

and a conjugate term. We finally obtain the following approximate expressions of R_b^c and R_a^c , when ν lies along the cut ($\nu = i\eta$)

$$R_b^c(i\eta) = \frac{\hbar^{-2}A_a^c A_b^a}{i(\eta + \omega_{cb})} \frac{1}{i(\eta + 2\gamma_a)} \left(\frac{1}{i(\eta + \omega_{ca} + \beta_a) \pm \gamma_a} + \frac{1}{i(\eta + \omega_{ab} - \beta_a) \pm \gamma_a} \right), \tag{4.12}$$

$$R_a^c(i\eta) = (i\eta \pm 2\gamma_a)^{-1}. \tag{4.13}$$

Calculation of the time-dependent original functions is elementary. From (4.13)

$$\rho_a^c(t) = \exp(-2\gamma_a t), \tag{4.14}$$

and the case of $R_b^c(\nu)$ can be treated using the same method as in previous publications (Fortini 1979, 1981). The result is as follows

$$\rho_b^c(t) = U_a^c(t)U_b^{+a}(t), \quad (4.15)$$

with

$$U_a^c(t) = \frac{A_a^c}{\hbar} e^{-i\omega_c t} \frac{\exp[i(\omega_{ca} + \beta_a)t - \gamma_a t] - 1}{i(\omega_{ca} + \beta_a) - \gamma_a},$$

and a related expression for $U_b^{+a}(t)$.

We have therefore reconstructed the product of the corresponding solutions of the evolution operator previously given in Fortini (1981). This is not at all surprising, but it must be pointed out that the result is obtained by using the detailed reduced form, (4.7), instead of the first one, (4.3).

From (4.15) the current diagonal element is written as

$$\rho_b^b(t) = \frac{|A_a^b|^2}{\hbar^2} \frac{e^{-2\gamma_a t} - 2e^{-\gamma_a t} \cos(\omega_{ba} + \beta_a)t + 1}{(\omega_{ba} + \beta_a)^2 + \gamma_a^2}$$

which is formally identical with the result (24) of Fortini (1979), and leads, with (4.14), to the trace conservation at any time of the second-order determinantal solution

$$\rho_a^a(t) + \sum_{b \neq a} \rho_b^b(t) = 1.$$

This is the original of equation (4.9). The latter, however, is valid far beyond the simplifying assumptions of the present application.

5. Conclusion

By means of an appropriate definition of the commutation kernel in the pair-of-states representation, we have been able to formulate a determinantal solution of the density matrix time-dependent problem, derived from the initial solution of the Laplace transformed Schrödinger equation, in the case of constant external perturbation. An elementary mathematical presentation has been used throughout, allowing a transparent monitoring of the trace conservation theorem at any time and any order of the kernel, even in the continuum limit. Practical methods for calculating explicit expressions of the response, in increasing orders, have been given. Although the illustration is restricted here to a simple model, the determinantal formalism is likely to be relevant in a wide range of physical situations.

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