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## Resolvent operator theory of sequential quantum processes

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**Abstract.** The Mower sequential decay theory of quantum processes has been extended in order formally to remove certain spurious poles in the matrix elements of the resolvent operator, and to recast the results into a more symmetrical general form. A special choice of intermediate manifolds of states leads to a further simplification. An illustrative application of the theory is given.

### 1. Introduction

The resolvent operator method has been widely used to treat time-dependent processes in atomic and molecular physics (Lambropoulos 1976, Freed 1977, Kay 1978, Mukamel and Jortner 1976, Bardsley and Mandl 1968, Smith 1966), in nuclear physics (Feshbach 1962) and in quantum optics (Cohen-Tannoudji 1975, Agarwal 1974, Kroll 1964).

The resolvent operator formalism (Goldberger and Watson 1964) allows the calculation of the probability amplitude  $I_{ba}(t)$  for finding the quantum-mechanical system in some final state  $|b\rangle$  at time  $t$ , given that at time  $t = 0$  it was in an initial state  $|a\rangle$ . This involves the matrix elements  $\langle b|G(z)|a\rangle$  of the resolvent operator  $G(z) = (z - H)^{-1}$ , where  $H$  is the time-independent Hamiltonian for the system. Thus

$$I_{ba}(t) = \frac{1}{2\pi i} \int_c dz e^{-izt/\hbar} \langle b|G(z)|a\rangle \quad t \geq 0 \quad (1)$$

where  $c$  is the usual contour in the complex  $z$  plane just above the real axis, that goes from  $+\infty$  to  $-\infty$ .

The basic approach in the application of the method is to develop good approximate forms which exhibit all the significant  $z$  variation of  $\langle b|G(z)|a\rangle$  and which enable the contour integral in (1) to be evaluated.

Mower (1966, 1968) developed a general approach using projection operators (Messiah 1964) to treat this problem, extending earlier work by Feshbach (1962) and Goldberger and Watson (1964). The Hamiltonian  $H$  is written as  $K + V$ , where  $|a\rangle, |b\rangle$  are eigenstates of  $K$  (or linear combinations of physically similar eigenstates of  $K$ ) and  $V$  is the interaction causing transitions to occur.

In his second paper Mower dealt with a general case where the quantum system passes through various intermediate states en route to the final state of interest,  $|b\rangle$ . To treat this case, the eigenstates of  $K$  are divided up into sets, each set containing states that play a physically similar role during the overall quantum process. Each set of

eigenstates of  $K$  defines a linear vector space or manifold orthogonal to that associated with any of the other sets. In each such linear vector space a projector is determined yielding the set  $\Lambda_0, \Lambda_1, \Lambda_2, \dots, \Lambda_i, \dots$ .  $\Lambda_0$  is the projector associated with the manifold containing the initial state  $|a\rangle$ ,  $\Lambda_1, \Lambda_2, \dots, \Lambda_{i-1}$  are those for various intermediate manifolds,  $\Lambda_i$  refers to the manifold containing the final state  $|b\rangle$  of interest.

The projectors so determined thus obey

$$\Lambda_j \Lambda_k = \delta_{jk} \Lambda_j \quad j, k = 0, 1, 2, \dots \quad (2)$$

$$\Lambda_j K = K \Lambda_j \quad (3)$$

Other complementary projectors  $Q_0, Q_1, \dots, Q_i$  are introduced via

$$\begin{aligned} Q_0 &= 1 - \Lambda_0 \\ Q_1 &= 1 - \Lambda_0 - \Lambda_1 \\ &\vdots \\ Q_i &= 1 - \sum_{j=0}^i \Lambda_j \end{aligned} \quad (4)$$

Mower did not need to specify the detailed way in which the  $\Lambda_j$  are to be chosen, provided (2) and (3) are satisfied. However, the choice of the manifolds of states that determine the  $\Lambda_j$  must be physically appropriate to the process of interest in order to fulfil the aim of making the  $z$  dependence of  $\langle b|G(z)|a\rangle$  as explicit as possible. One special way of choosing the  $\Lambda_j$  which leads to a very simple result in many cases is outlined in § 3; for the present we restrict ourselves to Mower's general choice.

Since  $\langle b|G(z)|a\rangle = \langle b|\Lambda_i G(z)\Lambda_0|a\rangle$  it is important to consider the quantity  $\Lambda_i G(z)\Lambda_0$  where  $i = 1, 2, \dots$  for transitions to states outside the initial manifold of states, and  $i = 0$  for transitions within the initial manifold.

In his second paper, Mower obtained the following results (his equations (10b) and (30)):

$$\Lambda_0 G(z)\Lambda_0 = \Lambda_0 G^0(z)\Lambda_0 \quad i = 0 \quad (5a)$$

$$\begin{aligned} \Lambda_i G(z)\Lambda_0 &= \Lambda_i (z - \Lambda_i K \Lambda_i)^{-1} \Lambda_i R^i(z) \\ &\times \prod_{j=1}^i (1 + \Lambda_j G^j(z)\Lambda_j \Lambda_j R^j(z)) \Lambda_0 G^0(z)\Lambda_0 \quad i \geq 1 \end{aligned} \quad (5b)$$

where in the last equation the factors in the product are ordered  $j = i, i-1, \dots, 2, 1$  from left to right.

The  $R^j(z)$  are the generalised level shift operators

$$\begin{aligned} R^j(z) &= V + V Q_j (z - Q_j H Q_j)^{-1} Q_j V \\ &= V + V Q_j (z - Q_j K Q_j)^{-1} Q_j R^j(z) \quad j = 0, 1, \dots \end{aligned} \quad (6)$$

and the quantities  $\Lambda_j G^j(z)\Lambda_j$  are the reduced resolvent operators

$$\Lambda_j G^j(z)\Lambda_j = \Lambda_j (z - K - \Lambda_j R^j(z)\Lambda_j)^{-1} \Lambda_j \quad (7)$$

The result (5b) is obtained from Mower's earlier paper by use of the important relationship

$$R^{i-1}(z) = R^i(z) + R^i(z)\Lambda_j G^j(z)\Lambda_j R^i(z) \quad j = 1, 2, \dots \quad (8)$$

The problem with the form (5b) is that it seems to imply that  $\langle b|G(z)|a\rangle$  will have a pole on the real axis, associated with the eigenvalue  $z = E_b$ . In the case where the level state  $|b\rangle$  is stable, and no further transitions occur to states in the manifold given by  $Q_i$ , this would be correct. However, as Mower himself pointed out, the state  $|b\rangle$  may itself be unstable, in which case the pole at  $E_b$  is spurious. It would then be necessary to remove this artificial pole in the details of the application of the formula (5b) to the specific problem.

## 2. Modification of Mower's results for $\Lambda_i G(z) \Lambda_0$ : formal removal of spurious poles

It turns out that (5b) can be recast into a more satisfactory form in which no spurious pole can arise. The result is also of a far more symmetrical form than (5b).

Consider the factor  $\Lambda_i R^i (1 + \Lambda_i G^i \Lambda_i \Lambda_i R^i)$  in (5b) which occurs via the  $j = i$  term in the product and the factor next on its left. We have, using the definition of  $\Lambda_i G^i \Lambda_i$ :

$$\begin{aligned} \Lambda_i R^i (1 + \Lambda_i G^i \Lambda_i \Lambda_i R^i) &= \Lambda_i (\Lambda_i + \Lambda_i R^i \Lambda_i \Lambda_i G^i \Lambda_i) \Lambda_i R^i \\ &= \Lambda_i [\Lambda_i (z - \Lambda_i K \Lambda_i - \Lambda_i R^i \Lambda_i) \Lambda_i G^i \Lambda_i + \Lambda_i R^i \Lambda_i \Lambda_i G^i \Lambda_i] \Lambda_i R^i \\ &= \Lambda_i (z - \Lambda_i K \Lambda_i) \Lambda_i \Lambda_i G^i \Lambda_i \Lambda_i R^i. \end{aligned}$$

Hence

$$\Lambda_i (z - \Lambda_i K \Lambda_i)^{-1} \Lambda_i R^i (1 + \Lambda_i G^i \Lambda_i \Lambda_i R^i) = \Lambda_i G^i \Lambda_i \Lambda_i R^i. \quad (9)$$

Substituting this result back into (5b) we then obtain

$$\Lambda_i G(z) \Lambda_0 = \Lambda_i G^i(z) \Lambda_i \Lambda_i R^i(z) \prod_{j=1}^{i-1} (1 + \Lambda_j G^j(z) \Lambda_j \Lambda_j R^j(z)) \Lambda_0 G^0(z) \Lambda_0. \quad (10)$$

In particular:

$$\Lambda_1 G(z) \Lambda_0 = \Lambda_1 G^1 \Lambda_1 \Lambda_1 R^1 \Lambda_0 \Lambda_0 G^0 \Lambda_0 \quad (11a)$$

$$\begin{aligned} \Lambda_2 G(z) \Lambda_0 &= \Lambda_2 G^2 \Lambda_2 \Lambda_2 R^2 \Lambda_0 \Lambda_0 G^0 \Lambda_0 \\ &\quad + \Lambda_2 G^2 \Lambda_2 \Lambda_2 R^2 \Lambda_1 \Lambda_1 G^1 \Lambda_1 \Lambda_1 R^1 \Lambda_0 \Lambda_0 G^0 \Lambda_0. \end{aligned} \quad (11b)$$

Defining a path from 0 to  $i$  to be specified by a sequence of numbers  $i, j, k, \dots, 0$  such that

$$i > j > k > \dots > 0$$

we see that the result (10) can be put in an interesting form from which  $\langle b|G(z)|a\rangle$  can be determined. This form also applies to  $i = 0$  (see (11a)).

$$\Lambda_i G(z) \Lambda_0 = \sum_{\substack{\text{paths} \\ \{i, j, \dots, 0\}}} \Lambda_i G^i(z) \Lambda_i \Lambda_i R^i \Lambda_j \Lambda_j G^j(z) \Lambda_j \dots \Lambda_0 G^0(z) \Lambda_0 \quad i = 0, 1, \dots \quad (12)$$

The result for  $i = 2$  given above involves a contribution from a direct path  $\{2, 0\}$  and an indirect path  $\{2, 1, 0\}$ .

Also we notice that the left-hand factor in  $\Lambda_i G(z) \Lambda_0$  is now  $\Lambda_i G^i(z) \Lambda_i$ . In general then  $\langle b | G(z) | a \rangle$  (or more precisely, its analytic continuation from the upper half-plane into the second Riemann sheet) will have poles below the real axis, thereby removing any spurious poles. In the case where the states in  $\Lambda_i$  are subject to no further transitions,  $\Lambda_i G^i \Lambda_i$  reduces to  $\Lambda_i (z - K)^{-1} \Lambda_i$  and the non-spurious pole on the real axis at  $E_b$  leads to oscillating factors  $e^{-iE_b t/\hbar}$  in the probability amplitude  $I_{ba}(t)$ .

### 3. Further simplification for $\Lambda_i G(z) \Lambda_0$ due to special choice of $\Lambda_i$

A further simplification occurs if we choose the manifolds so that matrix elements of  $V$  are only non-zero between states in successive manifolds or between states within one manifold.

The precise method by which the successive manifolds are chosen is as follows.

(a) The initial manifold is a linear vector space, defining projector  $\Lambda_0$ , consisting of all physically equivalent eigenstates of  $K$ , plus all their linear combinations and which must include the initial state  $|a\rangle$ . With this choice of initial manifold  $\Lambda_0 K = K \Lambda_0$ .

(b) Operating with  $V$  on the states in the initial manifold yields a vector space, in which certain of the eigenstates of  $K$  form an orthogonal basis. Excluding those eigenstates of  $K$  already included in the initial manifold we obtain the basis for the second manifold. This defines the projector  $\Lambda_1$ .

(c) Operating with  $V$  on the states of the second manifold yields another vector space, again in which certain of the eigenstates of  $K$  form an orthogonal basis. Excluding those already included in the first two manifolds we obtain the basis for the third manifold, which defines the projector  $\Lambda_2$ .

(d) The process is continued as long as necessary. The  $(j+1)$ th manifold is spanned by such eigenstates of  $K$  not already included in the  $j$ th or  $(j-1)$ th manifolds. By the construction process, the matrix elements of  $V$  are only non-zero between states in successive manifolds or within the same manifold.

Depending on the system under consideration, a stage may be reached at which further repetition of the process of operating with  $V$  yields only states already included in previous manifolds. If this is the case the sequence of projector operators will terminate. Otherwise the sequence will continue indefinitely.

With this choice of manifolds we then have

$$\Lambda_j V \Lambda_k = 0 \quad \text{if } j \neq k-1, k, k+1 \quad (13a)$$

$$Q_j V \Lambda_k = 0 \quad \text{if } j \geq k+1. \quad (13b)$$

It is then easily shown that for a typical  $j > k$  term that occurs in (12)

$$\begin{aligned} \Lambda_j R^j(z) \Lambda_k &= \Lambda_j V \Lambda_{j-1} & \text{for } k = j-1 \\ &= 0 & \text{otherwise.} \end{aligned} \quad (14)$$

Expression (12) then reduces to a contribution from the single path  $\{i, i-1, i-2, \dots, 2, 1, 0\}$

$$\Lambda_i G(z) \Lambda_0 = \Lambda_i G^i \Lambda_i \Lambda_i V \Lambda_{i-1} \Lambda_{i-1} G^{i-1} \Lambda_{i-1} \dots \Lambda_1 G^1 \Lambda_1 \Lambda_1 V \Lambda_0 \Lambda_0 G^0 \Lambda_0 \quad (15)$$

which is obviously a valuable simplification.

It should be pointed out, however, that it is not always desirable to choose the projectors in accordance with (13). For example,  $V$  may consist of a large term  $V_1$  and a small term  $V_2$ . If  $V_2$  causes transitions in first order between different types of states than does  $V_1$  it may be better to define  $\Lambda_1, \Lambda_2, \dots$ , using the method described above, but with  $V_1$  as the interaction rather than  $V$ . This would lead to simpler manifolds containing fewer types of states. In this situation (15) would no longer apply and the general result (12) would have to be used. Nevertheless, the direct path  $\{i, i-1, \dots, 1, 0\}$  would still give the dominant contribution, with other paths contributing smaller corrections due to  $V_2$ .

#### 4. Continued fraction expression for $\Lambda_j R^j(z) \Lambda_j$

In evaluating the  $\Lambda_j G^j(z) \Lambda_j$  we obviously need to determine  $\Lambda_j R^j \Lambda_j$ . In the case where we have chosen the manifolds to conform to (13) this quantity  $\Lambda_j R^j \Lambda_j$  can be evaluated as a continued fraction by making use of the result (8):

$$\begin{aligned} \Lambda_j R^j \Lambda_j &= \Lambda_j V \Lambda_j + \Lambda_j V \Lambda_{j+1} \left( \frac{1}{z - K - \Lambda_{j+1} R^{j+1} \Lambda_{j+1}} \right) \Lambda_{j+1} V \Lambda_j \\ &= \Lambda_j V \Lambda_j + \Lambda_j V \Lambda_{j+1} \\ &\quad \times \left( \frac{1}{z - K - \Lambda_{j+1} V \Lambda_{j+1} - \Lambda_{j+1} V \Lambda_{j+2} \left( \frac{1}{z - K - \Lambda_{j+2} R^{j+2} \Lambda_{j+2}} \right) \Lambda_{j+2} V \Lambda_{j+1}} \right) \\ &\quad \times \Lambda_{j+1} V \Lambda_j \end{aligned} \quad (16)$$

etc. where, in order to highlight the continued fraction form of the expression, operators of the form  $A^{-1}$  have been written as  $1/A$ .

Swain (1975) has obtained a continued fraction expression for the natural width and shift of an excited atomic state, using a somewhat similar method.

#### 5. Illustrative application

As an example illustrating the simplification described in § 3 we consider the case in quantum optics of a harmonic oscillator coupled to the radiation field.

In the rotating wave approximation

$$V = \sum_{m=0}^{\infty} i g_{m\lambda} (|m+1\rangle \langle m| a_\lambda - |m\rangle \langle m+1| a_\lambda^\dagger) \quad (17)$$

where  $|m\rangle$  are the harmonic oscillator states,  $a_\lambda, a_\lambda^\dagger$  are the annihilation and creation operators for the radiation field and  $g_{m\lambda}$  is a real coupling constant, proportional to the dipole matrix element between the states  $|m\rangle, |m+1\rangle$ . Thus in first order  $V$  allows for transitions from the  $m$  to the  $m+1$  harmonic oscillator states accompanied by the absorption of one photon, and transitions from the  $m+1$  to the  $m$  harmonic oscillator states accompanied by the emission of one photon.

Consider a process beginning with the state  $|a\rangle = |n\rangle|0_\lambda\rangle$ . With the notation  $|n; 0_\lambda\rangle = |n\rangle|0_\lambda\rangle$ ,  $|n-1; 1_\xi\rangle = |n-1\rangle|1_\xi\rangle$ , etc, the successive projectors are:

$$\begin{aligned}\Lambda_0 &= |n; 0_\lambda\rangle\langle n; 0_\lambda| \\ \Lambda_1 &= \sum_{\xi} |n-1; 1_\xi\rangle\langle n-1; 1_\xi| \\ \Lambda_2 &= \sum_{\xi\theta} |n-2; 1_\xi 1_\theta\rangle\langle n-2; 1_\xi 1_\theta|\end{aligned}\tag{18}$$

etc.

Suppose we wish to calculate the probability amplitude  $I_{n-1, \xi; n}(t)$  for finding the system in the state  $|n-1; 1_\xi\rangle$ . The relevant matrix element is, from (15):

$$\begin{aligned}\langle n-1; 1_\xi | \Lambda_1 G(z) \Lambda_0 | n; 0_\lambda \rangle \\ = \sum_{\xi'} \langle n-1; 1_\xi | \Lambda_1 G^1(z) \Lambda_1 | n-1; 1_{\xi'} \rangle \langle n-1; 1_{\xi'} | \Lambda_1 V \Lambda_0 | n; 0_\lambda \rangle \\ \times \langle n; 0_\lambda | \Lambda_0 G^0(z) \Lambda_0 | n; 0_\lambda \rangle.\end{aligned}\tag{19}$$

To determine the reduced resolvent operator matrix elements we first determine the matrix elements of the level shift operators. We have, from (6), correct to second order:

$$\begin{aligned}\langle n; 0_\lambda | \Lambda_0 R^0(z) \Lambda_0 | n; 0_\lambda \rangle \\ \doteq \langle n; 0_\lambda | V \Lambda_1 (z - K)^{-1} \Lambda_1 V | n; 0_\lambda \rangle \\ \doteq \sum_{\theta} \frac{\langle n; 0_\lambda | V | n-1; 1_\theta \rangle \langle n-1; 1_\theta | V | n; 0_\lambda \rangle}{z - \hbar\omega(n-1+\frac{1}{2}) - \hbar\omega_\theta} \\ \doteq \sum_{\theta} \frac{g_{n-1\theta}^2}{z - \hbar\omega(n-\frac{1}{2}) - \hbar\omega_\theta}.\end{aligned}$$

As  $z = x + i\epsilon$  ( $x$  real,  $\epsilon > 0$  small) is restricted to contour  $c$  and the matrix element  $\langle n; 0_\lambda | \Lambda_0 G^0(z) \Lambda_0 | n; 0_\lambda \rangle$  will be largest near  $z = \hbar\omega(n+\frac{1}{2}) + i\epsilon$ , we can replace  $\langle n; 0_\lambda | \Lambda_0 R^0(z) \Lambda_0 | n; 0_\lambda \rangle$  by its value obtained from the last expression with  $z = \hbar\omega(n+\frac{1}{2}) + i\epsilon$ . This procedure is essentially equivalent to the more rigorous determination of the poles of  $\langle n; 0_\lambda | \Lambda_0 G^0(z) \Lambda_0 | n; 0_\lambda \rangle$  in the second Riemann sheet via analytic continuation (Mower 1966).

Hence

$$\langle n; 0_\lambda | \Lambda_0 R^0(z) \Lambda_0 | n; 0_\lambda \rangle \doteq -\frac{1}{2}i\hbar\Gamma_n\tag{20}$$

where, as usual, the level shift has been ignored and  $\Gamma_n$  is the lifetime width of the  $n$ th harmonic oscillator level (independent of  $z$ ). A similar procedure is followed for  $\langle n-1; 1_\xi | \Lambda_1 R^1(z) \Lambda_1 | n-1; 1_\xi \rangle$ :

$$\begin{aligned}\langle n-1; 1_\xi | \Lambda_1 R^1(z) \Lambda_1 | n-1; 1_\xi \rangle \\ \doteq \delta_{\xi\xi'} \sum_{\theta} \frac{g_{n-2\theta}^2}{z - \hbar\omega(n-\frac{3}{2}) - \hbar\omega_\theta - \hbar\omega_\xi} \\ \doteq \delta_{\xi\xi'} (-\frac{1}{2}i\hbar\Gamma_{n-1}).\end{aligned}\tag{21}$$

Hence the reduced resolvent operators  $\Lambda_1 G^1(z)\Lambda_1$ ,  $\Lambda_0 G^0(z)\Lambda_0$  are diagonal and we obtain, using (7), (20), (21) and

$$\langle n-1; 1_\xi | \Lambda_1 V \Lambda_0 | n; 0_\lambda \rangle = -ig_{n-1\xi} \quad (22)$$

the following result:

$$\begin{aligned} & \langle n-1; 1_\xi | \Lambda_1 G(z) \Lambda_0 | n; 0_\lambda \rangle \\ & \doteq \frac{1}{z - \hbar\omega(n-1 + \frac{1}{2}) - \hbar\omega_\xi + \frac{1}{2}i\hbar\Gamma_{n-1}} \\ & \quad \times (-ig_{n-1\xi}) \frac{1}{z - \hbar\omega(n + \frac{1}{2}) + \frac{1}{2}i\hbar\Gamma_n}. \end{aligned} \quad (23)$$

Thus, no spurious pole on the real axis has appeared in the resolvent matrix element, but instead the physically correct pole at  $z = \hbar\omega(n - \frac{1}{2}) + \hbar\omega_\xi - \frac{1}{2}i\hbar\Gamma_{n-1}$  in the lower half-plane, corresponding to the final harmonic oscillator state  $n-1$  having a finite lifetime related to  $\Gamma_{n-1}$ .

The probability amplitude  $I_{n-1,\xi;n}(t)$  will decay with time with two damping factors  $\Gamma_{n-1}$ ,  $\Gamma_n$ .

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