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## A PARTITION METHOD FOR THE QUANTUM-MECHANICAL EQUATION OF MOTION\*

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## ABSTRACT

A method is developed for determining the effect of an additional time-dependent interaction  $V(t)$  on a quantum mechanical system described by a wave function  $\psi(t)$  satisfying  $i\hbar\partial\psi(t)/\partial t = H_0(t)\psi(t)$ . It is shown that if an operator  $\Omega(t)$  can be found such that the wave function  $\Psi(t)$  satisfying  $i\hbar\partial\Psi(t)/\partial t = [H_0(t) + V(t)]\Psi(t)$  can be obtained from  $\psi(t)$  as  $\Psi(t) = \Omega(t)\psi(t)$ , then separating  $\psi(t)$  into two parts  $[\psi_1(t), \psi_2(t)]$  allows the separation of  $\Psi(t)$  into two parts  $[\Psi_1(t), \Psi_2(t)]$ , each satisfying the equation

$$i\hbar \frac{\partial \Psi_n}{\partial t} = \left[ H_n + V_{nn} + V_{nm} \Omega_{mn} \frac{1}{\Omega_{nn}} \right] \Psi_n + V_{nm} \left[ \Omega_{mm} - \Omega_{mn} \frac{1}{\Omega_{nn}} \Omega_{nm} \right] \Psi_m$$

with  $n = 1, 2$  and  $m = 2, 1$ , and in which  $\Omega_{mn}$ ,  $1/\Omega_{nn} \equiv \Omega_{nn}^{-1}$ , etc. are known time-dependent operators. Under certain weakly restrictive conditions, the second term vanishes, and  $\Psi_n$  satisfies

$$i\hbar \frac{\partial \Psi_n}{\partial t} = [H_n + \delta H_n] \Psi_n$$

in which  $\delta H_n$  is an "effective hamiltonian" for level  $n$  ( $\Psi_m$  is still governed by a more complicated equation).  $\delta H_n$  gives rise to energy level

shifts, transitions, and other effects attributable to the additional interaction  $V(t)$ . These results are exact. So long as  $\Omega(t)$  is small compared to  $H_0(t)$ , an explicit formula for  $\Omega(t)$  is obtained from ordinary perturbation theory. An application of these formulas to optical effects in free atoms is presented.

## INTRODUCTION

There exists in mathematical physics a powerful technique of broad applicability for calculating properties of systems that divide themselves naturally into two (or more) relatively non-interacting parts, each of which has relatively simple properties. This technique, called partitioning, consists of separating the governing equations into two (or more) coupled equations, one for each part of the system, each containing terms describing the independent parts and terms describing interactions between the parts. Perhaps the best example of this technique is the separation of the Dirac equation into two equations, one describing electrons of positive energy, the other describing electrons of negative energy. Recently, Löwdin<sup>1</sup> has extensively explored the partitioning method for bound-state perturbations.

In this paper we apply this technique to the quantum-mechanical equation of motion in hamiltonian form. The result is a pair of quasi-coupled equations of a rather unusual form. We show how the interaction terms can lead to an effective hamiltonian which can be simply interpreted. We also present an example of the application of these equations to an atomic system.

DERIVATION

Consider a quantum-mechanical system described by a wave function  $\psi(t)$  which obeys the equation of motion

$$i\hbar \frac{\partial \psi(t)}{\partial t} = H_0(t) \psi(t) \quad (1)$$

where  $H_0(t)$  is a (possibly) time-dependent hamiltonian. We assume Eq. (1) can be solved exactly in terms of an evolution operator<sup>2</sup>  $U(t, t_0)$ :

$$\psi(t) = U(t, t_0) \psi(t_0) \quad (2)$$

Now consider the addition of an interaction  $V(t)$  to this system, resulting in a new system described by a new wave function  $\Psi(t)$  which satisfies

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = [H_0(t) + V(t)] \Psi(t) \quad (3)$$

Again, we assume the general solution of Eq. (3) is expressible in terms of an evolution operator  $\mathcal{U}(t, t_0)$ :

$$\Psi(t) = \mathcal{U}(t, t_0) \Psi(t_0) \quad (4)$$

Now let us assume that there exists an operator  $\Omega(t)$  that produces the system  $\Psi(t)$  from the system  $\psi(t)$ , i.e., such that

$$\Psi(t) = \Omega(t) \psi(t) \quad (5)$$

is satisfied for all times  $t$ . We defer for the moment any discussion of the conditions of existence or behavior of  $\Omega(t)$ .

At this point we partition Eqs. (1), (3), and (5). We assume that the system  $\psi(t)$  can be separated naturally into two parts,

$$\psi(t) = \begin{pmatrix} \psi_1(t) \\ \psi_2(t) \end{pmatrix} . \quad (6a)$$

and that  $\Psi(t)$  can be correspondingly separated:

$$\Psi(t) = \begin{pmatrix} \Psi_1(t) \\ \Psi_2(t) \end{pmatrix} . \quad (6b)$$

We assume that the operator  $H_0(t)$  has no matrix elements between  $\psi_1(t)$  and  $\psi_2(t)$ , and so can be written

$$H_0(t) = \begin{pmatrix} H_1(t) & 0 \\ 0 & H_2(t) \end{pmatrix} , \quad (7)$$

whereas the additional operator  $V(t)$  has the general form

$$V(t) = \begin{pmatrix} v_{11}(t) & v_{12}(t) \\ v_{21}(t) & v_{22}(t) \end{pmatrix} . \quad (8)$$

Finally, the operator  $\Omega(t)$  is written



$$\Omega(t) = \begin{pmatrix} \Omega_{11}(t) & \Omega_{12}(t) \\ \Omega_{21}(t) & \Omega_{22}(t) \end{pmatrix} \quad (9)$$

The elements of the  $2 \times 2$  matrices in Eqs.(7)-(9) are themselves matrices. The matrices  $H_n$ ,  $V_{nn}$ , and  $\Omega_{nn}$  are square and of the dimension of  $\psi_n$ , whereas  $V_{nm}$  and  $\Omega_{nm}$  are not necessarily square.

Combining Eqs. (3), (6b), (7), and (8) yields

$$i\hbar \frac{\partial \Psi_1}{\partial t} = (H_1 + V_{11}) \Psi_1 + V_{12} \Psi_2 \quad (10a)$$

$$i\hbar \frac{\partial \Psi_2}{\partial t} = (H_2 + V_{22}) \Psi_2 + V_{21} \Psi_1 \quad (10b)$$

where we now omit the argument  $t$  for brevity. Combining Eqs. (5), (6), (7) and (9) yields

$$\Psi_1 = \Omega_{11} \psi_1 + \Omega_{12} \psi_2 \quad (11a)$$

$$\Psi_2 = \Omega_{21} \psi_1 + \Omega_{22} \psi_2 \quad (11b)$$

Now let us assume that the inverse operators  $\Omega_{11}^{-1}$  and  $\Omega_{22}^{-1}$  exist, so that we can invert Eqs. (11) to obtain

$$\psi_1 = \Omega_{11}^{-1} (\Psi_1 - \Omega_{12} \psi_2) \quad (12a)$$

$$\psi_2 = \Omega_{22}^{-1} (\Psi_2 - \Omega_{21} \psi_1) \quad (12b)$$

Finally, combining Eqs. (10a), (11b), and (12a), and Eqs. (10b), (11a), and (12b), we find

$$i\hbar \frac{\partial \psi_1}{\partial t} = \left( H_1 + V_{11} + V_{12} \Omega_{21} \frac{1}{\Omega_{11}} \right) \psi_1 + V_{12} \left( \Omega_{22} - \Omega_{21} \frac{1}{\Omega_{11}} \Omega_{12} \right) \psi_2 \quad (13a)$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = \left( H_2 + V_{22} + V_{21} \Omega_{12} \frac{1}{\Omega_{22}} \right) \psi_2 + V_{21} \left( \Omega_{11} - \Omega_{12} \frac{1}{\Omega_{22}} \Omega_{21} \right) \psi_1 \quad (13b)$$

where we used  $1/\Omega_{nn} \equiv \Omega_{nn}^{-1}$ . Equations (13a) and (13b) can both be written as

$$i\hbar \frac{\partial \psi_n}{\partial t} = \left( H_n + V_{nn} + V_{nm} \Omega_{mn} \frac{1}{\Omega_{nn}} \right) \psi_n \quad (14)$$

$$+ V_{nm} \left( \Omega_{mm} - \Omega_{mn} \frac{1}{\Omega_{nn}} \Omega_{nm} \right) \psi_m$$

for  $n = 1, 2$  and  $m = 2, 1$ . Equations (14) constitute the principle results of this paper. These equations, plus the equations of motion for  $\psi_1$  and  $\psi_2$  (from Eqs. (1), (6a), (7))

$$i\hbar \frac{\partial \psi_n}{\partial t} = H_n \psi_n \quad (15)$$

constitute a complete description of the system  $\Psi$  governed by Eqs. (1), (3), and (5).

## DISCUSSION

Equations (14) are exact; they are valid for any  $V(t)$  so long as  $\Omega(t)$  and  $\Omega_{nn}^{-1}(t)$  exist. It is not necessary that  $V(t)$  be considered a small perturbation on  $H_0(t)$ , although for that case (discussed below),  $\Omega(t)$  is easily found and is well-behaved.

The two equations (14) for states 1, 2 are coupled; i.e., each involves both states 1, and 2. However, the coupling is of a very unusual nature, since it is only via the states for  $V(t) = 0$ . That is, the state  $\Psi_1$  is coupled to level 2 only via  $\psi_1$ , and  $\Psi_2$  to level 1 only via  $\psi_1$ . But  $\psi_1$  and  $\psi_2$  evolve totally independently (Eqs. (15)), so there is no nonlinear recoupling of  $\Psi_n$  (through  $\Psi_m$ ) back to  $\Psi_n$ . This is quite different than the usual set of coupled equations (10a, b). In fact, since we assume the solution for  $\psi_n$  is available (from Eqs. (15)), the levels 1, 2 are not really coupled in Eqs. (14), which are in the form

$$i\hbar \frac{\partial \Psi_n(t)}{\partial t} + f(t)\Psi_n(t) = g(t) \quad (16)$$

in which  $f(t)$  is an operator and  $g(t)$  is a function of  $t$ . Thus, we have completely decoupled levels 1, 2, since we have two independent equations, one involving  $\Psi_1$ , the other involving  $\Psi_2$ , but neither involving both.

Naturally, we pay a price for decoupling the states  $\Psi_1, \Psi_2$ : The differential equations now involve very complicated (operator) functions of  $t$ , and it is necessary not only to find  $\Omega(t)$  but to invert its diagonal part as well. Even more important is the fact that homogeneity has been lost--the homogeneous equation (3) is replaced by the inhomogeneous equation (16). We

could also see this in Eqs. (15), where addition of  $V(t)$  converts  $\psi_n(t)$  into  $\Psi_n(t)$ , and makes the right hand side inhomogeneous. Finally, we have also given up hermiticity, since the operators  $V \Omega_{nm} \Omega_{nn}^{-1}$  will have anti-hermitian parts.

An especially interesting aspect of Eqs. (14) is the occurrence of  $\Omega_{mm}$ ,  $\Omega_{mn}$ , etc. in the particular combination in the coefficient of  $\psi_m$ . In fact this is related to the inverse of a partitioned matrix:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A-BD^{-1}C)^{-1} & -A^{-1}B(D-CA^{-1}B)^{-1} \\ -D^{-1}C(A-BD^{-1}C)^{-1} & (D-CA^{-1}B)^{-1} \end{pmatrix} \quad (17)$$

in which  $A$ ,  $B$ ,  $C$ , and  $D$  are matrices. Equation (17) can be proved by direct multiplication.

## EFFECTIVE HAMILTONIAN

For a very general class of problems, Eqs. (14) simplify considerably. Suppose in the distant past, for  $t < t_0$ , the system was entirely in level 1. That is, before the application of  $V(t)$ ,  $\psi_2(t)$  was zero and  $\psi_1(t)$  was unity. Such is the case, for instance, for an ensemble of atoms in their ground state before the application of an external field. But since  $\psi_1$  and  $\psi_2$  evolve totally independently, we can say that any state  $\psi_m(t)$  that is zero at  $t = t_0$ , remains zero for  $t > t_0$ . This follows immediately from Eqs. (15) and (2). Thus we may drop the  $\psi_2(t)$  term in Eq. (13a) and write

$$i\hbar \frac{\partial \Psi_1}{\partial t} = (H_1 + \delta H_1) \Psi_1 \quad (18)$$

in which we define the effective hamiltonian

$$\delta H_1 = V_{11} + V_{12} \Omega_{21} \Omega_{11}^{-1} \quad (19)$$

It is clear why we call  $\delta H_1$  an "effective" operator: its domain of operation is restricted to level 1, whereas it produces all the physical effects within that domain as does the actual interaction  $H_1 + V$ . Furthermore, Eq. (18) is in precisely the hamiltonian form of the equation of motion, hence the interpretation of  $\delta H_1$  as a hamiltonian operator. No such interpretation is possible for the more general case of Eq. (13a). Thus, only when  $\psi_2(t)$  is zero, can we ascribe physical meaning to  $\delta H_1$  in terms of level shifts, transitions, etc. Of course,  $\Psi_1(t)$  is correctly governed by Eq. (13a) even when  $\psi_2(t) \neq 0$ , but in that case,  $\delta H_1$  is not simply related to the energy levels, etc., of level 1.

The wave function  $\Psi_2(t)$  obeys Eq. (13b), which does not reduce to the simple form of Eq. (18). By considering the relative magnitudes of each operator on the r.h.s., it should be possible to obtain an equation simple enough to be solved, even if only approximately.

There is another general class of problems for which an equation of the form

$$i\hbar \frac{\partial \Psi_n}{\partial t} = (H_n + \delta H_n) \Psi_n \quad (20)$$

is obtained. This occurs when  $\psi_m$  satisfies

$$\left( \Omega_{mm} - \Omega_{mn} \frac{1}{\Omega_{nn}} \Omega_{nm} \right) \psi_m = 0 \quad (21)$$

which we may write as an operator identity:

$$\Omega_{mm}^{-1} \Omega_{mn} \Omega_{nn}^{-1} \Omega_{nm} = 1 \quad (22)$$

This condition imposes serious constraints on  $V(t)$  but is independent of any assumed initial conditions. It remains to be seen whether any physically interesting interaction  $V(t)$  can be found that satisfies Eq. (22).

## PERTURBATION THEORY

We now consider the particular case when  $V(t)$  can be regarded as small and treated by perturbation theory. Substituting Eq. (4) into Eq. (3) yields the differential equation satisfied by  $\mathcal{U}(t, t_0)$ :

$$i\hbar \frac{\partial \mathcal{U}(t, t_0)}{\partial t} = [H_0(t) + V(t)] \mathcal{U}(t, t_0) \quad (23)$$

subject to the initial condition

$$\mathcal{U}(t_0, t_0) = 1 \quad (24)$$

The iterative solution of Eqs. (23), (24) is well known<sup>3</sup> to be

$$\mathcal{U}(t, t_0) = U(t, t_0) + \frac{1}{i\hbar} \int_{t_0}^t dt' U(t, t') V(t') U(t', t_0) \quad (25)$$

$$+ \frac{1}{(i\hbar)^2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' U(t, t') V(t') U(t', t'') V(t'') U(t'', t_0) + \dots$$

where the perturbation  $V(t)$  is assumed small enough so the series converges, and also  $V(t < t_0) = 0$ . The general solution for  $\Psi(t)$  (Eq. (4)) requires we know  $\Psi(t_0)$ . However, since the perturbation is "off" until  $t_0$ , the perturbed state at the onset of the perturbation is simply the unperturbed state:

$$\Psi(t_0) = \psi(t_0) \quad (26)$$

Furthermore we require the continuity condition

$$U(t', t_0) = U(t', t)U(t, t_0) \quad (27)$$

and recalling the definition

$$U(t, t_0)\psi(t_0) = \psi(t) \quad (28)$$

we find

$$\Psi(t) = U(t, t_0)\psi(t_0) + \frac{1}{i\hbar} \int_{t_0}^t dt' U(t, t')V(t')U(t', t)U(t, t_0)\psi(t_0) + \dots \quad (29a)$$

$$= \psi(t) + \frac{1}{i\hbar} \int_{t_0}^t dt' U(t, t')V(t')U(t', t)\psi(t) + \dots \quad (29b)$$

$$\equiv \Omega(t)\psi(t) \quad (29c)$$

where we defined

$$\Omega(t) = 1 + \frac{1}{i\hbar} \int_{t_0}^t dt' U(t, t')V(t')U(t', t) \quad (30)$$

$$+ \frac{1}{(i\hbar)^2} \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' U(t, t')V(t')U(t', t'')V(t'')U(t'', t) + \dots$$



In order to simplify notation, we use a bar to denote the time integrals and powers of  $(i\hbar)^{-1}$ :

$$\Omega = 1 + \overline{UVU} + \overline{UVUVU} + \dots \quad (31)$$

The partitioning of  $\Omega$  into  $\Omega_{11}, \Omega_{12}, \dots$  is easy if we note that the unperturbed evolution operator is diagonal:

$$U = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix} \quad (32)$$

We also assume  $V$  is only off-diagonal ( $V_{nn} = 0$ ). From Eqs. (31) and (32), we find

$$\Omega_{nn} = 1 + \overline{U V_n U V_m U V_n} \quad (33)$$

$$+ \overline{U V_n U V_m U V_n U V_m U V_n} + \dots$$

$$\Omega_{mn} = \overline{U V_m U V_n} + \overline{U V_m U V_n U V_m U V_n} + \dots \quad (34)$$

for  $n = 1, 2$  and  $m = 2, 1$ . It is clear that  $\Omega_{nn}$  involves only even multiples of  $V$ , and  $\Omega_{mn}$  only odd multiples. Note that the general Eqs. (14) require  $\Omega_{nn}^{-1}$  but not  $\Omega_{mn}^{-1}$ . The former exists due to the presence of the 1, but latter does not exist, in the limit  $V \rightarrow 0$ .

For the former, we can use the operator identity<sup>4</sup>

$$(A + B)^{-1} = A^{-1} - A^{-1}B(A + B)^{-1} \quad (35a)$$

$$= A^{-1} - A^{-1}BA^{-1} + A^{-1}BA^{-1}BA^{-1} - \dots \quad (35b)$$

to find the approximate expression

$$\Omega_{nn}^{-1} \cong 1 - \frac{U V U V U}{n \quad nm \quad m \quad mn \quad n} + \dots \quad (36)$$

Finally, substituting Eqs. (33), (34) and (36) in Eq. (14) we find

$$\begin{aligned} i\hbar \frac{\partial \psi_n}{\partial t} = & \left( H_n + V_{nm} \frac{U V U}{m \quad mn \quad n} + V_{nm} \frac{U V U V U V U}{m \quad mn \quad n \quad nm \quad m \quad mn \quad n} \right. \\ & \left. - V_{nm} \frac{U V U}{m \quad mn \quad n} \frac{U V U V U}{n \quad nm \quad m \quad mn \quad n} + \dots \right) \psi_n \\ & + V_{nm} \left( 1 + \frac{U V U V U}{m \quad mn \quad n \quad nm} - \frac{U V U}{m \quad mn \quad n} \frac{U V U}{n \quad nm \quad m} \right. \\ & + \frac{U V U V U V U V U}{m \quad mn \quad n \quad nm \quad m \quad mn \quad n \quad nm \quad m} \\ & + \frac{U V U}{m \quad mn \quad n} \frac{U V U V U}{n \quad nm \quad m \quad mn \quad n} \frac{U V U}{n \quad nm \quad m} \\ & - \frac{U V U}{m \quad mn \quad n} \frac{U V U V U V U}{n \quad nm \quad m \quad mn \quad n \quad nm \quad m} \\ & \left. - \frac{U V U V U V U V U}{m \quad mn \quad n \quad nm \quad m \quad mn \quad n} \frac{U V U}{n \quad nm \quad m} + \dots \right) \psi_m \end{aligned} \quad (37)$$

in which we have kept terms up to fourth order in V.

## APPLICATION: OPTICAL RADIATION IN AN ATOMIC VAPOR

To illustrate the usefulness of these formulas, we examine a fairly simple system: an atomic vapor is irradiated with a beam of light. We are interested in such effects as how the light affects the atomic energy levels and how the vapor affects the intensity and polarization of the light. If we write the atom-light coupling as  $V(t) = -\vec{\mathcal{E}}(t) \cdot \vec{p}$ , where  $\vec{\mathcal{E}}(t)$  is the (classical) electric field of the light, and  $\vec{p}$  is the atomic electric dipole moment operator, and if we assume that all the atoms were in their ground state when the light was applied in the distant past, Eq. (37) gives the (approximate) equation of motion of the atomic ground state

$$i\hbar \frac{\partial \psi_1}{\partial t} \cong (H_1 + \delta H_1) \psi_1 \quad (38)$$

where

$$\delta H_1 = \frac{1}{i\hbar} \int_{-\infty}^t dt' \vec{\mathcal{E}}(t) \cdot \vec{p} U_2(t, t') \vec{\mathcal{E}}(t') \cdot \vec{p} U_1(t', t_0) \quad (39)$$

is the effective ground state operator. If we use

$$\vec{\mathcal{E}}(t) = \frac{1}{2} \vec{\mathcal{E}} e^{-i\omega t} + \frac{1}{2} \vec{\mathcal{E}}^* e^{+i\omega t} \quad (40)$$

and save only the DC components of  $\delta H_1$  (terms oscillating at  $2\omega$  will average to zero), we can write Eq. (39) as

$$\delta H_1 = \frac{1}{4} \vec{e} \cdot \overleftrightarrow{\alpha}_+ \cdot \vec{e}^* + \frac{1}{4} \vec{e}^* \cdot \overleftrightarrow{\alpha}_- \cdot \vec{e} \quad (41)$$

where

$$\overleftrightarrow{\alpha}_\pm = \frac{i}{\hbar} \int_0^\infty d\tau e^{\pm i\omega\tau} \vec{p} U_2(t, t-\tau) \vec{p} U_1(t-\tau, t) \quad (42)$$

is a polarization dyadic operator for the atomic ground state. The properties of the individual atoms are contained entirely in  $\overleftrightarrow{\alpha}_\pm$ . It is necessary to solve Eqs. (1), (2) for  $U_2$  and  $U_1$ , and to perform collisional and velocity distribution averages of  $\overleftrightarrow{\alpha}_\pm$  to obtain the polarizability of the vapor. Performing the integration over  $\tau$  will produce a resonant denominator in  $\overleftrightarrow{\alpha}_+$ , but a non-resonant denominator in  $\overleftrightarrow{\alpha}_-$ , so the latter contribution to  $\delta H_1$  can be neglected for  $\omega$  near resonance. The hermitian part of  $\delta H_1$  gives the energy level shifts of the atomic states, whereas the antihermitian parts represent a loss of ground state atoms due to photon absorption. The macroscopic average of  $\overleftrightarrow{\alpha}_\pm$  is the electric susceptibility of the vapor, from which we can find the dielectric constant. The presence of magnetic fields is accounted for in  $U_{2,1}(t, t_0)$ , and if these fields are sinusoidally varying we find  $\overleftrightarrow{\alpha}_\pm$  is modulated at multiples of the field frequency, giving rise to sidebands characteristic of magnetic resonance phenomena. These relations have been discussed in detail by Happer and Mathur<sup>5</sup> for zero magnetic field, by Happer<sup>6</sup> and Happer and Schmieder<sup>7</sup> for a static field, and by Schmieder<sup>8</sup> for static plus rotating or oscillating fields.

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