Systematic method for deriving effective Hamiltonians

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A systematic procedure for deriving effective Hamiltonians to any order is presented, which is applicable to any time-independent Hamiltonian. The method is based on a continued-fraction approach and avoids the singularities which may occur with perturbation theory. It is illustrated by deriving the effective Hamiltonian for the one-photon, dressed-state laser to second order.

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I. INTRODUCTION

Effective Hamiltonians find widespread use in theoretical physics. Within the fields of quantum and nonlinear optics for example, their use is extensive, and they have found a place in several textbooks [1]. In the literature, they are obtained by a variety of *ad hoc* approximations whose range of validity is often not apparent. A derivation of multiphoton effective Hamiltonians, based on perturbation theory, has been presented by Friedmann and Wilson-Gordon [2].

Here we present a systematic derivation, based on the continued-fraction method [3], which seems ideally suited to deal with this problem. This approach makes it clear that in principle the use of effective Hamiltonians is an exact technique, although the usual motivation for introducing effective Hamiltonians is to produce tractable approximations to difficult problems. It avoids some of the difficulties associated with perturbation theory, such as divergence of the expressions at exact resonance.

A general expression for the effective Hamiltonian is obtained, under the basic assumption that the original Hamiltonian is time independent. The expressions presented are valid even at exact resonance. The method is systematic, in the sense that there is a clear procedure for deriving the effective Hamiltonian to the next degree of accuracy if the given form should be thought inadequate. The approach is illustrated by deriving the effective Hamiltonian for the single-photon, dressed-state laser.

II. MATHEMATICAL REVIEW

First we review the continued-fraction theory necessary for the treatment of effective Hamiltonians. We consider the following mathematical problem. Given the set of N linear equations for the N unknowns x_i,

$$\sum_{j=1}^{N} A_{ij}x_j = B_i, \quad i,j \in \text{set } S \equiv (1,2,\ldots,N) , \tag{1}$$

where the set S can be expressed as the sum of disjoint sets W and U: $S = U + W$ (with the elements of W being labeled by the symbols $a,b,c,\ldots$ and those of U by symbols of the form $\alpha,\beta,\gamma,\ldots$) to obtain a reduced set of equations of the form

$$\sum_{b\in W} \bar{A}_{ab}x_b = \bar{B}_a, \quad a \in W \tag{2}$$

in which the only explicit reference is to the "wanted" variables a,b, etc.

We require explicit expressions for the reduced matrix $\bar{A}_{ab}$ and reduced vector $\bar{B}_b$. It has been shown [3] that the elimination of the "unwanted" set U can be performed exactly. The result is

$$\bar{A}_{ab} = A_{ab} - \sum_{\alpha\in U}^{*} \frac{A_{a\alpha}A_{\alpha b}}{D_{\alpha}^{W}} + \sum_{\alpha,\beta\in U}^{*} \frac{A_{a\alpha}A_{\alpha\beta}A_{\beta b}}{D_{\alpha\beta}^{W}} + \cdots , \tag{3}$$

$$\bar{B}_a = B_a - \sum_{\alpha\in U}^{*} \frac{A_{a\alpha}B_{\alpha}}{D_{\alpha}^{W}} + \sum_{\alpha,\beta\in U}^{*} \frac{A_{a\alpha}A_{\alpha\beta}B_{\beta}}{D_{\alpha\beta}^{W}} + \cdots , \tag{4}$$

where the D functions are defined recursively through the relations

$$D_{\alpha}^{W} \equiv A_{\alpha\alpha} - \sum_{\beta\in U}^{*} \frac{A_{\alpha\beta}A_{\beta\alpha}}{D_{\beta}^{W}} + \sum_{\beta,\gamma\in U}^{*} \frac{A_{a\alpha}A_{\alpha\beta}A_{\beta b}}{D_{\alpha\beta}^{W}} + \cdots , \tag{5}$$

$$D_{\alpha\beta}^{W} \equiv D_{\alpha}^{W}D_{\beta}^{W,\alpha}; \quad D_{\alpha\beta\gamma}^{W} \equiv D_{\alpha}^{W}D_{\beta}^{W,\alpha}D_{\gamma}^{W,\alpha,\beta} . \tag{6}$$

The asterisk on the summation signs means that none of the variables summed over can be equal to each other, nor can they take on any of the values in the superscripts of the D functions. Thus in the second term of (3), we have the restriction $\alpha \neq W$ (W, of course, stands for the set of all wanted variables), and in the third term we have the restrictions $\alpha \neq W$, $\beta \neq W,\alpha$, in the double sum. [In Eqs. (3)–(5) it is unnecessary to specify explicitly that $\alpha,\beta \in U$ as we have done, because this is implied by the superscript W on the D functions.] The conditions on the sums become more restrictive as more terms are included, so that finally the sums terminate (if N is finite) and our expressions are exact.

Note that the D functions with more than one subscript are defined as products of D functions with a single subscript with increasing numbers of superscripts. The latter impose increasing restrictions on the sums, which in turn implies that the corresponding D functions contain fewer and fewer terms.

III. EFFECTIVE HAMILTONIANS

In mathematical terms, the derivation of an effective Hamiltonian corresponds to the elimination of an unwanted set of states from the time-independent Schrödinger equation, which we assume to be of the form

$$(H-\lambda_I)|\psi_I\rangle=0 \tag{7}$$

for the eigenvectors and eigenvalues of the Hamiltonian H. We introduce a complete set of states

$$\sum_{i\in S}|i\rangle\langle i|=1 \tag{8}$$

and write the equation in the form

$$\sum_{j\in S}(H_{ij}-\lambda\delta_{ij})\langle j|\psi\rangle=0, \quad i\in S\ , \tag{9}$$

where for convenience we have dropped the label "I" which distinguishes the particular eigensolutions of Eq. (7).

Equation (9) is of the same form as (1) with $B_i=0$. Proceeding as in the previous section, we divide the full set of states S into the sum of disjoint "wanted" W and "unwanted" U parts. The subset of equations which contain unwanted states as labels are eliminated to leave the reduced eigenvalue equation

$$\sum_{b\in W}[\bar{H}_{ab}(\lambda)-\lambda\delta_{ab}]\langle b|\psi\rangle=0, \quad a\in W\ , \tag{10}$$

where $\bar{H}(\lambda)$ is the effective Hamiltonian, and is given explicitly from Eqs. (3)–(6) as

$$\bar{H}_{ab}(\lambda)=H_{ab}-\sum_{\alpha\in U}^{*}\frac{H_{a\alpha}H_{\alpha b}}{D_\alpha^W}+\sum_{\alpha,\beta\in U}^{*}\frac{H_{a\alpha}H_{\alpha\beta}H_{\beta b}}{D_{\alpha\beta}^W}+\cdots \tag{11}$$

where

$$D_\alpha^W\equiv H_{\alpha\alpha}-\lambda-\sum_{\beta\in U}^{*}\frac{H_{\alpha\beta}H_{\beta\alpha}}{D_\beta^W}+\sum_{\beta,\gamma\in U}^{*}\frac{H_{a\alpha}H_{\alpha\beta}H_{\beta b}}{D_{\alpha\beta}^W}+\cdots\ , \tag{12}$$

$$D_{\alpha\beta}^W\equiv D_\alpha^W D_\beta^{W,\alpha}, \quad D_{\alpha\beta\gamma}^W\equiv D_\alpha^W D_\beta^{W,\alpha}D_\gamma^{W,\alpha,\beta};\ \text{etc.} \tag{13}$$

The eigenvalues can be determined by solving the determinantal equation

$$|\bar{H}_{ab}(\lambda)-\lambda\delta_{ab}|=0\ , \tag{14}$$

and correspond with the eigenvalues of the original Hamiltonian. Note that the effective Hamiltonian is an implicit function of the eigenvalue λ through the definition of the D functions. For notational convenience, we henceforth write $\bar{H}(\lambda)$ as $\bar{H}$.

Alternatively, we may write Eq. (11) in operator form as

$$\bar{H}=H-\sum_{\alpha\in U}^{*}\frac{H|\alpha\rangle\langle\alpha|H}{D_\alpha^W}+\sum_{\alpha,\beta\in U}^{*}\frac{H|\alpha\rangle\langle\alpha|H|\beta\rangle\langle\beta|H}{D_{\alpha\beta}^W}+\cdots\ , \tag{15}$$

it being understood that $\bar{H}$ acts only in the space spanned by the vectors of the wanted set W.

Equations (11)–(15) are the main results of the paper, and provide an exact procedure for calculating the effective Hamiltonian.

In practice, one usually takes an approximate form for $\bar{H}$. For example, if we take only the first two terms in Eqs. (11) and (12), we obtain the expression

$$\bar{H}_{ab}=H_{ab}-\sum_{\alpha\in U}^{*}\frac{H_{a\alpha}H_{\alpha b}}{H_{\alpha\alpha}-\lambda}\ , \tag{16}$$

which is the second-order perturbation-theory expression for the effective Hamiltonian, provided that λ is evaluated to zeroth order. This expression is valid if the off-diagonal elements $H_{a\alpha}$ are sufficiently small compared to the diagonal terms $H_{\alpha\alpha}-\lambda$.

While to lowest order, the systematic continued fraction approach we have presented here produces essentially the second-order perturbation-theory result, we should emphasize that in general it is a much more accurate procedure than perturbation theory. For example, a consistent third-order expression for the effective Hamiltonian obtained from Eqs. (11) and (12) is

$$\bar{H}_{ab}=H_{ab}-\sum_{\alpha\in U}^{*}\frac{H_{a\alpha}H_{\alpha b}}{H_{\alpha\alpha}-\lambda^{(1)}-\sum_{\beta\in U}^{*}H_{\alpha\beta}H_{\beta\alpha}/(H_{\beta\beta}-\lambda^{(0)})}+\sum_{a,\beta\in U}^{*}\frac{H_{a\alpha}H_{\alpha\beta}H_{\beta b}}{(H_{\alpha\alpha}-\lambda^{(0)})(H_{\beta\beta}-\lambda^{(0)})}\ , \tag{17}$$

where $\lambda^{(n)}$ indicates the nth-order approximation to the eigenvalue. We note that the presence of the term $\sum_{\beta\in U}^{*}H_{\alpha\beta}H_{\beta\alpha}/(H_{\beta\beta}-\lambda^{(0)})$ in the denominator of the second term of Eq. (17) represents the sum of an infinite subset of terms from the perturbation-theory power series.

The continued-fraction approach allows considerable flexibility in the manner in which approximations are introduced—an additional advantage over perturbation theory. Thus at resonance, such factors as $H_{\alpha\alpha}-\lambda^{(0)}$ in Eq. (17), which arise from taking the zeroth-order approximation to the D functions, may become zero, leading to singularities. These singularities may be eliminated by replacing the zeroth-order approximation to the D functions by the second-order approximation. A suitable second-order effective Hamiltonian to avoid these singularities is therefore

$$\bar{H}_{ab}=H_{ab}-\sum_{\alpha\in U}^{*}\frac{H_{a\alpha}H_{\alpha b}}{H_{\alpha\alpha}-\lambda^{(1)}-\sum_{\beta\in U}^{*}H_{\alpha\beta}H_{\beta\alpha}/(H_{\beta\beta}-\lambda^{(0)})}\ , \tag{18}$$

a nonperturbative result.

In many cases of interest we can decompose the original Hamiltonian into the sum of two terms:

$$H=H_0+V \tag{19}$$

where

$$(H_0)_{a\alpha}=(H_0)_{\alpha a}=0 \text{ for all } a \text{ and } \alpha ,$$
$$V_{aa}=0; \quad V_{\alpha\alpha}=0 \text{ for all } a \text{ and } \alpha . \tag{20}$$

That is, H_0 does not connect the W and U spaces, and V has no diagonal matrix elements in either space. Then we may write

$$\bar{H}=H_0-\sum_{\alpha\in U}^{*}\frac{V|\alpha\rangle\langle\alpha|V}{D_\alpha^W}+\sum_{\alpha,\beta\in U}^{*}\frac{V|\alpha\rangle\langle\alpha|V|\beta\rangle\langle\beta|V}{D_{\alpha\beta}^W}+\cdots , \tag{21}$$

$$D_\alpha^W\equiv(H_0)_{\alpha\alpha}-\lambda-\sum_{\beta\in U}^{*}\frac{V_{\alpha\beta}V_{\beta\alpha}}{D_\beta^W}+\sum_{\beta,\gamma\in U}^{*}\frac{V_{\alpha\alpha}V_{\alpha\beta}V_{\beta b}}{D_{\alpha\beta}^W}+\cdots . \tag{22}$$

IV. EXAMPLE: THE SINGLE-PHOTON DRESSED-STATE LASER

As a nontrivial example of the derivation of an effective Hamiltonian, we consider an ensemble of two-level atoms placed in a cavity and interacting with a transverse external pump whose Rabi frequency is Ω. This system was considered in detail by Zakrewski, Lewenstein, and Mossberg [4]. The Hamiltonian is

$$H=\tfrac{1}{2}\sum_\mu[\Delta_1\sigma_{3\mu}+\Omega(\sigma_\mu+\sigma_\mu^+)+g_\mu\sigma_\mu^+a+g_\mu\sigma_\mu a^\dagger+\Delta_2 a^\dagger a] \tag{23}$$

where $\Delta_1=\omega_a-\omega_L$ and $\Delta_2=\omega_c-\omega_L$ with ω_a, ω_c, and ω_L being the atomic, the cavity, and the pump frequencies, respectively. The σ's are the usual Pauli matrices used for describing two-level atoms and $a^\dagger$ is the creation operator for a cavity mode. The rotating-wave approximation has been used to eliminate the explicit time dependence at the pump frequency.

A transformation is now made to the dressed-state picture for the two-level atom:

$$|+\rangle=\cos\alpha[1\rangle+\sin\alpha|0\rangle ,$$
$$|-\rangle=-\sin\alpha|1\rangle+\cos\alpha|0\rangle , \tag{24}$$

where α is defined by

$$\sin2\alpha=\Omega/\Omega' \text{ and } \Omega'=(\Omega^2+\Delta_1^2)^{1/2} . \tag{25}$$

The Hamiltonian becomes $H=H_0+V$ with

$$H_0=\frac{\Omega'}{2}S_3+\Delta_2 a^\dagger a+a^\dagger G+G^\dagger a; \quad S_3\equiv\sum_\mu\sigma_{3\mu} , \tag{26}$$

$$V=a^\dagger(G_1+G_2^\dagger)+(G_1^\dagger+G_2)a , \tag{27}$$

where

$$G=\sum_\mu C_\mu g_\mu/4, \quad C_\mu\equiv g_\mu(1+\cos2\alpha)/4 ;$$
$$G_1=\sum_\mu A_\mu\sigma_{3\mu}, \quad A_\mu\equiv g_\mu\sin2\alpha/4 ; \tag{28}$$
$$G_2^\dagger=\sum_\mu B_\mu\sigma_{3\mu}, \quad B_\mu\equiv-g_\mu(1-\cos2\alpha)/4 .$$

The wanted set of states is defined to be the set of eigenfunctions of the "excitation number operator:"

$$N_{\text{ex}}\equiv a^\dagger a+\sum_\mu\sigma_\mu^\dagger\sigma_\mu \tag{29}$$

with eigenvalue M. These are of the form $|M-m;m\rangle$ where $M-m$ is the number of photons in the cavity mode and m is the number of two-level atoms in their excited state. The unwanted set is the set of vectors $\{|M'-m';m''\rangle$ where $m''\neq m'$ if $M'=M\}$. With these definitions for W and U, H_0 and V satisfy the conditions (20).

Noting the matrix elements

$$(H_0)_{\alpha\alpha}=\Delta_2(M-m')+\Omega'(m''-M/2) \quad \text{for } |\alpha\rangle=|M-m';m''\rangle \tag{30}$$

and

$$\begin{aligned}\langle M-m';m''|V|M-m;m\rangle=&\sqrt{M-m+1}(2m-M)\delta_{m',m-1}\delta_{m'',m}\sum_\mu A_\mu\\&+\sqrt{M-m+1}\,m\,\delta_{m',m-1}\delta_{m'',m+1}\theta(M-m-1)\sum_\mu B_\mu\\&+\sqrt{M-m}\,(2m-M)\delta_{m',m+1}\delta_{m'',m}\sum_\mu A_\mu\\&+\sqrt{M-m}\,(M-m)\delta_{m',m+1}\delta_{m'',m-1}\theta(m-1)\sum_\mu B_\mu ,\end{aligned} \tag{31}$$

where $\theta(x)$ is zero if $x \leq 0$ and takes the value unity otherwise. We may evaluate the second-order contribution to the effective Hamiltonian:

$$\Delta\bar{H}_{ab}^{(2)} = -\sum_{\alpha} \frac{V_{a\alpha}V_{\alpha b}}{(H_0)_{\alpha\alpha}-\lambda} \tag{32}$$

as

$$\Delta\bar{H}_{ab}^{(2)} = -\langle a| \left[\sum_{\mu,\mu'} \left[\frac{A_\mu A_{m'}^* \sigma_{3\mu}\sigma_{3\mu'}}{\Delta_2} + \frac{B_\mu B_{m'}^* \sigma_\mu \sigma_{\mu'}^\dagger}{\Delta_2+\Omega'} \right] - a^\dagger a \sum_{\mu} \frac{|B_\mu|^2 \sigma_{3\mu}}{\Delta_2+\Omega'} \right] |b\rangle \ . \tag{33}$$

We have assumed the zeroth-order approximation to the eigenvalue λ corresponding to the state $|M-m;m\rangle$:

$$\lambda^{(0)} \simeq \Delta_2(M-m)+\Omega'(m-M/2) \ . \tag{34}$$

If we further assume that the atomic dipoles have random phases, we recover the effective Hamiltonian derived by Zakrewski, Lewenstein, and Mossberg [4]:

$$\bar{H} = \Delta_2 a^\dagger a + \tfrac{1}{2}\Omega' S_3 + G^\dagger a + a^\dagger G^\dagger + \sum_{\mu} \frac{|B_\mu|^2}{\Delta_2+\Omega'} (a^\dagger a + \tfrac{1}{2})\sigma_{3\mu} \ . \tag{35}$$

By choosing different wanted and unwanted sets we can derive the two-photon effective Hamiltonian also employed by these authors.

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