Derivation of model Hamiltonians for interacting subsystems of nonidentical particles

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A method is given for deriving model Hamiltonians which describe the behavior of a subsystem in interaction with a set of different particles. The formalism is illustrated by reducing the Jaynes-Cummings Hamiltonian for an interacting fermion-boson system, to a fermion-only Hamiltonian. The conditions are discussed under which such elimination of degrees of freedom is possible.

I. INTRODUCTION

Many different kinds of experiments in atomic, molecular, nuclear, and solid-state physics are customarily described by giving values to adjustable parameters in suitable Hermitian model Hamiltonians H_{mod}. The spin Hamiltonians of Ising and Heisenberg, crystal fields, BCS theory, nuclear and atomic shell models, and the Hamiltonians of Hubbard and Anderson are but a few outstanding examples. These model Hamiltonians are extremely useful because a complete description of the experimental properties—albeit in a reduced energy range—can be given in terms of relatively few parameters. Sometimes H_{mod} is only an ansatz, but very often its analytical expression can be guessed from symmetry arguments, as long as one assumes it to be invariant under the symmetry group of the actual Hamiltonian H.[1] If Ω is the domain of H—Hilbert space for a single particle with only orbital degrees of freedom and Fock space in the general many-body case—H_{mod} always operates within a manifold $\Omega_{\text{mod}} \subset \Omega$. In paramagnetic resonance experiments, for instance, one takes the dimension of Ω_{mod} to be the number of levels connected by the experimentally observed transitions,[2] while for the Ising model[3] one takes into account only spin variables.

All in all, despite the fact that Ω_{mod} is quite different from Ω, one cannot get rid of the feeling that a well-formulated H_{mod} is a faithful though restricted representation of H and not just a convenient bookkeeping device. One thus expects that the behavior of the quasielectrons described by the atomic shell model[4] is uniquely related to that of the actual electrons. A rigorous mathematical justification of this belief requires proving the existence of a basis in which the system may be described as a set of noninteracting electrons. Whether or not such a basis exists is therefore a central problem for the discussion of the relationship between H_{mod} and H.

If one is willing to disregard convergence problems, and the ground state of the subsystem whose degrees of freedom one wishes to project out is nondegenerate, in some cases it is fairly straightforward to derive H_{mod} from H by using standard perturbation theory.[5] For example, the coupling constant J in the Heisenberg model can be thus related to the exchange integrals between neighboring atoms in an insulator.[6]

One would like to have a method for bridging the gap between model and actual Hamiltonians which does not have the aforementioned shortcomings. Such a method would provide both explicit expressions for the parameters in H_{mod} in terms of the interactions in H and a systematic way of deriving novel model Hamiltonians. Summarizing, the method's desired features are

(a) it should provide an explicit nonperturbative connection between H_{mod} and H;

(b) the model Hamiltonians thus obtained must be Hermitian and invariant under the symmetry group of H;

(c) one should be able to choose freely the manifold Ω_{mod} and to project out all unwanted degrees of freedom; and

(d) the eigenvalues of H_{mod} should coincide with a selected set of eigenvalues of H.

When the remaining and the left-out degrees of freedom do not belong to identical particles, all the previous requisites are fulfilled by suitably defined projections of effective Hamiltonians H_{eff}. When that is not the case, as when one defines valence-electrons-only model atomic Hamiltonians, or in crystal-field theory, further steps are required. In what follows we will concentrate upon the former case, leaving the latter for a later publication.

Several reviews have been made on the subject of effective Hamiltonians,[7–9] wherein abundant references may be found. In two previous works it was discussed how one may derive all effective Hamiltonians which satisfy three very general conditions[10] and how the defining equations may be solved in a nonperturbative fashion.[11] It should be stressed here that while some authors do not distinguish between model and effective Hamiltonians, in our terminology H_{mod} is empirically introduced, while H_{eff} is derived from *ab initio* calculations. Moreover, these two kinds of Hamiltonians should be distinguished from the equivalent Hamiltonians used in certain calculations.[12]

As the formalism used in the derivation of model Hamiltonians is rather abstract, we have chosen here to discuss a specific example, the Jaynes-Cummings Hamiltonian,[13–15] which is a simple example of the coupling between a fermion and a boson. As the exact solutions are known, one may check the results obtained before projecting out the bosonic degrees of freedom in order to write a dressed or renormalized fermion-only Hamiltonian. This

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Hamiltonian turns out to be an example of a class of systems where one expects to be able to solve exactly the nonlinear equation which determines H_{eff}.

The paper's organization is as follows. In Sec. II we give a short survey of the effective Hamiltonian formalism. Section III contains a discussion of the symmetry properties of H_{eff}, where some new results are derived. The Jaynes-Cummings Hamiltonian is briefly reviewed in Sec. IV, while in Sec. V we give the actual calculations leading to the fermion-only model Hamiltonian. Finally, in Sec. VI we briefly discuss the results obtained, as well as some possible generalizations.

II. EFFECTIVE HAMILTONIAN FORMALISM

An effective Hamiltonian associated with both H and a reference Hamiltonian H_0 is the operator H_{eff} that fulfills the following conditions.

(a) H and H_{eff} have the same set of eigenvalues; that is, if

$$H|\alpha\rangle=E_\alpha|\alpha\rangle ,$$

then

$$H_{\text{eff}}|\alpha\rangle_{\text{eff}}=E_\alpha|\alpha\rangle_{\text{eff}} . \tag{2.1}$$

(b) The eigenvectors $|\alpha\rangle$ and $|\alpha\rangle_{\text{eff}}$ are related by a nonsingular (and in general nonunitary) wave operator S,

$$|\alpha\rangle=S|\alpha\rangle_{\text{eff}} . \tag{2.2}$$

(c) H_{eff} is diagonal[16] with respect to H_0, i.e., it has no matrix elements connecting eigenvectors belonging to different eigenvalues of H_0.

From (2.1) and (2.2) it follows that

$$H_{\text{eff}}=S^{-1}HS . \tag{2.3}$$

The reference Hamiltonian H_0 does not have to represent any actual subsystem and is defined solely with respect to the set of experiments one is aiming to describe by H_{mod}, the only requirement being that the dimension of Ω_{mod} should be equal to the number of states experimentally involved. As one usually chooses as a basis for Ω_{mod} the best available approximations to the relevant eigenvectors of H, the spectral decomposition

$$H_0=\sum_j e_j P_j \tag{2.4}$$

is then fully determined.[17] Here P_j are the usual projection operators.

If one further requests that H_{eff} be Hermitian,

$$H_{\text{eff}}^\dagger=H_{\text{eff}} , \tag{2.5}$$

it then follows that

$$S=R(R^\dagger R)^{-1/2}U=(S^\dagger)^{-1} , \tag{2.6}$$

where U is a unitary operator, diagonal with respect to H_0 but otherwise arbitrary, and R satisfies the nonlinear Bloch equation[18,10]

$$R=1+h_0(R\langle VR\rangle-VR) , \tag{2.7}$$

where

$$V=H-H_0 , \tag{2.8}$$

$$h_0(A)=\sum_j\sum_{k\,(\neq j)} P_j A P_k/(e_j-e_k) , \tag{2.9}$$

and

$$\langle A\rangle=\sum_j P_j A P_j . \tag{2.10}$$

The simplest choice[19,20,8] is to take $U=1$ but this is not obligatory. In the basis of eigenvectors of H_0, Eq. (2.7) may be written[11]

$$\begin{aligned} &\underline{R}_{kk}=\underline{\mathbb{1}}_k , \\ &\underline{R}_{kj}=(e_k-e_j)^{-1}\sum_l(\underline{R}_{kj}\underline{V}_{jl}\underline{R}_{lj}-\underline{V}_{kl}\underline{R}_{lj}) , \end{aligned} \tag{2.11}$$

where $\underline{\mathbb{1}}_k$ is the unit $d_k\times d_k$ matrix, and $\underline{R}_{kj},\underline{V}_{kj}$ are rectangular $d_k\times d_j$ matrices, d_j being the degeneracy of e_j. Due to its nonlinear character Eq. (2.11) does, in general, have more than one solution. The adiabatic condition

$$\lim_{V\to 0}\underline{R}_{kj}=\underline{\mathbb{1}}_k\delta_{kj} \tag{2.12}$$

unambiguously identifies the proper solution.

In order to set up an effective Hamiltonian H_{eff}, the following steps are to be followed. Define first an appropriate reference Hamiltonian H_0 in accordance with the experimentally accessible energy levels and available approximate wave vectors; solve Eq. (2.7) or (2.11) for R, exactly if possible[21] or approximately otherwise;[11] make a choice of U in Eq. (2.6) if different from 1, thus obtaining S; write H_{eff} Eq. (2.3); solve the eigenvalue Eq. (2.1), thus obtaining the actual eigenvalues E_α; and obtain the actual eigenvectors from Eq. (2.2). One should notice that because of condition (c) of this section both Eqs. (2.11) and (2.1) may be solved within any chosen subspace with projector P_j, this being the foundation of standard perturbation theory.

III. SYMMETRY PROPERTIES OF EFFECTIVE HAMILTONIANS

Apart from the removal of a number of degrees of freedom, H and H_{mod} should have the same symmetries. Let G be the symmetry group of H and G_0 that of the reference Hamiltonian H_0. Practicality requires the degeneracy of H_0 to be as large as possible, that is,

$$G\subset G_0 . \tag{3.1}$$

With this choice symmetry is always lowered by the addition of V to H_0, which we take to be the rule. It is then obvious that any symmetry operator Q belonging to G satisfies

$$[Q,H]=[Q,H_0]=[Q,V]=0 . \tag{3.2}$$

As Q leaves invariant the manifold of eigenvectors of H_0

which belong to any given eigenvalue e_j, it immediately follows that

$$[Q,P_j]=0\ . \tag{3.3}$$

From Eqs. (3.2) and (3.3) the transformation properties of the operator R defined by Eq. (2.7) are immediately found to be given by

$$R'=QRQ^{-1}=Q\left[1+\sum_j \sum_{k\,(\neq j)} (P_jR\,P_kVR\,P_k-P_jVR\,P_k)/(e_j-e_k)\right]Q^{-1}=1+h_0(R'\langle VR'\rangle-VR')\ . \tag{3.4}$$

From the adiabatic condition Eq. (2.12)

$$\lim_{V\to 0} R'=1\ , \tag{3.5}$$

it follows that R and R' satisfy the same equation and should necessarily be equal, that is,

$$[Q,R]=0\ . \tag{3.6}$$

If H_{eff}, that is, H_{mod}, is to have the same symmetries as H it must then be

$$[Q,H_{\text{eff}}]=0\ , \tag{3.7}$$

which from Eqs. (2.3) and (3.6) leads to

$$[Q,U]=0\ . \tag{3.8}$$

As was previously pointed out, one may choose $U=1$, which fulfills Eq. (3.8), leading to the Hermitian symmetric effective Hamiltonian previously defined.[19,20,10] There is no general agreement on this point and several other choices have been made, notably that of Van Vleck,[22] who was the first to use effective Hamiltonians in solid-state physics. Although we do not intend to discuss the point at length here, we must stress that because of Schur's lemma[23] Eq. (3.8) imposes severe restrictions on U, which may only connect equal partners of identical irreducible representations. This partial freedom in the choice of U may perhaps be useful in some cases but it makes no difference here where we can take simply

$$U=1\ . \tag{3.9}$$

IV. JAYNES-CUMMINGS HAMILTONIAN

Exactly soluble Hamiltonians for coupled systems are exceedingly rare. One of the few known ones is the Jaynes-Cummings Hamiltonian, which was originally introduced in order to discuss the interaction of a two-level atom with a quantized radiation field.[13] Later on it was used in electron paramagnetic resonance,[14] its complicated dynamics having only recently been investigated by means of coherent states.[15] For our purposes the Jaynes-Cummings Hamiltonian H may be looked upon as describing a fermion (spin $\frac{1}{2}$, two-level electron, isospin doublet, etc.) which is capable of absorbing and emitting a boson (photon, phonon, meson, etc.), its expression being

$$H=\tfrac{1}{2}\omega_0\sigma_z+\omega a^\dagger a+k(a\sigma^+ +a^\dagger\sigma^-)\ , \tag{4.1}$$

where

$$\sigma_z=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},\quad \sigma^+=\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix},\quad \sigma^-=\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}$$

are the Pauli matrices, $a^\dagger$ and a the boson's creation and annihilation operators, ω the boson's single-mode energy, ω_0 the energy difference between the two possible fermion states $|+\rangle$ and $|-\rangle$, and k the fermion-boson coupling strength. The energy levels for the noninteracting case $k=0$ are shown in Fig. 1, where n is the boson's excitation number.

The Hamiltonian's eigenvectors and eigenfunctions are easily found if one knows all constants of motion (symmetries). These are given by the complete set of commuting operators C_1, C_2, and H, where[14]

$$C_1=\omega(a^\dagger a+\tfrac{1}{2}\sigma_z)\ , \tag{4.2}$$

$$C_2=k(\sigma^+a+\sigma^-a^\dagger)-\Delta\sigma_z\ , \tag{4.3}$$

$$[C_1,C_2]=[C_1,H]=[C_2,H]=0\ , \tag{4.4}$$

where

$$\Delta=\tfrac{1}{2}(\omega-\omega_0)\ . \tag{4.5}$$

The eigenvalues $E_n^\pm$ and eigenvectors $|\pm,n\rangle$ of H thus turn out to be

$$E_n^\pm=\omega(n+\tfrac{1}{2})\pm\lambda_n\ , \tag{4.6}$$

$$|+,n\rangle=\cos\theta_n\,|-\rangle\,|n+1\rangle+\sin\theta_n\,|+\rangle\,|n\rangle\ , \tag{4.7}$$

$$|-,n\rangle=-\sin\theta_n\,|-\rangle\,|n+1\rangle+\cos\theta_n\,|+\rangle\,|n\rangle\ , \tag{4.8}$$

where

$$\lambda_n=[\Delta^2+k^2(n+1)]^{1/2}\ . \tag{4.9}$$

and

$$\tan\theta_n=k(n+1)^{1/2}/(\lambda_n+\Delta)\ . \tag{4.10}$$

V. FERMION-ONLY MODEL HAMILTONIAN

We now set about the task of writing a fermion-only model Hamiltonian for the coupled fermion-boson system described by the Jaynes-Cummings Hamiltonian Eq. (4.1). H_{mod} will operate within the manifold

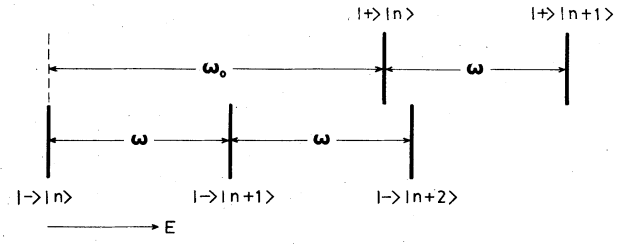

FIG. 1. Energy-levels scheme of the Jaynes-Cummings Hamiltonian in the uncoupled limit.

$$\Omega_{\text{mod}} \equiv \{ |+\rangle, |-\rangle \} , \tag{5.1}$$

its most general expression being

$$H_{\text{mod}} = C_0 \mathbb{1}_f + \vec{C} \cdot \vec{\sigma} , \tag{5.2}$$

where

$$\begin{aligned} \mathbb{1}_f &= |+\rangle\langle +| + |-\rangle\langle -| , \\ \vec{C} &= C_x \vec{i} + C_y \vec{j} + C_z \vec{k} , \\ \vec{\sigma} &= \sigma_x \vec{i} + \sigma_y \vec{j} + \sigma_z \vec{k} . \end{aligned} \tag{5.3}$$

The eigenvalues of H_{mod} are

$$E^{\pm} = C_0 \pm C , \tag{5.4}$$

where

$$C = |\vec{C}| = (C_x^2 + C_y^2 + C_z^2)^{1/2} . \tag{5.5}$$

If one is interested only in the energy splitting, taking C as the only adjustable parameter will do, but if directional properties are involved one should fit all three components of $\vec{C}$ from suitable experiments, C_0 usually being irrelevant because it gives only the zero of energies.

In order to derive H_{mod} from first principles we first have to write an appropriate effective Hamiltonian, which requires choosing the right reference Hamiltonian H_0. Decoupling the degrees of freedom requires the eigenvectors of H_{eff} to be direct products of fermionic and bosonic state vectors. It is then straightforward to project out the boson's degrees of freedom by taking matrix elements of H_{eff} with the bosonic state vectors. Property (c) of Sec. II shows that this goal may be achieved if H_0 is taken to be fully degenerate as regards the undesired degrees of freedom, so we may take it to be any purely fermionic operator.

It will prove convenient to write

$$H_0 = \Delta \sigma_z 1_b , \tag{5.6}$$

from which

$$V = \omega(a^\dagger a + \tfrac{1}{2}\sigma_z 1_b) + k(a^\dagger \sigma^- + a\sigma^+) , \tag{5.7}$$

where

$$1_b = \sum_n |n\rangle\langle n| \tag{5.8}$$

is the unit operator in the boson's space. The eigenvalues of H_0 are

$$e^{\pm} = \pm\Delta , \tag{5.9}$$

their degeneracies being infinite as the corresponding eigenvectors are $|\pm\rangle|n\rangle$ ($n=0, 1, 2, \ldots$). Using the notation discussed in connection with Eq. (2.11) one may write the Hermitian matrix

$$\underline{V} = \begin{matrix} \\ \langle + | \\ \langle - | \end{matrix} \begin{matrix} \begin{matrix} |+\rangle & |-\rangle \end{matrix} \\ \begin{bmatrix} V_{++} & V_{+-} \\ V_{-+} & V_{--} \end{bmatrix} \end{matrix} , \tag{5.10}$$

where

$$\begin{aligned} V_{++} &= \omega(a^\dagger a + \tfrac{1}{2}) , \\ V_{--} &= \omega(a^\dagger a - \tfrac{1}{2}) , \\ V_{+-} &= ka , \\ V_{-+} &= ka^\dagger . \end{aligned} \tag{5.11}$$

Equation (2.11) now reduces to

$$R_{+-}V_{-+}R_{+-} - V_{++}R_{+-} + R_{+-}V_{--} - V_{+-} + 2\Delta R_{+-} = 0 , \tag{5.12a}$$

$$R_{-+}V_{+-}R_{-+} - V_{--}R_{-+} + R_{-+}V_{++} - V_{-+} - 2\Delta R_{-+} = 0 , \tag{5.12b}$$

where we have used $R_{++} = R_{--} = 1_b$. From the symmetry property Eq. (3.6) with $Q = C_1$ it is straightforward to prove that

$$-V_{++}R_{+-} + R_{+-}V_{--} = 0 , \tag{5.13a}$$

$$-V_{--}R_{-+} + R_{-+}V_{++} = 0 . \tag{5.13b}$$

Equations (5.12) may then be rewritten

$$X_+^2 - 2\Delta X_+ = V_{+-}V_{-+} = k^2 aa^\dagger , \tag{5.14a}$$

$$X_-^2 + 2\Delta X_- = V_{-+}V_{+-} = k^2 a^\dagger a , \tag{5.14b}$$

where

$$X_\pm = V_{\pm\mp}R_{\mp\pm} \tag{5.15}$$

may be solved to give

$$X_+ = \Delta - (\Delta^2 + k^2 aa^\dagger)^{1/2} , \tag{5.16a}$$

$$X_- = -\Delta + (\Delta^2 + k^2 a^\dagger a)^{1/2} . \tag{5.16b}$$

The signs of the square roots have been chosen in accordance with Eq. (2.12). Equations (5.12) may now be written

$$R_{+-}X_- - ka + 2\Delta R_{+-} = 0 , \tag{5.17a}$$

$$R_{-+}X_+ - ka^\dagger - 2\Delta R_{-+} = 0 , \tag{5.17b}$$

which from Eqs. (5.16) immediately give

$$R_{+-} = kaI_1 , \tag{5.18a}$$

$$R_{-+} = ka^\dagger I_2 , \tag{5.18b}$$

where

$$I_1 = 1/[\Delta + (\Delta^2 + k^2 a^\dagger a)^{1/2}] = I_1^\dagger , \tag{5.19a}$$

$$I_2 = -1/[\Delta + (\Delta^2 + k^2 aa^\dagger)^{1/2}] = I_2^\dagger . \tag{5.19b}$$

Therefore

$$\underline{R} = \begin{bmatrix} 1_b & kaI_1 \\ ka^\dagger I_2 & 1_b \end{bmatrix} , \tag{5.20}$$

$$\underline{R} = \begin{bmatrix} 1_b & kI_2 a \\ kI_1 a^\dagger & 1_b \end{bmatrix} . \tag{5.21}$$

In order to find the wave operator S [Eq. (2.6)], which

defines both the effective Hamiltonian Eq. (2.3) and the actual eigenvectors Eq. (2.2), one needs

$$\underline{R}^{\dagger}\underline{R}=\begin{bmatrix}1_b+k^2I_2aa^{\dagger}I_2 & 0\\ 0 & 1+k^2I_1a^{\dagger}aI_1\end{bmatrix}, \tag{5.22}$$

where we have used some straightforward relations such as

$$(aI_1+I_2a)\,|\,n\,\rangle=0\,.$$

As $\underline{R}^{\dagger}\underline{R}$ is diagonal and positive definite[10] it follows at once that

$$\underline{S}=\underline{R}(\underline{R}^{\dagger}\underline{R})^{-1/2}=\begin{bmatrix}(1_b+k^2I_2aa^{\dagger}I_2)^{-1/2} & kaI_1(1_b+k^2I_1a^{\dagger}aI_1)^{-1/2}\\ ka^{\dagger}I_2(1_b+k^2I_2aa^{\dagger}I_2)^{-1/2} & (1_b+k^2I_1a^{\dagger}aI_1)^{-1/2}\end{bmatrix}. \tag{5.23}$$

The effective Hamiltonian Eq. (2.3) is thus given by

$$\begin{aligned}H_{\text{eff}}&=S^{-1}HS\\&=\tfrac{1}{2}\omega_0\sigma_z+\tfrac{1}{2}\omega a^{\dagger}a+\tfrac{1}{2}k^2(a^{\dagger}aI_1+aa^{\dagger}I_2)\\&\quad+\tfrac{1}{2}k^2\sigma_z(aa^{\dagger}I_2-a^{\dagger}aI_1)\,.\end{aligned} \tag{5.24}$$

The eigenvectors of H_{eff} are easily found to be

$$|\,+\,\rangle_{\text{eff}}=\begin{bmatrix}|\,n\,\rangle\\ 0\end{bmatrix},\quad |\,-\,\rangle_{\text{eff}}=\begin{bmatrix}0\\ |\,n\,\rangle\end{bmatrix}. \tag{5.25}$$

The eigenvectors of H are therefore

$$\underline{S}\begin{bmatrix}|\,n\,\rangle\\ 0\end{bmatrix}=\begin{bmatrix}S_{++}\,|\,n\,\rangle\\ S_{-+}\,|\,n\,\rangle\end{bmatrix}=\begin{bmatrix}\cos\theta_n\,|\,n\,\rangle\\ -\sin\theta_n\,|\,n+1\rangle\end{bmatrix}, \tag{5.26a}$$

$$\underline{S}\begin{bmatrix}0\\ |\,n\,\rangle\end{bmatrix}=\begin{bmatrix}S_{+-}\,|\,n\,\rangle\\ S_{--}\,|\,n\,\rangle\end{bmatrix}=\begin{bmatrix}\sin\theta_{n-1}\,|\,n-1\rangle\\ \cos\theta_{n-1}\,|\,n\,\rangle\end{bmatrix}, \tag{5.26b}$$

where θ_n is given by Eq. (4.10). In the same fashion it may be shown that the eigenvectors are those given by Eq. (4.6), thus verifying all the given results.

We now undertake the task of writing the model Hamiltonian H_{mod}. For that purpose it is fundamental to clearly establish what one expects from H_{mod}. From the eigenvalue equation

$$H_{\text{mod}}\,|\,\alpha\,\rangle_{\text{mod}}=(E_0+E_\alpha)\,|\,\alpha\,\rangle_{\text{mod}}\,, \tag{5.27}$$

one wishes to obtain the true eigenvalues E_α apart perhaps from a uniform energy shift E_0. In practice one also expects to be able to determine the expectation value of any physical fermionic operator F from the formula

$$\langle F\rangle={}_{\text{mod}}\langle\alpha\,|\,\tilde{F}\,|\,\alpha\,\rangle_{\text{mod}}=\langle\tilde{F}\rangle_{\text{mod}}\,, \tag{5.28}$$

where $\tilde{F}$ is a suitable renormalized operator.

One would moreover like $\langle\tilde{F}\rangle_{\text{mod}}$ to obey the standard equation of motion (Ehrenfest's theorem)

$$i\hbar\frac{d}{dt}\langle\tilde{F}\rangle_{\text{mod}}=\langle[\tilde{F},H_{\text{mod}}]\rangle_{\text{mod}}+i\hbar\left\langle\frac{\partial\tilde{F}}{\partial t}\right\rangle_{\text{mod}} \tag{5.29}$$

so that the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\,|\,\alpha\,\rangle_{\text{mod}}=H_{\text{mod}}\,|\,\alpha\,\rangle_{\text{mod}} \tag{5.30}$$

should be satisfied. Let us analyze how this may come about in our formulation. Assume the combined system to be in an arbitrary initial state

$$|\,\psi(0)\rangle=\sum_\alpha C_\alpha\,|\,\alpha\,\rangle\,. \tag{5.31}$$

It is then immediately found from Eqs. (2.2), (2.6), and (5.25) that

$$\begin{aligned}F(0)&=\langle\psi(0)\,|\,F\,|\,\psi(0)\rangle\\&=\sum_\alpha\sum_\beta c_\alpha^{*}c_\beta\langle\alpha\,|\,F\,|\,\beta\rangle\\&=\sum_\alpha\sum_\beta c_\alpha^{*}c_{\beta\,\text{eff}}\langle\alpha\,|\,S^{\dagger}FS\,|\,\beta\rangle_{\text{eff}}\\&=\sum_{j,n}\sum_{j',n'}c_{jn}^{*}c_{j'n'}\langle j\,|\,(\langle n\,|\,S^{\dagger}FS\,|\,n'\rangle)\,|\,j'\rangle\,,\end{aligned} \tag{5.32}$$

where

$$|\,j\,\rangle=|\,+\,\rangle,|\,-\,\rangle \tag{5.33}$$

are the fermionic state vectors. The fulfillment of Eq. (5.28) requires the existence of the fermion-only operator $\tilde{F}$, which in turn forces the factorization

$$c_{jn}=d_jd_n\,. \tag{5.34}$$

If such is the case, it follows at once that

$$\tilde{F}=\langle b\,|\,S^{\dagger}FS\,|\,b\,\rangle=\langle S^{\dagger}FS\rangle_{\text{boson}}\,, \tag{5.35}$$

where

$$|\,b\,\rangle=\sum_n d_n\,|\,n\,\rangle\,, \tag{5.36}$$

and Eq. (5.28) is satisfied with

$$|\,\alpha\,\rangle_{\text{mod}}=\sum_j d_j\,|\,j\,\rangle\,. \tag{5.37}$$

It may be shown that condition (5.34) is a necessary and sufficient condition for the fulfillment of Eq. (5.30) (see Appendix). The model Hamiltonian H_{mod} is but the renormalized fermion operator

$$H_{\text{mod}}=\tilde{H}=\langle H_{\text{eff}}\rangle_{\text{boson}}=C_0 1_f+\vec{\mathrm{C}}\cdot\vec{\sigma}\,, \tag{5.38}$$

where

$$\begin{aligned}C_0&=\tfrac{1}{2}\omega a^{\dagger}a+k^2\langle a^{\dagger}aI_1+aa^{\dagger}I_2\rangle_{\text{boson}}\,,\\C_x&=0=C_y\\C_z&=\tfrac{1}{2}\omega_0+\tfrac{1}{2}k^2\langle aa^{\dagger}I_2-a^{\dagger}aI_1\rangle_{\text{boson}}\end{aligned} \tag{5.39}$$

are the model's adjustable parameters Eq. (5.2). One may then say the fermion energy ω_0 is renormalized to

$$\omega_0' = \omega_0 + k^2 \langle aa^\dagger I_2 - a^\dagger a I_1 \rangle_{\text{boson}} \tag{5.40}$$

due to the interaction with the bosons, or that the particle described by H_{mod} is a quasifermion.

It is easy to realize that the only case in which c_{jn} may be factorized is when $|\psi(0)\rangle$ involves a single nondegenerate boson state. In this case no energy is exchanged between the fermions and the bosons, and the last subsystem acts only as a scleronomous constraint. One may then write a fermion-only Hamiltonian which satisfies the standard time-dependent Schrödinger equation. A detailed mathematical proof of these statements is given in the Appendix. Whether or not such a factorization is realized in practice depends on the experiments performed on the system, because if the excitation energies are such that the number n of bosons is fixed, H_{mod} is well defined, although its parameters will change if n changes. In the case where these requirements are not satisfied a model Hamiltonian can render only an approximate description of the actual fermion's behavior. If, for instance, energy transitions are allowed between boson states, the time evolution of the fermion-only Hamiltonian will not be given by the time-dependent Schrödinger equation, but by a more complicated nonlinear one corresponding to a dissipative system.[24] Although this problem is of great practical importance,[25] it is beyond the range of this work.

VI. CONCLUSIONS

The experience gained in the discussion of Sec. V makes it easier to generalize the method for writing model Hamiltonians, which is the goal of this section. Let H_a and H_b be the Hamiltonians corresponding to different sets of nonidentical particles and $H_{a\text{-}b}$ the interaction term. Thus the closed-system Hamiltonian is

$$H = H_a + H_b + H_{a\text{-}b} \ . \tag{6.1}$$

We are interested only in the a-type particles for which we wish to write a model Hamiltonian H_{mod} describing their properties in a certain energy range. This energy range is determined by the set of experiments made on the system, from which it should be possible to guess both the number of a states involved and its approximate nature. One should therefore have a set of approximate state vectors $\{|\varphi\rangle_a\}$ which define the domain Ω_{mod} of H_{mod},

$$\Omega_{\text{mod}} \equiv \{|\varphi\rangle_a\} \ . \tag{6.2}$$

In the case of the Jaynes-Cummings Hamiltonian Ω_{mod} has been taken to be the domain Ω_a of H_a, but this need not be so and in the general case

$$\Omega_a = \Omega_{\text{mod}} + \Omega_{\text{mod}}' \ , \tag{6.3}$$

where Ω_{mod}' is the orthogonal complement of Ω_{mod}.

One may now define an effective Hamiltonian H_{eff} associated with both H and the reference Hamiltonian

$$H_0 = O_a 1_b \ , \tag{6.4}$$

where O_a is any a-type operator and 1_b is the unit operator for b-type particles. In the simplest case one may take $O_a = H_a$, which is probably a good starting point for a perturbative determination of H_{eff} when $H_{a\text{-}b}$ is small, but this is not mandatory. In general one need only ask that the basis vectors $\{|\varphi\rangle_a\}$ which define Ω_{mod} be not only eigenvectors of H_0 with some set of eigenvalues $\{e_a\}$, but the only eigenvectors with those eigenvalues. This ensures that all the states required by the defining set of experiments are included in H_{mod}, and only them.

As H_{mod} should be both Hermitian and invariant under the symmetry group of H, so should H_{eff}. The simplest effective Hamiltonian fulfilling this condition is the Hermitian-symmetric one previously discussed.[10] One has now to find the exact or approximate solutions of Eq. (2.7) or (2.11) in order to obtain the wave operator S from Eq. (2.6) and H_{eff} from Eq. (2.3). Approximate solutions may be obtained by iterative methods, one of which is the degenerate Rayleigh-Schrödinger perturbation theory,[11] or by a self-consistent numerical solution of Eq. (2.7). The choice of Eq. (6.4) ensures that the eigenvalue Eq. (2.1) has the solutions

$$|\alpha_{\text{eff}}\rangle = |\varphi\rangle_a \, |\chi\rangle_b \ , \tag{6.5}$$

thus showing the a-type and b-type particles to be decoupled in this representation. This is not true if the two sets consist of identical particles because then one has still to deal with the mixing due to the symmetrical or antisymmetrical nature of the total state vector.

In the case where the experimental situation ensures that only a single state $|\chi\rangle_b$ is involved, the model Hamiltonian is given by

$$H_{\text{mod}} = {}_b\langle\chi| H_{\text{eff}} |\chi\rangle_b \tag{6.6}$$

and the expectation value of any physical magnitude A of the a system may be evaluated by the formula

$$\langle A \rangle = {}_a\langle\varphi| \tilde{A} |\varphi\rangle_a \ , \tag{6.7}$$

where

$$\tilde{A} = {}_b\langle\chi| S^\dagger A S |\chi\rangle_b \ . \tag{6.8}$$

Here $|\varphi\rangle_a$ satisfies the usual time-dependent Schrödinger equation and $\langle\tilde{A}\rangle_a$ satisfies Ehrenfest's theorem. If the state of the b subsystem is not uniquely determined by the experimental conditions, a model Hamiltonian can render only an approximate though perhaps very good description of the a subsystem, the nature of such an approximation being outside the scope of this paper.

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APPENDIX

In what follows we use the notation of Sec. VI. Let $|j\rangle_a$ and $|l\rangle_b$ be the eigenvectors of the separated subsystems

$$H_a |j\rangle_a = e_j^{(a)} |j\rangle_a, \quad H_b |l\rangle_b = e_l^{(b)} |l\rangle_b \ , \tag{A1}$$

where

$$ {}_{\alpha}\langle j \mid k \rangle_{\alpha} = \delta_{jk} \quad \text{for } \alpha = 1,2 \, . \tag{A2} $$

The eigenvector $|\psi\rangle$ of the combined system satisfies the time-dependent Schrödinger equation

$$ H \mid \psi \rangle = i\hbar \frac{\partial}{\partial t} \mid \psi \rangle \, , \tag{A3} $$

where H is given by Eq. (6.1). Assuming that

$$ \mid \psi \rangle = \sum_j \sum_l c_{jl}(t) \mid j \rangle_a \mid l \rangle_b \, , \tag{A4} $$

from the normalization condition $\langle \psi \mid \psi \rangle = 1$ it follows that

$$ \sum_j \sum_l \mid c_{jl}(t) \mid^2 = 1 \, . \tag{A5} $$

If A is any operator on subsystem a, its time-dependent expectation value is given by

$$ \langle A \rangle = \langle \psi \mid A \mid \psi \rangle = \sum_j \sum_k \rho^{(a)}_{kj}(t) \, {}_a\langle j \mid A \mid k \rangle_a \, , \tag{A6} $$

where

$$ \rho^{(a)}_{kj} = \sum_l c_{kl}(t) c^*_{jl}(t) \tag{A7} $$

is the reduced density matrix of subsystem a.[26] The necessary condition for subsystem a to be describable by a new Hamiltonian $\tilde{H}_a$ such that

$$ \tilde{H}_a \mid \psi \rangle_a = i\hbar \frac{\partial}{\partial t} \mid \psi \rangle_a \, , \tag{A8} $$

where

$$ \mid \psi \rangle_a = \sum_j a_j(t) \mid j \rangle_a \, , \tag{A9} $$

is that it should be possible to write

$$ \begin{aligned} \langle A \rangle &= \langle \psi \mid A \mid \psi \rangle = {}_a\langle \psi \mid \tilde{A} \mid \psi \rangle_a \\ &= \sum_j \sum_k a_j(t)^* a_k(t) \, {}_a\langle j \mid A \mid k \rangle_a \, . \end{aligned} \tag{A10} $$

Comparing Eqs. (A6) and (A10), it is therefore required that

$$ \rho^{(a)}_{kj} = a_k a^*_j \, . \tag{A11} $$

It is easily shown that condition (A11) is sufficient for the fulfillment of Eqs. (A8) and (A9) as it corresponds to the case of a pure state[27] where

$$ \mathrm{Tr}\{\rho^{(a)^2}\} = 1 \, . \tag{A12} $$

Because $\underline{\rho}^{(a)}$ is an Hermitian matrix it may be diagonalized by a unitary change of basis

$$ \mid J \rangle_a = \sum_j \mid j \rangle_a Q_{jJ} \tag{A13} $$

such that

$$ \underline{Q}^{\dagger} \underline{\rho}^{(a)} \underline{Q} = \underline{d} \, , \tag{A14} $$

where

$$ d_{JK} = \delta_{JK} d_{JJ} \, , \tag{A15} $$

and

$$ \underline{Q}^{\dagger} = \underline{Q}^{-1} \, . $$

From Eqs. (A14), (A11), (A9), and (A15) we obtain

$$ d_{JK} = f_J f^*_K = \delta_{JK} \mid f_J \mid^2 \, , \tag{A16} $$

where

$$ f_J = \sum_j a_j Q^*_{jJ} \, . \tag{A17} $$

Equation (A16) may be satisfied only if f_J differs from zero only for a single value of J, say $J = N$. In the new basis [Eq. (A13)] the effective state vector Eq. (A9) may be written

$$ \mid \psi \rangle_a = \sum_J f_J \mid J \rangle_a = f_N \mid N \rangle_a \, , \tag{A18} $$

where from normalization

$$ \mid f_N \mid = 1 \, . \tag{A19} $$

In the same fashion it is now straightforward to show that in the new representation the combined system's state vector may be written as the external product

$$ \mid \psi \rangle = \mid N \rangle_a \mid \phi \rangle_b \, , \tag{A20} $$

where

$$ \mid \phi \rangle_b = \sum_l C_{Nl} \mid l \rangle_b \, , \tag{A21} $$

$$ C_{Jl} = \sum_k Q^*_{kJ} C_{kl} \, . \tag{A22} $$

Equation (A10) is therefore satisifed if and only if the system's state vector is factorized. It would seem that such a stringent condition may only be satisfied for noninteracting subsystems, that is, $H_{a\text{-}b} = 0$. Actually, this is not necessarily so, as is shown below.

Let $T(t)$ be the time-development operator[28]

$$ T(t) \mid \psi(0) \rangle = \mid \psi(t) \rangle \tag{A23} $$

and $\Omega^{(0)}$ the manifold spanned by the time evolution of $|\psi(t)\rangle$,

$$ \Omega^{(0)} = \Omega^{(0)}_a \times \Omega^{(0)}_b \, . \tag{A24} $$

In order for the time evolution of subsystem a to be that of an isolated system within $\Omega^{(0)}$ it should be

$$ P_0 T(t) P_0 = e^{-iP_0 H P_0 t/\hbar} = e^{-i\tilde{H}_a t/\hbar} e^{-i\tilde{H}_b t/\hbar} \, , \tag{A25} $$

where

$$ [\tilde{H}_a, \tilde{H}_b] = 0 \, . $$

Therefore

$$ P_0 H P_0 = P_0 (H_a + H_b + H_{a\text{-}b}) P_0 = \tilde{H}_a + \tilde{H}_b \, , \tag{A26} $$

and it should be

$$ P_0 H_{a\text{-}b} P_0 = I_a 1_b + I_b 1_a \, . \tag{A27} $$

Equation (A27) is satisfied by a general interaction $H_{a\text{-}b}$ if and only if the manifold $\Omega^{(0)}_a$ is one dimensional.

Therefore, if subsystem a interacts with subsystem b

the time evolution of a is that of an isolated system if and only if the state of subsystem b remains constant. In practice this condition is fulfilled if b has a ground nondegenerate state and the energy of interaction with a is less than that required for a transition to b's first excited state. A little reflection shows that this condition is satisfied in all cases where model Hamiltonians successfully apply.

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