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A method to calculate effective Hamiltonians in quantum information*

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Effective Hamiltonian method is widely used in quantum information. We introduce a method to calculate effective Hamiltonians and give two examples in quantum information to demonstrate the method. We also give a relation between the effective Hamiltonian in the Shrödinger picture and the corresponding effective Hamiltonian in the interaction picture. Finally, we present a relation between our effective Hamiltonian method and the James–Jerke method which is currently used by many authors to calculate effective Hamiltonians in quantum information science.

Keywords: effective Hamiltonian, method, quantum information

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1. Introduction

Effective Hamiltonians may play important roles in analyzing quantum mechanical systems. When a complicated model Hamiltonian is studied, the method of effective Hamiltonian can be used to obtain some of its approximate eigenvalues and eigenstates, which can usually give some basic physics behind the model. Therefore it is an important problem to calculate the effective Hamiltonian from the original complicated Hamiltonian. Much progress has been made on this topic.[1,2]

As the development of quantum information and quantum optics, it becomes common to use effective Hamiltonians in quantum entangled state preparation and quantum gate construction.[3–9] The method to calculate effective Hamiltonians presented by James and Jerke has been widely used in the fields of quantum information and quantum optics.[10,11] Their basic idea is to consider a time-dependent Hamiltonian in the interaction picture and to delete the high frequency terms of the corresponding time evolution operator. Recently their effective Hamiltonian method has been generalized to the higher-order cases.[12]

In this paper, a new method is introduced to calculate effective Hamiltonians in the Shrödinger picture and in the interaction picture. The new method to calculate effective Hamiltonians is quite different from the one given by James and Jerke,[10] and our method is demonstrated by two examples in quantum information. Based on the second example, a caution of using the James–Jerke effective Hamiltonian method is given. Finally, we present a relation between the new effective Hamiltonian method and the James–Jerke method. The new method provides an alternative way to calculate effective Hamiltonians, which can be used in many fields such as quantum information science.

2. Effective Hamiltonian in the Shrödinger picture

Consider a Hamiltonian H acting on a D-dimensional Hilbert space Ω, which is divided into a subspace $P\Omega$ and the corresponding complementary subspace $Q\Omega$. The projectors onto the two subspaces, denoted by P and Q, satisfy the following conditions

$$P+Q=I, \quad PQ=0, \tag{1}$$

where I is the identity operator, and the dimension of the subspace $P\Omega$ is assumed to be d ($d<D$). Choose d normalized eigenstates of H satisfying

$$H|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle, \quad \alpha=1,2,\ldots,d. \tag{2}$$

The projections of these eigenstates onto the subspace $P\Omega$ are

$$|\phi_\alpha\rangle = P|\Psi_\alpha\rangle. \tag{3}$$

The effective Hamiltonian $H_{\rm eff}$ defined on the subspace $P\Omega$, i.e., $H_{\rm eff}=PH_{\rm eff}P$, is an operator satisfying[1,2]

$$H_{\rm eff}|\phi_\alpha\rangle = E_\alpha|\phi_\alpha\rangle, \quad \alpha=1,2,\ldots,d. \tag{4}$$

This definition of effective Hamiltonian is dependent on the choice of the projector P and the d eigenstates $|\Psi_\alpha\rangle$ of H.

The Hamiltonian researchers are interested in can be usually written as

$$H=H_0+V, \tag{5}$$

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where H_0 is assumed to have the known spectral decomposition

$$H_0 = \sum_{n=1}^{N} E_n P_n, \tag{6}$$

and V can be regarded as a perturbation. Define the projector onto the subspace $P\Omega$ as

$$P = \sum_{m \in S_P} P_m, \tag{7}$$

where P_m are projectors of Eq. (6) and S_P is a subset of $\{1,2,\ldots,N\}$. Equaiton (7) specifies the subspace $P\Omega$. The effective Hamiltonian $H_{\rm eff}$ on the subspace $P\Omega$ according to the definition in Eq. (4) can be written as

$$H_{\rm eff} = PH_0P + \nu, \tag{8}$$

where $\nu = P\nu P$ is called the effective interaction.[2] In the above, the eigenstates of H in defining the effective Hamiltonian are required to approach the eigenstates of PH_0P in the limit $V \to 0$.

The effective interaction ν can be expanded in powers of V,[2] i.e.,

$$\nu = \nu^{(1)} + \nu^{(2)} + \nu^{(3)} + \cdots, \tag{9}$$

where the first three terms are

$$\nu^{(1)} = PVP, \tag{10}$$

$$\nu^{(2)} = PV(V)P, \tag{11}$$

$$\nu^{(3)} = P[V(V(V)) - V((V)V)]P. \tag{12}$$

In the above, the notation (A) means that it is an operator only taking the states in subspace $P\Omega$ to its complementary subspace $Q\Omega$, and its definition is

$$(A) = \sum_{x \notin S_p} \sum_{y \in S_p} \frac{1}{E_y - E_x} P_x A P_y, \tag{13}$$

when E_x and E_y are eigenvalues of H_0; P_x and P_y are projectors given in Eq. (6). The above expression of (A) will be used to calculate the operator (V), $(V(V))$ and $((V)V)$ in the powers of V.

In principle, many terms of the effective interaction ν in Eq. (9) can be calculated. However when V can be considered as a perturbation, i.e., when there is

$$\frac{\max|\langle m|V|n\rangle|}{\min_{x\notin S_p, y\in S_p}|E_x - E_y|} \ll 1, \tag{14}$$

where $|m\rangle$ and $|n\rangle$ are the eigenstates of H_0, it will be a good approximation to take the first two terms of ν as its approximation. In this situation, the effective Hamiltonian $H_{\rm eff}$ is approximately

$$H_{\rm eff} = PH_0P + PVP + PV(V)P, \tag{15}$$

where the operator (V) can be calculated according to Eq. (13). The last term of $H_{\rm eff}$ in Eq. (15) represents the indirect interaction within the subspace $P\Omega$ with the help of states in the subspace $Q\Omega$, which can be seen from the fact that $PV(V)P = PVQ(V)P$.

3. Effective Hamiltonian in the interaction picture

Quantum problems are often considered in the interaction picture. The original Hamiltonian H of Eq. (5) in the Schrödinger picture will be changed into

$$H_I = {\rm e}^{{\rm i}H_0 t/\hbar} V {\rm e}^{-{\rm i}H_0 t/\hbar} \tag{16}$$

in the interaction picture.[13] As discussed in the above section, we will show how to calculate the effective Hamiltonian on the subspace $P\Omega$ that is specified by its projector P given in Eq. (7).

Denote the effective Hamiltonian of H_I on the subspace $P\Omega$ as $H_{I,\rm eff}$. Rewrite the interaction Hamiltonian H_I as

$$H_I = {\rm e}^{{\rm i}H_0 t/\hbar} H {\rm e}^{-{\rm i}H_0 t/\hbar} - H_0. \tag{17}$$

Noting that the effective Hamiltonian of H on the subspace $P\Omega$ is $H_{\rm eff}$ and the operator P commute with ${\rm e}^{{\rm i}H_0\, t/\hbar}$, we have

$$H_{I,\rm eff} = {\rm e}^{{\rm i}H_0 t/\hbar} H_{\rm eff} {\rm e}^{-{\rm i}H_0 t/\hbar} - PH_0P. \tag{18}$$

Equation (18) shows the relation between the effective Hamiltonian in the Schrödinger picture and that in the interaction picture. When V can be considered as a perturbation, substituting Eq. (15) into Eq. (18) yields

$$\begin{aligned} H_{I,\rm eff} &= {\rm e}^{{\rm i}H_0 t/\hbar}\{PVP + PV(V)P\}{\rm e}^{-{\rm i}H_0 t/\hbar} \\ &= PH_IP + PH_I(H_I)P \\ &= PH_IP + PH_IQ(QH_IP), \end{aligned} \tag{19}$$

where (QH_IP) should be calculated according to Eq. (13). It can be found that $H_{I,\rm eff}$ in Eq. (19) may not be a Hermitian operator. In the following the Hermitian operator

$$\mathscr{H}_{I,\rm eff} = \frac{1}{2}[H_{I,\rm eff} + H_{I,\rm eff}^{\dagger}] \tag{20}$$

will be used as the effective Hamiltonian similarly to the James–Jerke effective Hamiltonian method.[10]

4. Two demonstration examples

Now we give two examples to demonstrate how to get the effective Hamiltonian. These examples are often used in quantum information and quantum optics. The second example will give a caution about using the James–Jerke effective Hamiltonian method.

4.1. Raman transition

Consider the case of a three-level atom interacting with two classical optical fields. The Hamiltonian in the interaction picture is ($\hbar = 1$)

$$H_I = \frac{\Omega_1}{2}|3\rangle\langle 1|\exp(-\mathrm{i}\Delta_1 t) + \frac{\Omega_2}{2}|3\rangle\langle 2|\exp(-\mathrm{i}\Delta_2 t) + \mathrm{H.c.}, \quad (21)$$

which can be written as $H_I = \mathrm{e}^{\mathrm{i}H_0 t} V \mathrm{e}^{-\mathrm{i}H_0 t}$ with

$$H_0 = \Delta_1|1\rangle\langle 1| + \Delta_2|2\rangle\langle 2|, \quad (22)$$

$$V = \frac{\Omega_1}{2}|3\rangle\langle 1| + \frac{\Omega_2}{2}|3\rangle\langle 2| + \mathrm{H.c.} \quad (23)$$

In the above, H_0 is already in its spectral decomposition form. Specify the subspace $P\Omega$ and $Q\Omega$ by their projectors

$$P = |1\rangle\langle 1| + |2\rangle\langle 2|, \quad Q = |3\rangle\langle 3|. \quad (24)$$

When there is

$$\frac{\max\{|\Omega_1|, |\Omega_2|\}}{\min\{|\Delta_1|, |\Delta_2|\}} \ll 1, \quad (25)$$

we can use Eqs. (19) and (20) to calculate the effective Hamiltonian. Note that $PH_IP = 0$, from Eqs. (19) and (20) we can find that the effective Hamiltonian on the subspace $P\Omega$ is

$$\mathscr{H}_P = \frac{|\Omega_1|^2}{4\Delta_1}|1\rangle\langle 1| + \frac{|\Omega_2|^2}{4\Delta_2}|2\rangle\langle 2| + \frac{\Omega_1^*\Omega_2}{4\bar{\Delta}}|1\rangle\langle 2|\mathrm{e}^{\mathrm{i}\delta t} + \frac{\Omega_1\Omega_2^*}{4\bar{\Delta}}|2\rangle\langle 1|\mathrm{e}^{-\mathrm{i}\delta t}, \quad (26)$$

where $\delta = \Delta_1 - \Delta_2$ and

$$\frac{1}{\bar{\Delta}} = \frac{1}{2}\left(\frac{1}{\Delta_1} + \frac{1}{\Delta_2}\right). \quad (27)$$

Similarly, the effective Hamiltonian on the subspace $Q\Omega$ is

$$\mathscr{H}_Q = -\frac{|\Omega_1|^2}{4\Delta_1}|3\rangle\langle 3| - \frac{|\Omega_2|^2}{4\Delta_2}|3\rangle\langle 3|. \quad (28)$$

It can be found that $\mathscr{H}_P + \mathscr{H}_Q$ is the same as the effective Hamiltonian obtained from the James–Jerke method.[10] This result demonstrates a connection between the effective Hamiltonian method presented in this paper and the James–Jerke method, which will be discussed in the next section.

4.2. Two atoms interacting with one quantum optical field

Consider two same two-level atoms simultaneously interacting with one single-mode cavity field. This is a famous model that has been used to generate two-atom maximally entangled states and realize quantum logic gates.[14] The Hamiltonian in the interaction picture is ($\hbar = 1$)

$$H_I = g\sum_{j=1,2}(\hat{a}^\dagger\sigma_j\exp(-\mathrm{i}\Delta t) + \mathrm{H.c.}), \quad (29)$$

where $\sigma_j = |g_j\rangle\langle e_j|$, $\sigma_j^\dagger = |e_j\rangle\langle g_j|$, $|e_j\rangle$ and $|g_j\rangle$ are the excited and ground states of the jth atom, $\hat{a}^\dagger$ and $\hat{a}$ are the creation and annihilation operators of the cavity field, and g is the atom-cavity coupling strength.

The interaction Hamiltonian H_I can be written as $H_I = \mathrm{e}^{\mathrm{i}H_0 t} V \mathrm{e}^{-\mathrm{i}H_0 t}$ with

$$H_0 = \frac{1}{2}\Delta\sum_{j=1,2}(|e_j\rangle\langle e_j| - |g_j\rangle\langle g_j|), \quad (30)$$

$$V = g\sum_{j=1,2}(\hat{a}^\dagger\sigma_j + \hat{a}\sigma_j^\dagger). \quad (31)$$

The spectral decomposition of H_0 is

$$H_0 = \sum_{n=0}^{+\infty}E_{0n}P_{0n} + \sum_{n=0}^{+\infty}E_{1n}P_{1n} + \sum_{n=0}^{+\infty}E_{2n}P_{2n}, \quad (32)$$

with the eigenvalues

$$E_{0n} = -\Delta, \quad E_{1n} = 0, \quad E_{2n} = \Delta, \quad (33)$$

and the projectors

$$P_{0n} = |f_{gg}\rangle\langle f_{gg}| \otimes |n\rangle\langle n|, \quad (34)$$

$$P_{1n} = \{|f_{ge}\rangle\langle f_{ge}| + |f_{eg}\rangle\langle f_{eg}|\} \otimes |n\rangle\langle n|,$$

$$P_{2n} = |f_{ee}\rangle\langle f_{ee}| \otimes |n\rangle\langle n|, \quad (35)$$

where $|n\rangle$ is the Fock state for the cavity field and

$$|f_{gg}\rangle = |g_1\rangle \otimes |g_2\rangle, \quad |f_{ge}\rangle = |g_1\rangle \otimes |e_2\rangle, \quad (36)$$

$$|f_{eg}\rangle = |e_1\rangle \otimes |g_2\rangle, \quad |f_{ee}\rangle = |e_1\rangle \otimes |e_2\rangle. \quad (37)$$

We first consider the effective Hamiltonian on the subspace $P_{1n}\Omega$, which is an interesting subspace with one atom in the excitation state. Note that the interaction Hamiltonian H_I conserves the excitation number, i.e., the number of atoms in the excited state plus the number of photon in the cavity field, and the states in subspace $P_{in}\Omega$ have $i+n$ excitations, there is

$$P_{1n}H_I\bar{P}_{1n} = P_{1n}H_IP_{0(n+1)} + P_{1n}H_IP_{2(n-1)}, \quad (38)$$

$$(\bar{P}_{1n}H_IP_{1n}) = \frac{1}{\Delta}P_{0(n+1)}H_IP_{1n} - \frac{1}{\Delta}P_{2(n-1)}H_IP_{1n}, \quad (39)$$

where $\bar{P}_{1n} = I - P_{1n}$ is the projector onto the complementary subspace of $P_{1n}\Omega$. According to Eqs. (19) and (20) we can find that the effective Hamiltonian on the subspace $P_{1n}\Omega$ will be

$$\mathscr{H}_{P_{1n}} = P_{1n}H_I\bar{P}_{1n}(\bar{P}_{1n}H_IP_{1n}) = \frac{1}{\Delta}P_{1n}VP_{0(n+1)}VP_{1n} - \frac{1}{\Delta}P_{1n}VP_{2(n-1)}VP_{1n}. \quad (40)$$

Using Eqs. (38) and (39), we have obtained Eq. (40). It is not difficult to find

$$P_{0(n+1)}VP_{1n} = g\sqrt{n+1}|f_{gg}\rangle(\langle f_{eg}| + \langle f_{ge}|) \otimes |n+1\rangle\langle n|, \quad (41)$$

$$P_{2(n-1)}VP_{1n} = g\sqrt{n}|f_{ee}\rangle(\langle f_{eg}| + \langle f_{ge}|) \otimes |n-1\rangle\langle n|. \quad (42)$$

Substituting Eqs. (41) and (42) into Eq. (40) yields

$$\mathscr{H}_{P_{1n}} = \frac{g^2}{\Delta}(|f_{eg}\rangle + |f_{ge}\rangle)(\langle f_{eg}| + \langle f_{ge}|) \otimes |n\rangle\langle n|$$

$$= \frac{g^2}{\Delta}P_{1n} + \frac{g^2}{\Delta}\{\sigma_1^\dagger \otimes \sigma_2 + \sigma_1 \otimes \sigma_2^\dagger\} \otimes |n\rangle\langle n|, \quad (43)$$

which shows that there is a coupling between two atoms, this is because they both have a coupling with the cavity field in the interaction Hamiltonian. We note that the above effective Hamiltonian $\mathscr{H}_{P_{1n}}$ in Eq. (43) is acceptable only when there is

$$\left|\frac{g\sqrt{n+1}}{\Delta}\right| \ll 1, \quad (44)$$

i.e., the coupling strength between the subspace $P_{1n}\Omega$ and $P_{0(n+1)}\Omega$ given in Eq. (41) should be much smaller than the energy gap. Even if there is $|g/\Delta| \ll 1$, the effective Hamiltonian $\mathscr{H}_{P_{1n}}$ in Eq. (43) for large n will not be acceptable.

In a similar way, the effective Hamiltonian on the subspace $P_{0n}\Omega$ will be

$$\begin{aligned}\mathscr{H}_{P_{0n}} &= -\frac{2ng^2}{\Delta}|f_{gg}\rangle\langle f_{gg}| \otimes |n\rangle\langle n| \\ &= -\frac{2g^2}{\Delta}|f_{gg}\rangle\langle f_{gg}| \otimes a^\dagger a|n\rangle\langle n|. \end{aligned} \quad (45)$$

The effective Hamiltonian on the subspace $P_{2n}\Omega$ will be

$$\begin{aligned}\mathscr{H}_{P_{2n}} &= \frac{2(n+1)g^2}{\Delta}|f_{ee}\rangle\langle f_{ee}| \otimes |n\rangle\langle n| \\ &= \frac{2g^2}{\Delta}|f_{ee}\rangle\langle f_{ee}| \otimes aa^\dagger|n\rangle\langle n|. \end{aligned} \quad (46)$$

If we calculate the effective Hamiltonian on the subspace $P_n\Omega$ whose projector is

$$P_n = P_{0n} + P_{1n} + P_{2n} = I_1 \otimes I_2 \otimes |n\rangle\langle n|, \quad (47)$$

where $I_1 = |g_1\rangle\langle g_1| + |e_1\rangle\langle e_1|$ and $I_2 = |g_2\rangle\langle g_2| + |e_2\rangle\langle e_2|$ are the identity operators for atoms, then we can find that there is

$$\mathscr{H}_{P_n} = \mathscr{H}_{P_{0n}} + \mathscr{H}_{P_{1n}} + \mathscr{H}_{P_{2n}}. \quad (48)$$

This is because the states in subspace $P_{0n}\Omega$ have n excitations, states in subspace $P_{1n}\Omega$ have $n+1$ excitations and states in subspace $P_{2n}\Omega$ have $n+2$ excitations, so that the operator H_I can not couple them. We note that these effective Hamiltonians will be good approximations only when the condition (44) is satisfied.

The effective Hamiltonian methods introduced in the above section can not be used to define an effective Hamiltonian on the whole Hilbert space, whereas the effective Hamiltonian of James and Jerke is defined on the whole Hilbert space.[10] This is a difference between the two methods. For the example discussed above, if we check carefully the approximation conditions of the James–Jerke method, it can be found that their first condition can not be satisfied even when there is $|g/\Delta| \ll 1$ (as the large photon number will lead to a strong interaction), therefore we can not use the James–Jerke method to get an effective Hamiltonian for this example. We should be cautious on using the James–Jerke effective Hamiltonian method when a cavity quantum field is involved as the interaction strength is usually dependent on the photon number and the photon number can be large.

If the approximation conditions of James and Jerke are ignored, then according to their method an effective Hamiltonian

$$\begin{aligned}\mathscr{H}_{\text{James}} &= -\frac{g^2}{\Delta}\{|g_1\rangle\langle g_1| \otimes I_2 + I_1 \otimes |g_2\rangle\langle g_2|\} \otimes a^\dagger a \\ &\quad + \frac{g^2}{\Delta}\{|e_1\rangle\langle e_1| \otimes I_2 + I_1 \otimes |e_2\rangle\langle e_2|\} \otimes aa^\dagger \\ &\quad + \frac{g^2}{\Delta}\{\sigma_1^\dagger \otimes \sigma_2 + \sigma_1 \otimes \sigma_2^\dagger\} \otimes I_c \end{aligned} \quad (49)$$

will be obtained, where I_c is the identity operator for the cavity field. It can be found that $\mathscr{H}_{\text{James}}$ is the sum of our obtained effective Hamiltonians, i.e.,

$$\mathscr{H}_{\text{James}} = \sum_{n=0}^{+\infty}\mathscr{H}_{P_{0n}} + \sum_{n=0}^{+\infty}\mathscr{H}_{P_{1n}} + \sum_{n=0}^{+\infty}\mathscr{H}_{P_{2n}}. \quad (50)$$

This result also demonstrates a connection between the effective Hamiltonian method presented in this paper and the James–Jerke method.

5. Relation to the James–Jerke method

The two examples in the above section show that there is a connection between our effective Hamiltonian method presented and the James–Jerke method. Now we discuss it in some detail. We will show that in some special cases the two methods get the same result.

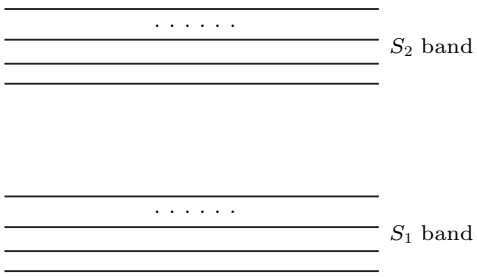


Fig. 1. Demonstration of the eigenvalues of H_0 in Eq. (52).

Consider a Hamiltonian in the Shrödinger picture

$$H = H_0 + V, \quad (51)$$

where the eigenvalues of H_0 can be divided into two energy bands S_1 and S_2 as shown in Fig. 1. The spectral decomposition of H_0 is

$$H_0 = \sum_{i\in S_1} E_i P_i + \sum_{j\in S_2} E_j P_j. \quad (52)$$

The whole Hilbert space Ω is divided into two subspaces $P_{S_1}\Omega$ and $P_{S_2}\Omega$ with the corresponding projectors

$$P_{S_1} = \sum_{i\in S_1} P_i, \quad P_{S_2} = \sum_{j\in S_2} P_j. \quad (53)$$

Assume the perturbation V can only couple states of the subspace $P_{S_1}\Omega$ with states of the subspace $P_{S_2}\Omega$, which means

$$V=\sum_{i\in S_1,j\in S_2}(P_iVP_j+P_jVP_i). \tag{54}$$

The corresponding Hamiltonian in the interaction picture is

$$\begin{aligned}H_I=&\mathrm{e}^{\mathrm{i}H_0t}V\mathrm{e}^{-\mathrm{i}H_0t}\\=&\sum_{i\in S_1,j\in S_2}(h_{ij}\mathrm{e}^{\mathrm{i}\omega_{ij}t}+h_{ji}\mathrm{e}^{\mathrm{i}\omega_{ji}t}),\end{aligned} \tag{55}$$

where we have used the following definitions

$$h_{ij}=P_iVP_j,\quad \omega_{ij}=E_i-E_j. \tag{56}$$

Under the condition that the elements of the operator V are much smaller than the energy gap between the two bands, the approximate effective Hamiltonian on the subspace $P_{S_1}\Omega$ and $P_{S_2}\Omega$ can be both calculated. According to Eqs. (19) and (20), the effective Hamiltonian on the subspace $P_{S_1}\Omega$ is

$$\mathscr{H}_{P_{S_1}}=\frac{1}{2}\{H_{P_{S_1}}+H_{P_{S_1}}^{\dagger}\}, \tag{57}$$

where

$$H_{P_{S_1}}=\textstyle\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{\omega_{nm}}h_{ij}h_{mn}\mathrm{e}^{\mathrm{i}(\omega_{ij}+\omega_{mn})t}. \tag{58}$$

The effective Hamiltonian on the subspace $P_{S_2}\Omega$ is

$$\mathscr{H}_{P_{S_2}}=\tfrac{1}{2}\{H_{P_{S_2}}+H_{P_{S_2}}^{\dagger}\}, \tag{59}$$

where

$$H_{P_{S_2}}=\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{\omega_{mn}}h_{ji}h_{nm}\mathrm{e}^{\mathrm{i}(\omega_{ji}+\omega_{nm})t}. \tag{60}$$

To give a relation to the James–Jerke method, it is necessary to define an effective Hamiltonian on the whole Hilbert as the James–Jerke method. As the whole Hilbert space Ω is a direct sum of the subspace $P_{S_1}\Omega$ and $P_{S_2}\Omega$, the effective Hamiltonian $\mathscr{H}$ on the whole Hilbert space Ω can be defined as the sum of the effective Hamiltonian on the subspace $P_{S_1}\Omega$ and $P_{S_2}\Omega$, i.e.,

$$\begin{aligned}\mathscr{H}=&\mathscr{H}_{P_{S_1}}+\mathscr{H}_{P_{S_2}}\\=&\frac{1}{2}\{H_{P_{S_1}}+H_{P_{S_2}}^{\dagger}\}+\frac{1}{2}\{H_{P_{S_2}}+H_{P_{S_1}}^{\dagger}\}.\end{aligned} \tag{61}$$

Now we show that the above effective Hamiltonian $\mathscr{H}$ is the same as that calculated by the James–Jerke method. From Eq. (60) we can find

$$H_{P_{S_2}}^{\dagger}=-\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{\omega_{nm}}h_{mn}h_{ij}\mathrm{e}^{\mathrm{i}(\omega_{ij}+\omega_{mn})t}, \tag{62}$$

which together with Eq. (58) leads to

$$\begin{aligned}&\frac{1}{2}\{H_{P_{S_1}}+H_{P_{S_2}}^{\dagger}\}\\=&\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{2\omega_{nm}}[h_{ij},h_{mn}]\mathrm{e}^{\mathrm{i}(\omega_{ij}+\omega_{mn})t}.\end{aligned} \tag{63}$$

Similarly there is

$$\begin{aligned}&\frac{1}{2}\{H_{P_{S_2}}+H_{P_{S_1}}^{\dagger}\}\\=&\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{2\omega_{mn}}[h_{ji},h_{nm}]\mathrm{e}^{\mathrm{i}(\omega_{ji}+\omega_{nm})t}\\=&\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{2\omega_{nm}}[h_{nm},h_{ji}]\mathrm{e}^{\mathrm{i}(\omega_{nm}+\omega_{ji})t}\\=&\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{2\omega_{ij}}[h_{ij},h_{mn}]\mathrm{e}^{\mathrm{i}(\omega_{ij}+\omega_{mn})t}.\end{aligned} \tag{64}$$

From Eqs. (61), (63), and (64), it can be found that the effective Hamiltonian on the whole Hilbert space is

$$\mathscr{H}=\textstyle\sum_{i\in S_1,j\in S_2}\sum_{n\in S_1,m\in S_2}\frac{1}{\omega_{ij,nm}}[h_{ij},h_{mn}]\mathrm{e}^{\mathrm{i}(\omega_{ij}+\omega_{mn})t}, \tag{65}$$

where $\omega_{ij,nm}$ is the harmonic mean of ω_{ij} and ω_{nm}, i.e.,

$$\frac{1}{\omega_{ij,nm}}=\frac{1}{2}\Big\{\frac{1}{\omega_{ij}}+\frac{1}{\omega_{nm}}\Big\}. \tag{66}$$

The effective Hamiltonian of Eq. (65) is the same as the James–Jerke method. The first example in the above section belongs to the case that the eigenvalues of H_0 can be divided into two energy bands, which is the reason why its effective Hamiltonian on the whole Hilbert space is the same as that obtained by the James–Jerke method. The result in Eq. (65) is obtained by assuming the eigenvalues of H_0 forming two energy bands, but it can be extended to the cases that the eigenvalues of H_0 form more than two bands. Suppose that there are s bands, i.e.,

$$H_0=\sum_{a=1}^{s}\sum_{i\in S_a}E_iP_i, \tag{67}$$

where a is the band index, and the interaction is

$$V=\sum_{a,b(a\neq b)}P_{S_a}VP_{S_b}, \tag{68}$$

where P_{S_a} means a projector of band S_a,

$$P_{S_a}=\sum_{i\in S_a}P_i. \tag{69}$$

The interaction V in Eq. (68) means that there are only couplings between different bands. Assume that the coupling strengths are much smaller than the band gaps. From Eqs. (19) and (20), the effective Hamiltonian of band S_a in the interaction picture is

$$\mathscr{H}_{P_{S_a}}=\frac{1}{2}\{H_{P_{S_a}}+H_{P_{S_a}}^{\dagger}\}, \tag{70}$$

where

$$H_{P_{S_a}}=\sum_{b=1(b\neq a)}^{s}U^{\dagger}P_{S_a}VP_{S_b}(P_{S_b}VP_{S_a})U \tag{71}$$

with $U = \mathrm{e}^{-\mathrm{i}H_0 t}$. Thus, the effective Hamiltonian of the whole space in the interaction picture is

$$\begin{aligned}\mathscr{H} &= \sum_{a=1}^{s} \mathscr{H}_{P_{S_a}} \\ &= \frac{1}{2}\sum_{a=1}^{s}\sum_{b=1(b\neq a)}^{s} U^{\dagger} P_{S_a} V P_{S_b} (P_{S_b} V P_{S_a}) U + \mathrm{H.c.} \\ &= \frac{1}{4}\sum_{a=1}^{s}\sum_{b=1(b\neq a)}^{s} U^{\dagger}\{P_{S_a} V P_{S_b} (P_{S_b} V P_{S_a}) \\ &\quad + P_{S_b} V P_{S_a} (P_{S_a} V P_{S_b})\} U + \mathrm{H.c.} \\ &= \frac{1}{4}\sum_{a=1}^{s}\sum_{b=1(b\neq a)}^{s} \{H_{\mathrm{ab}} + H_{\mathrm{ab}}^{\dagger}\} \\ &= \frac{1}{2}\sum_{a=1}^{s}\sum_{b=1(b\neq a)}^{s} \mathscr{H}_{\mathrm{ab}} \end{aligned} \tag{72}$$

with

$$H_{\mathrm{ab}} = U^{\dagger}\{P_{S_a} V P_{S_b} (P_{S_b} V P_{S_a}) + P_{S_b} V P_{S_a} (P_{S_a} V P_{S_b})\} U, \tag{73}$$

$$\mathscr{H}_{\mathrm{ab}} = \frac{1}{2}\{H_{\mathrm{ab}} + H_{\mathrm{ab}}^{\dagger}\}. \tag{74}$$

It can be found that $\mathscr{H}_{ab}$ is the effective Hamiltonian when there are only bands a and b. The last expression in Eq. (72) shows that the effective Hamiltonian of the whole space can be written as the sum of two-band results, which has been shown to be equivalent to the result of James and Jerke. Therefore the effective Hamiltonian of the whole space is the same as that obtained by the James–Jerke method when the eigenvalues of H_0 form two or more bands and there are only couplings between different bands. The eigenvalues of H_0 in the second example in the above section form three bands and there are no couplings within one band. This is the reason why the two methods can obtain the same result when the approximation condition is ignored.

6. Summary

We have introduced a new method to calculate the effective Hamiltonian in the Shrödinger picture as well as in the interaction picture, and given two examples in quantum information to demonstrate it. The new method can discuss effective Hamiltonian in more general cases than the James–Jerke method, and they can give the same result in some special cases, which reveals the deep connection between the two seemingly different methods.

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