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The Invariant Eigen-Operator Method for Hamiltonians with Coordinates-Coordinates Coupling Terms

Yong-mei Liu · Ying-hua Ji

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Abstract In this paper, we apply the method of "invariant eigen-operator" to study the Hamiltonian of harmonic oscillator with couplings and derive their invariant eigen-operator. We first discuss decoupling of coupled harmonic oscillators with the two different quality and frequencies. And then, we propose an operator Hamiltonian to describe the linear lattice chain with Born–von Karman boundary condition. The vibrating spectrum is thus obtained. The results show that, for the system of coupled harmonic oscillators by coordinate coupling or momentum coupling, the invariant eigen operator $\hat{Q}$ of system always has the form of $\hat{Q} = \sum_j g_j \hat{x}_j$ or $\hat{Q} = \sum_j \lambda_j \hat{p}_j$.

Keywords Heisenberg equation · Invariant eigen-operator method · Coupled harmonic oscillators

1 Introduction

The model of coupled harmonic oscillators has been studied, being applied to various problems of quantum mechanics and quantum optics. For instance, it was used to describe quantum amplifiers and converters [1, 2]. Explicit exact solutions and propagators of the Schrödinger equations as well as solutions of the Heisenberg equations of motion were considered and applied to different problems [3, 4]. As a result, in [5], the solution for coupled identical oscillators has been found through a unitary transformation approach. In general, solving various stationary Schrödinger equations leads to eigenvalues and eigenvectors of dynamic Hamiltonians. Though the Heisenberg equation stands on the same footing as the Schrödinger equation, it is seldom employed for the purpose of directly deriving energy

Y.-M. Liu
Education College, Jiangxi Normal University, Nanchang, Jiangxi 330022, China

Y.-H. Ji
College of Physics and Communication Electronics, Jiangxi Normal University, Nanchang, Jiangxi 33002, China
e-mail: jyh2006@jxnu.edu.cn

eigenvalues. In a very recent paper [6] author has introduced a new method, i.e. the "invariant eigen-operator" (IEO) method to explore energy-level gap of dynamic Hamiltonians, which is based on both the concept of Schrödinger operator and the Heisenberg equation of motion. In this manuscript, we apply the method of "invariant eigen-operator" to obtain the decoupling of the quantum system for some kinds of coupled harmonic oscillators and give the corresponding eigenvalue of energy. The method is different from those presented in the published before on the same problem.

2 The Invariant Eigen-Operator Method

In quantum mechanics, the discrete energy levels and simultaneously the eigenstates of dynamic systems are usually derived by solving the appropriate Schrödinger equation $i\hbar(d/dt)\psi = \hat{H}\psi$. However, owing to the Heisenberg equation of motion,

$$i\hbar\frac{d}{dt}\hat{Q} = [\hat{Q}, \hat{H}] \tag{1}$$

which is of the same form and importance as the Schrödinger equation. Since (1) does not involve wavefunctions or eigenvectors, it can hardly be straightforwardly employed to derive energy-level formulas. In [7], the authors reported that the Heisenberg equation of motion can also be used to deduce the energy-level gap of certain dynamic systems if one can find some appropriate eigen-operators $\hat{Q}$ of the square of the Schrödinger operator $i\hbar(d/dt)$. Its main idea is as follows. For the certain quantum system, there is $\hat{Q}$ satisfying the following eigenvector-like equation

$$\left(i\hbar\frac{d}{dt}\right)^2\hat{Q} = G^2\hat{Q} \tag{2}$$

where G is real. We can judge that G is the gap between two adjacent energy levels of the dynamic Hamiltonian $\hat{H}$.

To clarify this point of view, we assume that $|m\rangle$ and $|n\rangle$ are two adjacent different stationary eigen-states of Hamiltonian $\hat{H}$ with eigen-values E_m and E_n, respectively. Using the Heisenberg equation, we obtain

$$\begin{aligned}\langle m|\left(i\hbar\frac{d}{dt}\right)^2\hat{Q}\,|n\rangle &= \langle m|\,[[\hat{Q}, \hat{H}_0], \hat{H}_0]\,|n\rangle \\ &= \langle m|\,(\hat{Q}\hat{H}_0^2 - 2\hat{H}_0\hat{Q}\hat{H}_0 + \hat{H}_0^2\hat{Q})\,|n\rangle \\ &= (E_m - E_n)^2\,\langle m|\,\hat{Q}\,|n\rangle \\ &= G^2\,\langle m|\,\hat{Q}\,|n\rangle\end{aligned}$$

where

$$G = |E_m - E_n|$$

Whenever $\langle m|\hat{Q}|n\rangle$ is nonzero matrix element, the energy gap between $|m\rangle$ and $|n\rangle$ can be obtained as $G = |E_m - E_n|$. Thus, this new method is named as the invariant eigen-operator method.

3 The Invariant Eigen-Operator Method for Some Hamiltonians

In this section we shall apply the invariant eigen-operator method to derive the energy level of the coupled harmonic oscillator. The Hamiltonian of coupled harmonic oscillators is usually used to describe the molecular with many binding atoms. The simplest Hamiltonian of two coupled harmonic oscillators is written as

$$\hat{H}_1 = \sum_{j=1}^{2}\left(\frac{1}{2m_j}\hat{p}_j^2 + \frac{1}{2}m_j\omega_j^2\hat{x}_j^2\right) - k_1\hat{p}_1\hat{p}_2 - k_2\hat{x}_1\hat{x}_2$$

In most of the books on quantum mechanics, the ways solving eigenvalues of $\hat{H}_1$ are introduced on containing only coordinate-coupling or momentum-coupling both the same quality and frequency. Obviously, the Hamiltonian getting from $\hat{H}_1$ is more general form.

For another example, the Hamiltonian of the lattice chain model is

$$\hat{H}_2 = \frac{1}{2m}\sum_{l=1}^{N}\hat{p}_l^2 + \frac{\beta}{2}\sum_{l=1}^{N}(\hat{x}_l - \hat{x}_{l+1})^2$$

It is well known that the lattice chain model has been a basic theory for understanding vibrating mode of phonon and energy-band in solid state physics. The last term in $\hat{H}_2$ reflects that an atomic ring is formed by connecting the lattermost atom with first atom. Because of forming a ring, we also consider that this chain is endless so as to every atom being in the same environment.

The last the Hamiltonian of harmonic oscillators with bilinear coupling is written as

$$\hat{H}_3 = \sum_{j=1}^{2}\left(\frac{1}{2m_j}\hat{p}_j^2 + \frac{1}{2}m_j\omega_j^2\hat{x}_j^2\right) + k_1\hat{x}_1\hat{p}_2 + k_2\hat{x}_2\hat{p}_1 + k_3\hat{p}_1\hat{x}_2 + k_4\hat{p}_2\hat{x}_1$$

Case 1 The Hamiltonian is

$$\hat{H}_1 = \sum_{j=1}^{2}\left(\frac{1}{2m_j}\hat{p}_j^2 + \frac{1}{2}m_j\omega_j^2\hat{x}_j^2\right) - k_1\hat{p}_1\hat{p}_2 - k_2\hat{x}_1\hat{x}_2 \tag{3}$$

According to the invariant eigen-operator method, firstly we should consider the basic commutative relations using the Heisenberg equation

$$[\hat{x}_1, \hat{H}_1] = i\hbar\left(\frac{1}{m_1}\hat{p}_1 - k_1\hat{p}_2\right) \tag{4}$$

$$[\hat{x}_2, \hat{H}_1] = i\hbar\left(\frac{1}{m_2}\hat{p}_2 - k_1\hat{p}_1\right) \tag{5}$$

$$[\hat{p}_1, \hat{H}_1] = -i\hbar\left(m_1\omega_1^2\hat{x}_1 - k_2\hat{x}_2\right) \tag{6}$$

$$[\hat{p}_2, \hat{H}_1] = -i\hbar\left(m_2\omega_2^2\hat{x}_1 - k_2\hat{x}_1\right) \tag{7}$$

Based on Hamiltonian $\hat{H}_1$ in (3), we suppose that the invariant eigen-operator in the case is

$$\hat{Q}_1 = \hat{x}_1 + g_1\hat{x}_2 \tag{8}$$

The parameter $g_1$is to be determined.

Substituting (8) into (2), combing (4)–(7), we have

$$\left(i\hbar\frac{d}{dt}\right)^2\hat{Q}_1 = \hbar^2(\omega_1^2 + m_1k_1\omega_1^2g_1 - k_1k_2 - m_2^{-1}k_2g_1)\hat{x}_1 + \hbar^2(\omega_2^2g_1 + m_2k_1\omega_2^2 - k_1k_2g_1 - m_1^{-1}k_2)\hat{x}_2 \tag{9}$$

If the operator $\hat{Q}_1$ satisfies (2), comparing (8) and (9), we obtain

$$\frac{\omega_1^2 + m_1k_1\omega_1^2g_1 - k_1k_2 - m_2^{-1}k_2g_1}{1} = \frac{\omega_2^2g_1 + m_2k_1\omega_2^2 - k_1k_2g_1 - m_1^{-1}k_2}{g_1} \tag{10}$$

As a consequence of (10) we have

$$g_1(\pm) = \frac{(\omega_2^2 - \omega_1^2) \pm \sqrt{(\omega_2^2 - \omega_1^2)^2 + 4(m_1k_1\omega_1^2 - m_2^{-1}k_2)(m_2k_1\omega_2^2 - m_1^{-1}k_2)}}{2(m_1k_1\omega_1^2 - m_2^{-1}k_2)} \tag{11}$$

Substituting (11) into (9) and comparing with (2), we can get level gap

$$G^2 = \frac{1}{2}\hbar^2\left[(\omega_2^2 + \omega_1^2 - 2k_1k_2) \pm \sqrt{(\omega_2^2 - \omega_1^2)^2 + 4(m_1k_1\omega_1^2 - m_2^{-1}k_2)(m_2k_1\omega_2^2 - m_1^{-1}k_2)}\right] \tag{12}$$

As the coupled quantum system of two harmonic oscillators is described by (3), we can easily see that the energy level gap of quantum system is given by G, but after decoupling, the frequency of two independent harmonic oscillators is given by $\hbar^{-1}G$. Writing as

$$\Omega_1 = \hbar^{-1}G_+, \qquad \Omega_2 = \hbar^{-1}G_-$$

The energy eigen-value of the system reads

$$E = \left(n_1 + \frac{1}{2}\right)\hbar\Omega_1 + \left(n_2 + \frac{1}{2}\right)\hbar\Omega_2 \tag{13}$$

where

$$\Omega_1^2 = \frac{1}{2}\left[(\omega_2^2 + \omega_1^2 - 2k_1k_2) + \sqrt{(\omega_2^2 - \omega_1^2)^2 + 4(m_1k_1\omega_1^2 - m_2^{-1}k_2)(m_2k_1\omega_2^2 - m_1^{-1}k_2)}\right] \tag{14}$$

$$\Omega_2^2 = \frac{1}{2}\left[(\omega_2^2 + \omega_1^2 - 2k_1k_2) - \sqrt{(\omega_2^2 - \omega_1^2)^2 + 4(m_1k_1\omega_1^2 - m_2^{-1}k_2)(m_2k_1\omega_2^2 - m_1^{-1}k_2)}\right] \tag{15}$$

In fact, for the quantum system describing by Hamiltonian (3), we can find that another invariant eigen-operator $\hat{Q}_1'$ is

$$\hat{Q}_1' = \hat{p}_1 + g_1'\hat{p}_2 \tag{16}$$

Here g_1' is to be determined. Substituting (16) into (2) and using (4)–(7), it is easy to get

$$\left(i\hbar\frac{d}{dt}\right)^2 \hat{Q}_1' = \hbar^2(\omega_1^2 + m_2k_1\omega_2^2g_1' - k_1k_2 - m_1^{-1}k_2g_1')\hat{p}_1 + \hbar^2(\omega_2^2g_1' + m_1k_1\omega_1^2 - k_1k_2g_1' - m_2^{-1}k_2)\hat{p}_2 \tag{17}$$

When the operator $\hat{Q}_1'$ meets (2), by comparing (17) with (16), we can get

$$\frac{\omega_1^2 + m_2k_1\omega_2^2g_1' - k_1k_2 - m_1^{-1}k_2g_1'}{1} = \frac{\omega_2^2g_1' + m_1k_1\omega_1^2 - k_1k_2g_1'' - m_2^{-1}k_2}{g_1'} \tag{18}$$

From (18), we may determine the two value of g_1'

$$g_1'(\pm) = \frac{(\omega_2^2 - \omega_1^2) \pm \sqrt{(\omega_2^2 - \omega_1^2)^2 + 4(m_1k_1\omega_1^2 - m_2^{-1}k_2)(m_2k_1\omega_2^2 - m_1^{-1}k_2)}}{2(m_2k_1\omega_2^2 - m_1^{-1}k_2)} \tag{19}$$

Substituting (19) into (17) and comparing with (2), we also obtain the energy level gap G determined by (12).

In order to be able to understand intuitively the method of "invariant eigen-operator", for the coupled quantum system of two harmonic oscillators, we discussed a simple case

$$m_1 = m_2 = m, \qquad \omega_1 = \omega_2 = \omega$$

Under these conditions, from (11), we can get

$$g_1 = \pm 1$$

When $g_1 = 1$, we can obtain from (14)

$$\Omega_1 = \sqrt{\omega^2 - m\omega^2k_1 - k_1k_2 - m^{-1}k_2} \tag{20}$$

When $g_1 = -1$, we can get from (15)

$$\Omega_2 = \sqrt{\omega^2 - m\omega^2k_1 - k_1k_2 + m^{-1}k_2} \tag{21}$$

Further, when $k_1 = 0$, we get

$$\Omega_{1,2} = \sqrt{\omega^2 \pm \frac{k_2}{m}}$$

When $k_2 = 0$, we also get

$$\Omega_{1,2} = \sqrt{\omega^2 \pm m\omega^2k_1}$$

Case 2 The Hamiltonian is

$$\hat{H}_2 = \frac{1}{2m}\sum_{l=1}^{N}\hat{p}_l^2 + \frac{\beta}{2}\sum_{l=1}^{N}(\hat{x}_l - \hat{x}_{l+1})^2 \tag{22}$$

Because of forming a ring, we can consider

$$\hat{p}_{N+l} = \hat{p}_l, \qquad x_{N+l} = x_l \tag{23}$$

Due to the difficulty and complicacy in directly diagonalizing quantum Hamiltonian operator of a long chain, in solid state physics textbooks people start to illustrate the vibrating modes of the lattice chain model in the context of classical dynamics together with the Born-von-Karman boundary condition. In [8], for the quantum system described by the Hamiltonian (22), authors give the invariant eigen-operator $\hat{Q}_2$ is

$$\hat{Q}_2 = \sum_{j=1}^{N} B_j \hat{p}_j \tag{24}$$

where

$$B_j = \cos(j\theta_l), \qquad \theta_l = \frac{2\pi}{N}(l-1)$$

In this section, we give another form of the invariant eigen-operator. Using the Heisenberg equation of motion we have

$$[\hat{x}_j, \hat{H}_2] = \frac{i\hbar}{m}\hat{p}_j \tag{25}$$

$$[\hat{p}_j, \hat{H}_2] = -i\hbar\beta(2\hat{x}_j - \hat{x}_{j+1} - \hat{x}_{j-1}) \tag{26}$$

From (25) and (26) we guess that the invariant eigen-operator of $\hat{H}_2$ is

$$\hat{Q}_2' = \sum_{j=1}^{N} A_j \hat{x}_j \tag{27}$$

The parameters A_js are to be determined. Substituting (27) into (2), combing (25) and (26), we have

$$\begin{aligned}\left(i\hbar\frac{d}{dt}\right)\hat{Q}_2' &= -i\hbar\beta\sum_{j=1}^{N} A_j[2\hat{x}_j - \hat{x}_{j+1} - \hat{x}_{j-1}] \\ &= -i\hbar\beta\left[2\sum_{j=1}^{N} A_j\hat{x}_j - \sum_{j=1}^{N} A_j\hat{x}_{j+1} - \sum_{j=1}^{N} A_j\hat{x}_{j-1}\right] \\ &= -i\hbar\beta\sum_{j=1}^{N}(2A_j - A_{j+1} - A_{j-1})\hat{x}_j\end{aligned}$$

Further, we evaluate

$$\left(i\hbar\frac{d}{dt}\right)^2\hat{Q}_2' = \frac{\beta\hbar^2}{m}\sum_{j=1}^{N}(2A_j - A_{j+1} - A_{j-1})\hat{x}_j \tag{28}$$

Comparing (28) with (2), it is necessary to ask for

$$A_{j+1} + A_{j-1} = \lambda A_j \tag{29}$$

λ is a coefficient has nothing to do with summation j. There is no doubt that a reasonable choice is

$$A_j = \cos(j\theta_l) \tag{30}$$

Substituting (30) into (29), we have

$$A_{j+1} + A_{j-1} = 2\cos\theta\cos(j\theta_l) \tag{31}$$

And then

$$\lambda = 2\cos\theta_l$$

The periodicity of the ring should be described by θ_l, so

$$\theta_l = \frac{2\pi}{N}(l-1), \quad l = 1, 2, \ldots, N \tag{32}$$

From (28)–(32), we obtain

$$\left(i\hbar\frac{d}{dt}\right)^2 \hat{Q}'_2 = \frac{2\beta\hbar^2}{m}(1-\cos\theta_l)\,\hat{Q}'_2 \tag{33}$$

here

$$\hat{Q}'_2 = \sum_{j=1}^{N} \hat{x}_j \cos(j\theta_l) \tag{34}$$

which means that $\hat{Q}'_2$ also is the invariant eigen-operator of $\hat{H}_2$. From (33), we can get the energy gap

$$G_2^2 = \frac{2\beta\hbar^2}{m}(1-\cos\theta_l)$$

The vibration modes of this chain is

$$\Omega_l = \sqrt{\frac{2\beta}{m}(1-\cos\theta_l)}, \quad l > 1 \tag{35}$$

We now analyze the physical meaning of diagonalized frequency Ω_l and the physical system represented by this circular type of Hamiltonian. We think that $\hat{H}_2$ is on behalf of a single atomic lattice model (described the single atomic crystal in the cell), of which the last term (the beginning and the end interaction) represents Born-von Karman boundary condition. After diagonalization of $\hat{H}_2$, Ω_l represents the phonon frequency of quantum lattice. We can see that using the invariant eigen-operator method we can obtain the result of the chain more easily and directly.

In brief, from above results, we can easily know that: for the quantum system of coupled harmonic oscillators by coordinate coupling, momentum coupling or both coordinate coupling and momentum coupling, the form of invariant eigen-operator $\hat{Q}$ is $\hat{Q} = \sum_j \alpha_j \hat{x}_j$ or $\hat{Q} = \sum_j \beta_j \hat{p}_j$. Coefficient α_js or β_js is determined by both the inherent parameters of coupled harmonic oscillators and coupling parameter.

Case 3 The Hamiltonian of oscillators with bilinear coupling is

$$\hat{H}_3 = \sum_{j=1}^{2}\left(\frac{1}{2m_j}\hat{p}_j^2 + \frac{1}{2}m_j\omega_j^2\hat{x}_j^2\right) + k_1\hat{x}_1\hat{p}_2 + k_2\hat{x}_2\hat{p}_1 + k_3\hat{p}_1\hat{x}_2 + k_4\hat{p}_2\hat{x}_1 \tag{36}$$

Using the basic commutative relations of coordinate and momentum, we have

$$[\hat{x}_1, \hat{H}_3] = i\hbar(m_1^{-1}\hat{p}_1 + k_2\hat{x}_2 + k_3\hat{x}_3) \tag{37}$$

$$[\hat{x}_2, \hat{H}_3] = i\hbar(m_2^{-1}\hat{p}_1 + k_1\hat{x}_1 + k_4\hat{x}_1) \tag{38}$$

$$[\hat{p}_1, \hat{H}_3] = -i\hbar(m_1\omega_1^2\hat{x}_1 + k_1\hat{p}_2 + k_4\hat{p}_2) \tag{39}$$

$$[\hat{p}_2, \hat{H}_3] = -i\hbar(m_2\omega_2^2\hat{x}_2 + k_2\hat{p}_1 + k_3\hat{p}_1) \tag{40}$$

Based on Hamiltonian $\hat{H}_3$ in (35), we suppose that the invariant eigen-operator in the case is

$$\hat{Q}_3 = \hat{x}_1 + g_3\hat{p}_2 \tag{41}$$

Substituting (41) into (2), combing (37)–(40), we have

$$\left(i\hbar\frac{d}{dt}\right)^2 \hat{Q}_3 = \hbar^2\{m_1\omega_1^2[m_1^{-1} - g_3(k_2+k_3)] - (k_1+k_4)[(k_2+k_3) - m_2\omega_2^2 g_3]\}\hat{x}_1$$
$$+ \hbar^2\{(k_1+k_4)[m_1^{-1} - g_3(k_2+k_3)] - m_2^{-1}[(k_2+k_3) - m_2\omega_2^2 g_3]\}\hat{p}_2 \tag{42}$$

If the operator $\hat{Q}_3$ is the invariant eigen-operator for $\hat{H}_3$, g_3 must satisfy the equation following

$$[m_1\omega_1^2(k_2+k_3) + m_2\omega_2^2(k_1+k_4)]g_3^2 + (\omega_2^2 - \omega_1^2)g_3 + m_1^{-1}(k_1+k_4) - m_2^{-1}(k_2+k_3) = 0 \tag{43}$$

It is necessary for us to solve this equation for g_3. Substituting g_3 into (42) and comparing with (2), we can obtain $\hat{Q}_3$, which is the invariant eigen-operator of $\hat{H}_3$. Thus, coupling between modes is eliminated and Hamiltonian $\hat{H}_3$ can be simplified as two mode independent harmonic oscillators, problem is solved.

In summary, we have adopted the invariant eigen-operator method to tackle some special coupled oscillator model. This approach seems concise and direct and can be extended to tackle other Hamiltonian models.

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