

# Normal coordinate in harmonic crystal obtained by virtue of the classical correspondence of the invariant eigen-operator\*

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Noticing that the equation

$$\frac{d^2 O_n}{dt^2} = \{H_c, \{H_c, O_n\}\} = \lambda O_n$$

with double-Poisson bracket, where  $O_n$  is normal coordinate,  $H_c$  is classical Hamiltonian, is the classical correspondence of the invariant eigen-operator equation (2004 *Phys. Lett. A* **321** 75), we can find normal coordinates in harmonic crystal by virtue of the invariant eigen-operator method.

**Keywords:** quantum impeller, vibration spectrum, invariant eigen-operator method

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## 1. Introduction

Usually for obtaining energy spectrum of dynamic systems in quantum mechanics, one appeals to solving the stationary Schrödinger equation.<sup>[1]</sup> In Refs. [2]–[6] we have proposed the invariant eigen-operator (IEO) method for deriving energy level of Hamiltonians, which is based on the original idea of the Schrödinger quantisation scheme and the Heisenberg equation of motion. Schrödinger took the identification  $i \frac{d}{dt} \longleftrightarrow \hat{H}$  (in this paper we assume  $\hbar = 1$  for simplicity), so  $i \frac{d}{dt}$  is named the Schrödinger operator in many reference papers. Similarly, we have  $\left(i \frac{d}{dt}\right)^n \longleftrightarrow \hat{H}^n$ , then set up the following equation for an operator  $\hat{O}_e$ ,

$$\left(i \frac{d}{dt}\right)^n \hat{O}_e = \lambda \hat{O}_e, \quad (1)$$

when  $n = 1$ , it looks similar in form to the Schrödinger equation  $i(d/dt)\psi = \hat{H}\psi$ . Thus we name Eq. (1) as  $n$ -order invariant eigen-operator equation, with the eigenvalue being  $\lambda$ . Using the Heisenberg equation

$$i \frac{d}{dt} \hat{O}_e = [\hat{O}_e, \hat{H}], \quad (2)$$

we can write Eq. (2) as

$$\left(i \frac{d}{dt}\right)^n \hat{O}_e = [\dots [[\hat{O}_e, \hat{H}], \hat{H}] \dots, \hat{H}] = \lambda \hat{O}_e. \quad (3)$$

If we can find such an  $\hat{O}_e$  that satisfies Eq. (3), we can say that  $\sqrt[n]{\lambda}$  is the energy-level gap of  $\hat{H}$ . To clarify this point of view, we take  $n = 2$  in Eq. (3) for example, assuming  $|\psi_a\rangle$  and  $|\psi_b\rangle$  are two adjacent eigenstates of Hamiltonian  $\hat{H}$  with eigen-values  $E_a$  and  $E_b$ , respectively, then we have

$$\begin{aligned} \langle \psi_a | (i \frac{d}{dt})^2 \hat{O}_e | \psi_b \rangle &= \langle \psi_a | [[\hat{O}_e, \hat{H}], \hat{H}] | \psi_b \rangle \\ &= (E_b - E_a)^2 \langle \psi_a | \hat{O}_e | \psi_b \rangle \\ &= \lambda \langle \psi_a | \hat{O}_e | \psi_b \rangle; \end{aligned} \quad (4)$$

whenever  $\langle \psi_a | \hat{O}_e | \psi_b \rangle$  is a nonzero matrix element, the energy gap between  $|\psi_a\rangle$  and  $|\psi_b\rangle$  can be obtained as  $|E_a - E_b| = \sqrt{\lambda}$ . So this IEO method may be used to derive the energy eigenvalues of some quantum systems, without directly solving the Schrödinger equation as did in Ref. [7].

In this work we point out that the classical correspondence of the IEO equation  $(i(d/dt))^2 \hat{O}_e = [[\hat{O}_e, \hat{H}], \hat{H}] = \lambda \hat{O}_e$  is useful to finding normal coordinates in harmonic crystal. This classical correspondence is composed of classical Poisson brackets. In

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turn, the normal coordinates in harmonic crystal can be derived by virtue of the IEO method, which seems convenient and effective.

## 2. Classical correspondence of IEO equation

By considering the classical correspondence of Eq. (3) in  $n = 2$  case. We are naturally led to the following equation composed of Poisson brackets

$$\frac{d^2 O}{dt^2} = \{H, \{H, O\}\} = \lambda O, \quad (5)$$

where  $O$  is a classical dynamic variable, which is not explicitly time-dependent,  $\partial O / \partial t = 0$ ,  $H$  is a classical Hamiltonian. The reason is as follows. The time evolution of  $O$  is<sup>[8]</sup>

$$\frac{dO}{dt} = \sum_i \left( \frac{\partial O}{\partial p_i} \dot{p}_i + \dot{q}_i \frac{\partial O}{\partial q_i} \right). \quad (6)$$

Using the Hamiltonian equation

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad (7)$$

and the definition of Poisson brackets

$$\{f, g\} = \sum_i \left( \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} - \frac{\partial g}{\partial p_i} \frac{\partial f}{\partial q_i} \right), \quad (8)$$

one can rewrite Eq. (6) as

$$\frac{dO}{dt} = \sum_i \left( \frac{\partial H}{\partial p_i} \frac{\partial O}{\partial q_i} - \frac{\partial O}{\partial p_i} \frac{\partial H}{\partial q_i} \right) = \{H, O\}, \quad (9)$$

which is very-well known. It then follows that

$$\begin{aligned} \frac{d^2 O}{dt^2} &= \frac{d}{dt} \frac{dO}{dt} = \sum_i \left[ \frac{\partial H}{\partial p_i} \frac{\partial \dot{O}}{\partial q_i} - \frac{\partial \dot{O}}{\partial p_i} \frac{\partial H}{\partial q_i} \right] \\ &= \sum_i \left[ \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \left( \frac{\partial H}{\partial p_i} \frac{\partial O}{\partial q_i} - \frac{\partial O}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \right. \\ &\quad \left. - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \left( \frac{\partial H}{\partial p_i} \frac{\partial O}{\partial q_i} - \frac{\partial O}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \right] \\ &= \{H, \{H, O\}\}, \end{aligned} \quad (10)$$

where  $\{H, \{H, O\}\}$  is a double-Poisson bracket, seldom used in analytical mechanics in the literature before, but now we pay attention to it since it is classical correspondence of IEO equation (3).

If we can find some  $O$  obeying

$$\{H, \{H, O\}\} = \lambda O, \quad (11)$$

then we name  $O$  the normal coordinate. Let us explain this.

For the multimode coupled oscillators whose classical Lagrangian is

$$\mathcal{L} = \frac{1}{2} \left( \sum_{i=1}^l m_i \dot{x}_i^2 - \sum_{i,j=1}^l k_{ij} x_i x_j \right), \quad (12)$$

an important task is to find its collective vibration (normal vibration) modes. Normal vibration means that  $l$ -particles located at  $x_i$ ,  $i = 1, 2, \dots, l$ , vibrate with the same frequency  $\omega_\alpha$ ,  $\alpha = 1, 2, \dots, l$ , i.e., there are  $l$  collective vibration modes. The real vibration is the linear superposition of these  $l$ -collective modes. Thus one can introduce normal coordinate (generalized coordinate), for which  $\mathcal{L}$  exhibits  $l$  independent vibrations

$$\mathcal{L} = \frac{1}{2} \left( \sum_{\alpha=1}^l \dot{Q}^{(\alpha)2} - \sum_{\alpha=1}^l \omega_\alpha^2 Q^{(\alpha)2} \right), \quad (13)$$

so the Lagrangian equation

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{Q}^{(\alpha)}} - \frac{\partial \mathcal{L}}{\partial Q^{(\alpha)}} = 0$$

leads to the Newton equation

$$\frac{d^2}{dt^2} Q^{(\alpha)} = \omega_\alpha^2 Q^{(\alpha)}. \quad (14)$$

Comparing Eq. (14) with Eq. (5), we see that  $\lambda$  in Eq. (5) corresponds to  $\omega_\alpha^2$  in Eq. (14), so  $O$  just represents the normal coordinate for the Hamiltonian  $\mathcal{H}$ .

On the other hand, since  $O$  is the classical correspondence of  $O$  in the formalism of the IEO method, we can find normal coordinates of the dynamic systems by virtue of the IEO method (finding  $O$  in Eq. (3) first). This approach seems convenient and efficient. In solid state physics,<sup>[9–11]</sup> an analysis of the classical normal modes of a lattice of ions is of great utility. In the next section, as an example, we will search for normal coordinates of a harmonic crystal.

## 3. Normal coordinates of a diatomic linear chain in which alternate ions having different masses

We consider a diatomic linear chain in which alternate  $N$  ions (located at  $x_n$  and  $x'_n$  respectively) have masses  $m$  and  $m'$  and only nearest neighbours

interact, whose Hamiltonian is

$$H = \sum_{n=1}^N \left[ \frac{P_n^2}{2m} + \frac{P_n'^2}{2m'} + \frac{\beta}{2}(x_n - x_n')^2 + \frac{\beta}{2}(x_n' - x_{n+1})^2 \right]. \quad (15)$$

To derive its normal coordinates we impose the quantisation condition

$$[P_n, x_j] = [P_n', x_j'] = -i\delta_{j,n}, \quad (16)$$

while other commutators are zero, i.e.,

$$\begin{aligned} [P_n, P_j'] &= [x_n, x_j'] = [P_n, x_j'] \\ &= [P_n', x_j] = [P_n, P_j] = [x_n, x_j] = 0, \end{aligned} \quad (17)$$

so  $H$  becomes a quantum mechanical Hamiltonian and we search for its invariant eigen-operator  $O$ . Assuming  $O$  is

$$O = \sum_{n=1}^N (f_n P_n + f_n' P_n'), \quad (18)$$

where  $f_n$  and  $f_n'$  are to be determined, hoping  $O$  satisfying

$$[[O, H], H] = \varpi^2 O. \quad (19)$$

From

$$\begin{aligned} [P_n, H] &= \left[ P_n, \frac{\beta}{2}(x_n - x_n')^2 + \frac{\beta}{2}(x_n - x_{n-1}')^2 \right] \\ &= i\beta(x_n' + x_{n-1}' - 2x_n), \end{aligned} \quad (20)$$

$$[x_n, H] = \left[ x_n, \frac{P_n^2}{2m} \right] = \frac{i}{m} P_n, \quad [x_n', H] = \frac{i}{m'} P_n', \quad (21)$$

and

$$[P_n', H] = i\beta(x_n + x_{n+1} - 2x_n'), \quad (22)$$

we calculate

$$\begin{aligned} [O, H] &= \sum_{n=1}^N i\beta[(f_n' + f_{n-1}' - 2f_n)x_n \\ &\quad + (f_n + f_{n+1} - 2f_n')x_n']. \end{aligned} \quad (23)$$

It then follows that

$$\begin{aligned} [[O, H], H] &= \sum_{n=1}^N \left[ -\frac{\beta}{m}(f_n' + f_{n-1}' - 2f_n)P_n \right. \\ &\quad \left. - \frac{\beta}{m'}(f_n + f_{n+1} - 2f_n')P_n' \right]. \end{aligned} \quad (24)$$

Comparing Eq. (24) with Eq. (19), we have

$$\begin{aligned} \bar{\omega}^2 &= -\frac{\beta}{mf_n}(f_n' + f_{n-1}' - 2f_n) \\ &= -\frac{\beta}{m'f_n'}(f_n + f_{n+1} - 2f_n'), \end{aligned} \quad (25)$$

which means

$$\frac{1}{m} \left( 1 - \frac{f_n' + f_{n-1}'}{2f_n} \right) = \frac{1}{m'} \left( 1 - \frac{f_n + f_{n+1}}{2f_n'} \right), \quad n = 1, 2, \dots, N. \quad (26)$$

Analysing Eq. (26), we set up equations for determining  $f_n$  and  $f_n'$ ,

$$f_n = \xi \cos(2n\theta_l), \quad f_n' = \xi' \cos((2n+1)\theta_l), \quad (27)$$

where

$$\theta_l = \frac{l}{N}\pi, \quad l = 1, 2, \dots, 2N. \quad (28)$$

Substituting Eq. (27) into Eq. (25) yields

$$\bar{\omega}^2 = \frac{2\beta}{m} \left( 1 - \frac{\xi'}{\xi} \cos \theta_l \right) = \frac{2\beta}{m'} \left( 1 - \frac{\xi}{\xi'} \cos \theta_l \right). \quad (29)$$

Then we have

$$\frac{\xi'}{\xi} = \frac{2\beta \cos \theta_l}{2\beta - m'\bar{\omega}^2} = \frac{2\beta - m\bar{\omega}^2}{2\beta \cos \theta_l}, \quad (30)$$

from which we further have

$$m'\bar{\omega}^4 - 2\beta(m + m')\bar{\omega}^2 + 4\beta^2 \sin^2 \theta_l = 0, \quad (31)$$

with the solution

$$\begin{aligned} \bar{\omega}_{\pm} &= \left\{ \beta \left( \frac{1}{m} + \frac{1}{m'} \right) \pm \beta \left[ \left( \frac{1}{m} + \frac{1}{m'} \right)^2 \right. \right. \\ &\quad \left. \left. - \frac{4 \sin^2 \theta}{mm'} \right]^{1/2} \right\}^{1/2}; \end{aligned} \quad (32)$$

this is the normal mode which conforms with that in Ref. [4]. Not only we have obtained the normal frequency, we can also know the normal coordinates. In fact, from Eqs. (27) and (29) we can determine the invariant eigen-operator

$$O = \sum_{n=1}^N [\xi P_n \cos(2n\theta_l) + \xi' P_n' \cos((2n+1)\theta_l)]. \quad (33)$$

Correspondingly, let  $P_n$  and  $P_n'$  be classical variables, then we obtain the normal coordinate (generalised coordinate) for the diatomic chain-lattice

$$O_n = \sum_{n=1}^N [\xi P_n \cos(2n\theta_l) + \xi' P_n' \cos((2n+1)\theta_l)]. \quad (34)$$

This method for deriving the normal coordinates seems convenient and effective. Actually, without this IEO method, the normal coordinates for the classical

Hamiltonian (15) can hardly be derived, because one should make ansatz (some lattice wave solution) to the second-order differential equation in Eq. (10) (the only existing method to derive normal coordinates), and then solve it; however, for the complicated lattice structure one has no good idea about what the correct ansatz is.

In summary, in this paper we have introduced a new method to find normal coordinates for classical Hamiltonians, i.e. by virtue of the IEO method;

in other words, adopting the IEO method not only can help us to derive energy spectrum for some quantum mechanical Hamiltonians, but also works well for finding normal coordinates which may be the classical correspondence of the invariant eigen-operators. It seems that the IEO method can significantly simplify the derivation because calculating quantum commutators sometimes are easier than solving differential equations.

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