Applying invariant eigen-operator method to deriving normal coordinates of general classical Hamiltonian*

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For classical Hamiltonian with general form $H = \frac{1}{2}\sum_{ij} M_{ij}p_ip_j + \frac{1}{2}\sum_{ij} L_{ij}q_iq_j$ we find a new convenient way to obtain its normal coordinates, namely, let H be quantised and then employ the invariant eigen-operator (IEO) method (Fan *et al.* 2004 *Phys. Lett.* A **321** 75) to derive them. The general matrix equation, which relies on $\boldsymbol{M}$ and $\boldsymbol{L}$, for obtaining the normal coordinates of H is derived.

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1. Introduction

Obtaining normal coordinates for dynamic systems is a common task both in classical dynamics and solid state physics, because they represent vibration modes or energy spectrum. Usually for obtaining normal coordinates of a classical quadratic dynamic system in terms of canonical coordinators q_i and p_i,

$$H = \frac{1}{2}\sum_{ij} M_{ij}p_ip_j + \frac{1}{2}\sum_{ij} L_{ij}q_iq_j, \tag{1}$$

where $M_{ij} = M_{ji}$, $L_{ij} = L_{ji}$, one uses Legendre transformation to have the corresponding Lagrangian, then derives the Lagrangian equations of motion (second-order differential equations), which are further converted to a set of correlated algebraic equations with solution being assumed of an oscillatory form, then applying the principal axis transformation[1] to obtain the fundamental frequencies of periodic oscillations. A simply periodic function involving only one of the resonant frequencies is related to a normal coordinate. In this work we adopt an alternate approach for obtaining normal coordinates of classical systems, we suppose H in Eq. (1) is quantised, and then use the newly developed invariant eigen-operator (IEO) method in quantum mechanics to obtain the normal coordinates of H. The paper is arranged as follows. In Section 2 we briefly review the IEO method. In Section 3 we derive the matrix equation for obtaining the second-order IEO for Hamiltonians of a general quadratic dynamic system. In Section 4 the general form of normal are presented. In the last section, we study some examples as the application of the above conclusions.

2. Brief review of the IEO method

The IEO method[2,3] is invented for deriving the energy level of quantum Hamiltonians, (without directly appealing to the stationary Schrödinger equation for solving wave functions), which is based on the original idea of Heisenberg equation of motion and the concept of Schrödinger operator $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}$.[4] Schrödinger took the identification $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} \longleftrightarrow \hat{H}$ (in this paper we assume $\hbar = 1$ for simplicity). Similarly, we have $\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \longleftrightarrow \hat{H}^n$. If we can find an operator $\hat{O}_e$ which obeys the following equation,

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \hat{O}_e = \lambda \hat{O}_e, \tag{2}$$

where λ is a number (or a diagonal matrix), then Eq. (2) is called n-order invariant eigen-operator equation, when $n = 1$, it looks similar in form to the Schrödinger equation $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi = \hat{H}\psi$. Thus we name $\hat{O}_e$ as n-order invariant eigen-operator, with the eigen-

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value being λ. Using the Heisenberg equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_e = \left[\hat{O}_e, \hat{H}\right], \tag{3}$$

we can write Eq. (2) as

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \hat{O}_e = \left[\ldots\left[\left[\hat{O}_e, \hat{H}\right], \hat{H}\right]\ldots, \hat{H}\right] = \lambda\hat{O}_e. \tag{4}$$

If we can find such an $\hat{O}_e$ that satisfies Eq. (4), 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. (4) 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

$$\begin{aligned}\langle\psi_a|\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^2\hat{O}_e|\psi_b\rangle &= \langle\psi_a|\left[\left[\hat{O}_e, \hat{H}\right], \hat{H}\right]|\psi_b\rangle \\ &= (E_b - E_a)^2\langle\psi_a|\hat{O}_e|\psi_b\rangle \\ &= \lambda\langle\psi_a|\hat{O}_e|\psi_b\rangle;\end{aligned} \tag{5}$$

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. [4]. We point out that the classical correspondence of the second-order IEO equation $\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^2\hat{O}_e = \left[\left[\hat{O}_e, \hat{H}\right], \hat{H}\right] = \lambda\hat{O}_e$ is useful for finding normal coordinates in classical dynamics. This is because $\left[\left[\hat{O}_e, \hat{H}\right], \hat{H}\right]$ corresponds to the classical Newton equation (see the Appendix). Thus the classical normal coordinates can be derived by virtue of the IEO method, which seems convenient and effective.

3. Matrix equation for obtaining the second-order IEO for the quantised Hamiltonian

Now we tackle the quantised Hamiltonian

$$\hat{H} = \frac{1}{2}\sum_{ij}^{n} M_{ij}\hat{p}_i\hat{p}_j + \frac{1}{2}\sum_{ij}^{n} L_{ij}\hat{q}_i\hat{q}_j, \tag{6}$$

the Hermiticity of $\hat{H}$ requires $M_{ij} = M_{ji}^*$, $L_{ij} = L_{ji}^*$. Note that there is no cross term of $\hat{p}_i$ and $\hat{q}_i$ in the Hamiltonian. And $\hat{q}_i$, $\hat{p}_i$ satisfy the following commutation relationship

$$[\hat{q}_i, \hat{p}_j] = \mathrm{i}\,\delta_{ij}, \quad [\hat{q}_i, \hat{q}_j] = [\hat{p}_i, p_j] = 0. \tag{7}$$

It then follows

$$\left[\hat{q}_i, \hat{H}\right] = \mathrm{i}\sum_j M_{ji}\hat{p}_j, \tag{8}$$

$$\left[\hat{p}_i, \hat{H}\right] = -\mathrm{i}\sum_j L_{ji}\hat{q}_j. \tag{9}$$

The above equations can be written in matrix form

$$\left[(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}), \hat{H}\right] = (\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{K}, \tag{10}$$

where

$$(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}) \equiv (\hat{q}_1, \ldots, \hat{q}_n, \hat{p}_1, \ldots, \hat{p}_n) \tag{11}$$

and $\boldsymbol{K}$ is a 2n×2n matrix

$$\boldsymbol{K} = \mathrm{i}\begin{pmatrix} 0 & -L \\ M & 0 \end{pmatrix}. \tag{12}$$

Without loss of generality, an invariant eigen-operator can be expressed as

$$\hat{\boldsymbol{O}}_e = (\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{V}, \tag{13}$$

where the matrix $\boldsymbol{V}$ is to be determined by the equation

$$\begin{aligned}\mathrm{i}\frac{\partial}{\partial t}\left[(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{V}\right] &= \left[(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{V}, \hat{H}\right] = (\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{K}\boldsymbol{V} \\ &= \lambda\,(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{V},\end{aligned} \tag{14}$$

so we arrive at the eigen-equation

$$\boldsymbol{K}\boldsymbol{V} = \lambda\boldsymbol{V}. \tag{15}$$

As we have seen in the introduction that the normal coordinates come for solving the second-order differential equations, which correspond to communication relation $\left[\left[(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}), \hat{H}\right], \hat{H}\right]$, so from Eqs. (10) and (12) we have

$$\begin{aligned}\left[\left[(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}}), \hat{H}\right], \hat{H}\right] &= \left[(\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{K}, \hat{H}\right] = (\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\,\boldsymbol{K}^2 \\ &= (\hat{\boldsymbol{q}}, \hat{\boldsymbol{p}})\begin{pmatrix} \boldsymbol{L}\boldsymbol{M} & 0 \\ 0 & \boldsymbol{M}\boldsymbol{L} \end{pmatrix},\end{aligned} \tag{16}$$

$\boldsymbol{K}^2$ is in diagonalised form, in other words, $\hat{\boldsymbol{q}}$ and $\hat{\boldsymbol{p}}$ are separated in its second communication relation with $\hat{H}$, i.e.,

$$\left[\left[\hat{\boldsymbol{q}}, \hat{H}\right], \hat{H}\right] = \hat{\boldsymbol{q}}\boldsymbol{L}\boldsymbol{M}, \tag{17}$$

$$\left[\left[\hat{\boldsymbol{p}}, \hat{H}\right], \hat{H}\right] = \hat{\boldsymbol{p}}\boldsymbol{M}\boldsymbol{L}, \tag{18}$$

so we can use $\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^2\hat{O}_e = \left[\left[\hat{O}_e, \hat{H}\right], \hat{H}\right] = \lambda\hat{O}_e$ to calculate second-order invariant operators with the form $\hat{\boldsymbol{O}}_e = \hat{\boldsymbol{q}}\boldsymbol{V}_q$ or $\hat{\boldsymbol{O}}_e = \hat{\boldsymbol{p}}\boldsymbol{V}_p$,

$$\left[\left[\hat{\boldsymbol{q}}\boldsymbol{V}_q, \hat{H}\right], \hat{H}\right] = \lambda\hat{\boldsymbol{q}}\boldsymbol{V}_q, \tag{19}$$

$$\left[\left[\hat{\boldsymbol{p}}\boldsymbol{V}_q, \hat{H}\right], \hat{H}\right] = \lambda \hat{\boldsymbol{p}}\boldsymbol{V}_q. \tag{20}$$

Combining Eqs. (17) and (18) with Eqs. (19) and (20) respectively, we find that $\boldsymbol{V_q}$ and $\boldsymbol{V_p}$ satisfy the eigenvalue equations

$$\boldsymbol{LMV_q} = \boldsymbol{\lambda_q V_q}, \tag{21}$$

and

$$\boldsymbol{MLV_p} = \boldsymbol{\lambda_p V_p}, \tag{22}$$

respectively. This is the matrix equation for obtaining the second-order invariant eigen-operator for the quantised Hamiltonian $\hat{H}$. Once $\boldsymbol{V_q}$ (and simultaneously λ_q) is determined, $\boldsymbol{O_e}$ will be obtained.

4. The general form of normal coordinates

We can rewrite $\boldsymbol{LMV_q} = \boldsymbol{\lambda_q V_q}$ as

$$\left(\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}\right)\left(\boldsymbol{M}^{1/2}\boldsymbol{V}_q\right) = \boldsymbol{\lambda_q}\left(\boldsymbol{M}^{1/2}\boldsymbol{V_q}\right). \tag{23}$$

Now since $\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}$ is symmetric, we can find an orthogonal matrix $\boldsymbol{R}$ such that

$$\boldsymbol{R}^{\mathrm{T}}\left(\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}\right)\boldsymbol{R} = \mathrm{diag}\left(\boldsymbol{\lambda}_q\right). \tag{24}$$

Then by introducing the new canonical coordinates

$$\hat{\boldsymbol{q}}' = \hat{\boldsymbol{q}}\boldsymbol{M}^{-1/2}\boldsymbol{R}, \quad \hat{\boldsymbol{p}}' = \hat{\boldsymbol{p}}\boldsymbol{M}^{1/2}\boldsymbol{R}, \tag{25}$$

which satisfy

$$\left[\hat{q}'_j, \hat{p}'_k\right] = \mathrm{i}\,\delta_{jk}, \tag{26}$$

and using Eq. (24), we have

$$\begin{aligned}\hat{H} &= \frac{1}{2}\hat{\boldsymbol{p}}\boldsymbol{M}\hat{\boldsymbol{p}}^{\mathrm{T}} + \frac{1}{2}\hat{\boldsymbol{q}}\boldsymbol{L}\hat{\boldsymbol{q}}^{\mathrm{T}} \\ &= \frac{1}{2}\hat{\boldsymbol{p}}'\boldsymbol{R}^{\mathrm{T}}\boldsymbol{M}^{-1/2}\boldsymbol{M}\boldsymbol{M}^{-1/2}\boldsymbol{R}\hat{\boldsymbol{p}}'^{T} \\ &\quad + \frac{1}{2}\hat{\boldsymbol{q}}'\boldsymbol{R}^{\mathrm{T}}\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}\boldsymbol{R}\hat{\boldsymbol{q}}'^{\mathrm{T}} \\ &= \frac{1}{2}\hat{\boldsymbol{p}}'\hat{\boldsymbol{p}}'^{\mathrm{T}} + \frac{1}{2}\hat{\boldsymbol{q}}'\mathrm{diag}\left(\boldsymbol{\lambda}_q\right)\hat{\boldsymbol{q}}'^{T}. \end{aligned} \tag{27}$$

In other words, $\boldsymbol{q}' = \boldsymbol{q}\boldsymbol{M}^{-1/2}\boldsymbol{R}$ are exactly the normal coordinates we need. One can confirm this by calculating

$$\begin{aligned}\left[\left[\hat{\boldsymbol{q}}', \hat{H}\right], \hat{H}\right] &= \left[\left[\hat{\boldsymbol{q}}, \hat{H}\right], \hat{H}\right]\boldsymbol{M}^{-1/2}\boldsymbol{R} \\ &= \hat{\boldsymbol{q}}\boldsymbol{L}\boldsymbol{M}\boldsymbol{M}^{-1/2}\boldsymbol{R} \\ &= \hat{\boldsymbol{q}}'\boldsymbol{R}^{\mathrm{T}}\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}\boldsymbol{R} \\ &= \hat{\boldsymbol{q}}'\mathrm{diag}\left(\boldsymbol{\lambda}_q\right), \end{aligned} \tag{28}$$

and

$$\begin{aligned}\left[\left[\hat{\boldsymbol{p}}', \hat{H}\right], \hat{H}\right] &= \left[\left[\hat{\boldsymbol{p}}, \hat{H}\right], \hat{H}\right]\boldsymbol{M}^{1/2}\boldsymbol{R} \\ &= \hat{\boldsymbol{p}}\boldsymbol{M}\boldsymbol{L}\boldsymbol{M}^{1/2}\boldsymbol{R} \\ &= \hat{\boldsymbol{p}}'\boldsymbol{R}^{\mathrm{T}}\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}\boldsymbol{R} \\ &= \hat{\boldsymbol{p}}'\mathrm{diag}\left(\boldsymbol{\lambda}_q\right), \end{aligned} \tag{29}$$

i.e.

$$\left[\left[\hat{q}'_i, \hat{H}\right], \hat{H}\right] = \lambda_{qi}\hat{q}'_i, \quad \left[\left[\hat{p}'_i, \hat{H}\right], \hat{H}\right] = \lambda_{qi}\hat{p}'_i, \tag{30}$$

where $\hat{q}'_i$ and $\hat{p}'_i$ are the second-order invariant eigenvector with the same eigenvalue λ_{qi}. The standard procedure for obtaining normal coordinates are summarised as: 1) Read off matrices $\boldsymbol{M}$ and $\boldsymbol{L}$ straightforwardly from Hamiltonian H itself. 2) Calculate the eigenvalues and eigenvectors of the numerical matrix $\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}$, then write down normal coordinates according to Eq. (25). If we are interested in the energy-gaps only, then we do not need to calculate $\boldsymbol{M}^{1/2}$, let alone the eigenvectors of $\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}$. The energy-gaps are the square roots of eigenvalues of $\boldsymbol{ML}$ (or equivalently, $\boldsymbol{LM}$).

5. Some examples

Now we list some examples as applications of the above conclusion. When we consider a triatomic molecule with the Hamiltonian[5]

$$\begin{aligned}\hat{H}_1 &= \frac{\hat{p}_1^2}{2\nu} + \frac{\hat{p}_2^2}{2\mu} + \frac{\hat{p}_3^2}{2\nu} + \frac{\tau}{2}\left(\hat{q}_1 - \hat{q}_2\right)^2 \\ &\quad + \frac{\tau}{2}\left(\hat{q}_3 - \hat{q}_2\right)^2, \end{aligned} \tag{31}$$

by comparing Eq. (31) with the standard form Eq. (1) we find

$$\boldsymbol{L} = \tau\begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}, \quad \boldsymbol{M} = \begin{pmatrix} \frac{1}{\nu} & 0 & 0 \\ 0 & \frac{1}{\mu} & 0 \\ 0 & 0 & \frac{1}{\nu} \end{pmatrix}, \tag{32}$$

it follows

$$\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2} = \tau\begin{pmatrix} \frac{1}{\nu} & -\sqrt{\frac{1}{\mu\nu}} & 0 \\ -\sqrt{\frac{1}{\mu\nu}} & \frac{2}{\mu} & -\sqrt{\frac{1}{\mu\nu}} \\ 0 & -\sqrt{\frac{1}{\mu\nu}} & \frac{1}{\nu} \end{pmatrix}. \tag{33}$$

Using Eq. (24), we can derive the diagonalising matrix for $\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}$

$$\boldsymbol{R}=\begin{pmatrix} \sqrt{\dfrac{\nu}{\mu+2\nu}} & -\sqrt{1/2} & \sqrt{\dfrac{\mu}{2\mu+4\nu}} \\ \sqrt{\dfrac{\mu}{\mu+2\nu}} & 0 & -2\sqrt{\dfrac{\nu}{2\mu+4\nu}} \\ \sqrt{\dfrac{\nu}{\mu+2\nu}} & \sqrt{1/2} & \sqrt{\dfrac{\mu}{2\mu+4\nu}} \end{pmatrix}, \tag{34}$$

and

$$\boldsymbol{R}^{\mathrm{T}}\left(\boldsymbol{M}^{1/2}\boldsymbol{L}\boldsymbol{M}^{1/2}\right)\boldsymbol{R}=\mathrm{diag}\left(0,\frac{\tau}{\nu},\frac{2\tau}{\mu}+\frac{\tau}{\nu}\right). \tag{35}$$

Then according to Eq. (25) we further calculate

$$(\hat{q}_1,\hat{q}_2,\hat{q}_3)\,\boldsymbol{M}^{-1/2}\boldsymbol{R}=\left(\frac{\nu\hat{q}_1+\mu\hat{q}_2+\nu\hat{q}_3}{\sqrt{\mu+2\nu}},\ \sqrt{\nu/2}\,(\hat{q}_1-\hat{q}_3)\,,\ \sqrt{\frac{\mu\nu}{2\mu+4\nu}}\,(\hat{q}_1-2\hat{q}_2+\hat{q}_3)\right), \tag{36}$$

where $\dfrac{\nu\hat{q}_1+\mu\hat{q}_2+\nu\hat{q}_3}{\sqrt{\mu+2\nu}}$ just denotes the centre of mass coordinate, so it corresponds to $\sqrt{\lambda_1}=0$; The two normal coordinates (up to an inconsequential constant) are

$$\hat{q}_1-\hat{q}_3, \tag{37}$$

and

$$\hat{q}_1-2\hat{q}_2+\hat{q}_3, \tag{38}$$

which correspond to

$$\sqrt{\lambda_2}=\sqrt{\frac{\tau}{\nu}},\ \sqrt{\lambda_3}=\sqrt{\frac{\tau}{\nu}\left(1+\frac{2\nu}{\mu}\right)}, \tag{39}$$

respectively. In the normal mode $(\hat{q}_1-\hat{q}_3)$, $\hat{q}_1$ and $\hat{q}_3$ are displaced equally in opposite directions, while in the second normal mode, the two end masses move in the same direction. One can check Eq. (28) by Eq. (36).

Example 2: when the Hamiltonian is[6]

$$\hat{H}_2=\sum_{n=1}^{N}\left[\frac{\hat{p}_n^2}{2m}+\frac{\beta}{2}\left(\hat{q}_n-\hat{q}_{n-1}\right)^2+\gamma\hat{q}_n^2\right], \tag{40}$$

under the periodic condition

$$\hat{p}_{N+n}=\hat{p}_n,\quad \hat{q}_{N+n}=\hat{q}_n, \tag{41}$$

according to the standard form Eq. (1) we obtain in this case $\boldsymbol{M}=\boldsymbol{I}_N/m$, so $\boldsymbol{M}\boldsymbol{L}=\boldsymbol{L}\boldsymbol{M}=\boldsymbol{L}/m$, the problem is ascribed to searching for the eigenvector of $\boldsymbol{L}$, and $\boldsymbol{L}$ is a cyclic matrix, its N-eigenvectors are

$$\sum_{n=1}^{N}\hat{q}_n\cos(n\theta_l),\quad \theta_l=\frac{l\pi}{N},\quad l=1,2\ldots N, \tag{42}$$

which are just the N-normal coordinates. Taking $\sum\limits_{n=1}^{N}\hat{q}_n\cos(n\theta_l)=\hat{O}_e$ as an IEO, then from

$$[\hat{q}_n,H_2]=\frac{\mathrm{i}\,\hat{p}_n}{m}, \tag{43}$$

and

$$[\mathrm{i}\,\hat{p}_n,H_2]=\beta\left(2\hat{q}_n-\hat{q}_{n-1}-\hat{q}_{n+1}\right)+2\gamma\hat{q}_n, \tag{44}$$

we have

$$\begin{aligned}\left[\left[\sum_{n=1}^{N}\hat{q}_n\cos(n\theta_l),H_2\right],H_2\right] &= \sum_{n=1}^{N}\cos(n\theta_l)\left[\frac{\beta}{m}\left(2\hat{q}_n-\hat{q}_{n-1}-\hat{q}_{n+1}\right)+\frac{2\gamma}{m}\hat{q}_n\right] \\ &= \frac{2\beta\left(1-\cos\theta_l\right)+2\gamma}{m}\sum_{n=1}^{N}\hat{q}_n\cos(n\theta_l),\end{aligned} \tag{45}$$

so the vibration mode is

$$\omega_l = \sqrt{\frac{2\beta\left(1-\cos\theta_l\right)+2\gamma}{m}}. \tag{46}$$

In summary, we have introduced a new method to derive the normal coordinates, which seems convenient and effective and can be applied to studying vibration in lattice. Actually without this IEO method, the normal coordinates for the classical Hamiltonian in Eq. (1) was hardly derived, because one should make ansatz (some lattice wave solution) to the Lagrangian equation of motion (second-order differential equation) and then solve it; however, for the complicated lattice structure one has no good idea about what the correct ansatz is.

Also it seems that the IEO method can significantly simplify the derivation of vibration modes because calculating quantum commutators in many cases are easier than solving differential equations.

Appendix

For the classical Lagrangian

$$\mathcal{L} = \frac{1}{2}\left(\sum_{i=1}^{n} m_i x_i^2 - \sum_{i,j=1}^{n} k_{ij} x_i x_j\right), \tag{A1}$$

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

$$\mathcal{L} = \frac{1}{2}\left(\sum_{\alpha=1}^{n} \dot{Q}^{(\alpha)2} - \sum_{\alpha=1}^{n} \omega_\alpha^2 Q^{(\alpha)2}\right), \tag{A2}$$

so the Lagrangian equation $\dfrac{\mathrm{d}}{\mathrm{d}t}\dfrac{\partial \mathcal{L}}{\partial \dot{Q}^{(\alpha)}} - \dfrac{\partial \mathcal{L}}{\partial Q^{(\alpha)}} = 0$ leads to the Newton equation (second order differential equation)

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} Q^{(\alpha)} = \omega_\alpha^2 Q^{(\alpha)}. \tag{A3}$$

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