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N-Mode Hamiltonians with Coordinate-Momentum Coupling Terms

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Abstract The Virial theorem, which is related to the Feynman-Hellmann (FH) theorem, usually applies to Hamiltonians without coordinate-momentum coupling terms. In this paper we discuss when there are coordinate-momentum coupling terms in N-mode Hamiltonians, how the Virial theorem should be modified, and the energy contribution arising from the coordinate-momentum coupling is also be discussed.

Keywords Feynman-Hellmann theorem · Invariant 'eigen-operator'

1 Introduction

The Feynman-Hellmann (FH) theorem has been widely employed in quantum chemistry, quantum statistics, molecular physics, and elementary particle physics [1–3]. In quantum mechanics the Feynman-Hellmann theorem states that for pure normalized states $|\psi_n\rangle$

$$\frac{\partial E_n}{\partial \lambda} =_n \langle\psi|\frac{\partial H}{\partial \lambda}|\psi\rangle_n, \quad {}_n\langle\psi|\psi\rangle_n = 1, \tag{1}$$

here H is the Hamiltonian relying on the parameter λ, $|\psi\rangle_n$ is H's eigenvectors, $H|\psi\rangle_n = E_n|\psi\rangle_n$. This theorem can be extended to the case for mixed state ensemble average [4]. We can derive the Virial theorem which states that for Hamiltonians

$$H = \frac{\vec{P}^2}{2m} + V(\vec{r}), \tag{2}$$

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the following formula is valid for kinetic energy and potential energy,

$$ {}_n\langle\psi|\frac{\vec{P}^2}{2m}|\psi\rangle_n = \frac{1}{2}{}_n\langle\psi|\vec{r}.\nabla V(\vec{r})|\psi\rangle_n. \tag{3} $$

Especially, when $V(\vec{r})$ is a υ-order homogeneous function of $\vec{r}$, then (3) leads to

$$ {}_n\langle\psi|\frac{P^2}{2m}|\psi\rangle_n = \frac{\upsilon}{2}{}_n\langle\psi|V(\vec{r})|\psi\rangle_n. \tag{4} $$

N-mode Hamiltonian has the form as:

$$ H = \sum_{i=1}^{n}\left(\frac{P_i^2}{2m} + \frac{1}{2}m\omega^2 Q_i^2\right). \tag{5} $$

When there are coordinates-momentum couplings terms, e.g.

$$ H_1 = \sum_{i=1}^{n}\left(\frac{P_i^2}{2m} + \frac{1}{2}m\omega^2 Q_i^2\right) + \lambda\left(\prod_{i=1}^{n} P_i + \prod_{i=1}^{n} Q_i\right) \tag{6} $$

or

$$ H_2 = \sum_{i=1}^{n}\left(\frac{P_i^2}{2m} + \frac{1}{2}m\omega^2 Q_i^2\right) + \lambda\left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1\right) \tag{7} $$

in Hamiltonians, then the Virial theorem needs to be modified, the contribution of coordinates-momentum couplings terms to energy for a definite energy level also should be discussed. We will give some information about these question.

2 The Modified Virial Theorem for N-Mode Hamiltonians

Let us recall that one approach to the Virial theorem for

$$ H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 Q^2 \tag{8} $$

is selecting the operator PQ and writing down its Heisenberg equation of motion,

$$ \frac{d(PQ)}{dt} = -i[PQ, H] = \frac{P^2}{m} - m\omega^2 Q^2. \tag{9} $$

Due to

$$ \left\langle\frac{d(PQ)}{dt}\right\rangle_n = -i\langle[PQ, H]\rangle_n = 0, \tag{10} $$

so

$$ \left\langle\frac{P^2}{m}\right\rangle_n = \langle m\omega^2 Q^2\rangle_n. \tag{11} $$

It can be extend to the N-mode Hamiltonian, i.e.,

$$H=\sum_{i=1}^{n}\left(\frac{P_i^2}{2m}+\frac{1}{2}m\omega^2Q_i^2\right). \tag{12}$$

We select the operator $\sum_{i=1}^{n}P_iQ_i$ and write down its Heisenberg equation of motion

$$\frac{d(\sum_{i=1}^{n}P_iQ_i)}{dt}=-i\left[\sum_{i=1}^{n}P_iQ_i,H\right]=\sum_{i=1}^{n}\left(\frac{P_i^2}{m}+m\omega^2Q_i^2\right), \tag{13}$$

for

$$\frac{d(\sum_{i=1}^{n}P_iQ_i)}{dt}=-i\left[\sum_{i=1}^{n}P_iQ_i,H\right]=0, \tag{14}$$

so

$$\left\langle\sum_{i=1}^{n}\frac{P_i^2}{m}\right\rangle_n=m\omega^2\left\langle\sum_{i=1}^{n}Q_i^2\right\rangle_n. \tag{15}$$

When there are different kinds of coordinate-momentum couplings in Hamiltonians, the Virial theorem needs to be reconsidered. Now we will discuss three cases:

Case 1: The Hamiltonian is

$$H_1=\sum_{i=1}^{n}\left(\frac{P_i^2}{2m}+\frac{1}{2}m\omega^2Q_i^2\right)+\lambda\left(\prod_{i=1}^{n}P_i+\prod_{i=1}^{n}Q_i\right). \tag{16}$$

We consider

$$-i\sum_{i=1}^{n}\left[P_iQ_i,\frac{P_i^2}{2m}+\frac{1}{2}m\omega^2Q_i^2\right]=\sum_{i=1}^{n}\left(\frac{P_i^2}{m}-m\omega^2Q_i^2\right), \tag{17}$$

and

$$-i\left[\sum_{i=1}^{n}P_iQ_i,\lambda\left(\prod_{i=1}^{n}P_i+\prod_{i=1}^{n}Q_i\right)\right]=2\lambda\left(\prod_{i=1}^{n}P_i-\prod_{i=1}^{n}Q_i\right). \tag{18}$$

Then

$$\begin{aligned}\frac{d}{dt}\left(\sum_{i=1}^{n}P_iQ_i\right)&=-i\left[\sum_{i=1}^{n}P_iQ_i,H_1\right]\\&=\sum_{i=1}^{n}\left(\frac{P_i^2}{m}-m\omega^2Q_i^2\right)+2\lambda\left(\prod_{i=1}^{n}P_i-\prod_{i=1}^{n}Q_i\right).\end{aligned} \tag{19}$$

For bound states of H_1,

$$\left\langle\frac{d}{dt}\left(\sum_{i=1}^{n}P_iQ_i\right)\right\rangle_n=\left\langle-i\left[\sum_{i=1}^{n}P_iQ_i,H_1\right]\right\rangle_n=0, \tag{20}$$

so we can have

$$\left\langle \sum_{i=1}^{n} \frac{P_i^2}{m} + 2\lambda \prod_{i=1}^{n} P_i \right\rangle = \left\langle \sum_{i=1}^{n} m\omega^2 Q_i^2 + 2\lambda \prod_{i=1}^{n} Q_i \right\rangle. \tag{21}$$

This is a non-trivial generalization of the Virial theorem for H_1.

Case 2: When the N-mode Hamiltonian is [5]

$$H_2 = \sum_{i=1}^{n} \left(\frac{P_i^2}{2m} + \frac{1}{2} m\omega^2 Q_i^2 \right) + \lambda \left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1 \right), \tag{22}$$

in which the coordinates-momentum are cross coupled. Due to

$$\begin{aligned} \frac{d}{dt}\left(\prod_{i=1}^{n} Q_i \right) &= -i \left[\prod_{i=1}^{n} Q_i, H_2 \right] \\ &= \frac{1}{m} \left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1 \right) + \lambda \sum_{i=1}^{n} Q_i^2, \end{aligned} \tag{23}$$

for the bounded states of H_2,

$$\left\langle \frac{d}{dt}\left(\prod_{i=1}^{n} Q_i \right) \right\rangle_n = -i \left\langle \left[\prod_{i=1}^{n} Q_i, H_2 \right] \right\rangle_n = 0, \tag{24}$$

so

$$\left\langle \left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1 \right) \right\rangle_n =_n \langle \Psi | \frac{\partial H_2}{\partial \lambda} | \Psi \rangle_n = -\lambda m \left\langle \left(\sum_{i=1}^{n} Q_i^2 \right) \right\rangle_n = \frac{\partial E_n}{\partial \lambda}. \tag{25}$$

Thus $\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1$ decreases the energy. On the other hand, from

$$\begin{aligned} \frac{d}{dt}\left(\prod_{i=1}^{n} P_i \right) &= -i \left[\prod_{i=1}^{n} P_i, H_2 \right] \\ &= -m\omega^2 \left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1 \right) - \lambda \sum_{i=1}^{n} P_i^2, \end{aligned} \tag{26}$$

and that for bounded states

$$\left\langle \frac{d}{dt}\left(\prod_{i=1}^{n} P_i \right) \right\rangle_n = -i \left\langle \left[\prod_{i=1}^{n} P_i, H_2 \right] \right\rangle_n = 0, \tag{27}$$

we have

$$\frac{\partial E_n}{\partial \lambda} = \left\langle \sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1 \right\rangle_n = -\frac{\lambda}{m\omega^2} \left\langle \sum_{i=1}^{n} P_i^2 \right\rangle_n = -\lambda m \left\langle \sum_{i=1}^{n} Q_i^2 \right\rangle_n, \tag{28}$$

so in this case we have $m\omega^2\langle\sum_{i=1}^n Q_i^2\rangle = \frac{1}{m}\langle\sum_{i=1}^n P_i^2\rangle_n$. The total energy

$$\langle H_2\rangle_n = \left\langle \sum_{i=1}^n \frac{P_i^2}{m} + \lambda\left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1\right)\right\rangle_n = \left\langle \sum_{i=1}^n \frac{\omega^2-\lambda^2}{m\omega^2} P_i^2\right\rangle_n = E_n, \tag{29}$$

thus the contribution arising from $\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1$ is,

$$\left\langle \sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1\right\rangle = -\frac{\lambda}{\omega^2-\lambda^2} E_n. \tag{30}$$

From (28), we also have

$$E_n = -m\int \lambda \left\langle \sum_{i=1}^n Q_i^2\right\rangle_n d\lambda + C. \tag{31}$$

From $[\sum_{i=1}^N Q_i, H] = i\lambda\sum_{i=1}^N Q_i + i\sum_{n=1}^N P_i$ and $[\sum_{i=1}^N P_i, H] = -i\sum_{i=1}^N Q_i - i\lambda\times \sum_{i=1}^N P_i$, we suppose the 'invariant eigen-operator' [6] is

$$O_e = \sum_{i=1}^N Q_i + \left(\lambda + i\sqrt{1-\lambda^2}\right)\sum_{i=1}^N P_i. \tag{32}$$

Using the Heisenberg equation of motion we have

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2 O_e = [[O_e, H], H] = (1-\lambda^2)O_e, \tag{33}$$

so one of the energy-level gaps is

$$k = \sqrt{1-\lambda^2}. \tag{34}$$

Case 3: The Hamiltonian is

$$H_3 = \sum_{i=1}^n \left(\frac{P_i^2}{2m} + \frac{1}{2}m\omega^2 Q_i^2\right) + f\sum_{i=1}^n (P_i Q_i + Q_i P_i). \tag{35}$$

From $[\sum_{i=1}^n P_i^2, \sum_{i=1}^n Q_i^2] = -2i\sum_{i=1}^n (P_i Q_i + Q_i P_i)$, we know

$$\begin{aligned}\frac{d(\sum_{i=1}^n P_i^2)}{dt} &= -i\left[\sum_{i=n}^n P_i^2, \sum_{i=n}^n\left[\frac{1}{2}m\omega^2 Q_i^2 + f(P_i Q_i + Q_i P_i)\right]\right]\\ &= -m\omega^2\sum_{i=1}^n (P_i Q_i + Q_i P_i) - 4f\sum_{i=1}^n P_i^2,\end{aligned} \tag{36}$$

and

$$\begin{aligned}\frac{d(\sum_{i=1}^n Q_i^2)}{dt} &= -i\sum_{i=n}^n\left[Q_i^2, \frac{P_i^2}{2m} + f\left(\prod_{i=1}^n P_i + \prod_{i=1}^n Q_i\right)\right]\\ &= \frac{1}{m}\sum_{i=1}^n (P_i Q_i + Q_i P_i) + 4f\sum_{i=1}^n Q_i^2.\end{aligned} \tag{37}$$

For bound states $|\Psi\rangle_n$ of H_3 , we see

$$\left\langle \frac{d\sum_{i=1}^{n} P_i^2}{dt} \right\rangle_n = -i\left\langle \left[\sum_{i=1}^{n} P_i^2, H_3 \right] \right\rangle_n = 0,$$
$$\left\langle \frac{d\sum_{i=1}^{n} Q_i^2}{dt} \right\rangle_n = -i\left\langle \left[\sum_{i=1}^{n} Q_i^2, H_3 \right] \right\rangle_n = 0, \tag{38}$$

it then follows

$$\left\langle \sum_{i=1}^{n} (P_i Q_i + Q_i P_i) \right\rangle = -\frac{4f}{m\omega^2}\left\langle \sum_{i=1}^{n} P_i^2 \right\rangle = -4mf\left\langle \sum_{i=1}^{n} Q_i^2 \right\rangle, \tag{39}$$

and still we see $m\omega^2 \langle \sum_{i=1}^{n} Q_i^2 \rangle = \frac{1}{m}\langle \sum_{i=1}^{n} P_i^2 \rangle$. The total energy in the state $|\psi\rangle_n$ is

$$\begin{aligned} \langle H_3 \rangle_n &= \left\langle \sum_{i=1}^{n} \left(\frac{P_i^2}{2m} + \frac{1}{2} m\omega^2 Q_i^2 \right) + f \sum_{i=1}^{n} (P_i Q_i + Q_i P_i) \right\rangle_n \\ &= E_n = \frac{\omega^2 - 4f^2}{m\omega^2}\left\langle \sum_{i=1}^{n} P_i^2 \right\rangle_n, \end{aligned} \tag{40}$$

so

$$\left\langle \sum_{i=1}^{n} \frac{P_i^2}{2m} \right\rangle = \frac{\omega^2}{2(\omega^2 - 4f^2)} E_n. \tag{41}$$

Thus the contribution from the coordinate-momentum coupling term is

$$\langle f(P_i Q_i + Q_i P_i) \rangle_n = -\frac{8f^2}{\omega^2}\left\langle \sum_{i=1}^{n} \frac{P_i^2}{2m} \right\rangle_n = \frac{-4f^2}{(\omega^2 - 4f^2)} E_n, \tag{42}$$

which plays the role of decreasing the energy when $\omega^2 > 4f^2$, however, when $\omega^2 < 4f^2$, its contribution is positive.

3 Extending to the Mixed State Case

Equation (3) is the Virial theorem which is suitable for pure states. The generalized virial theorem relating the ensemble average values of kinetic energy and potential energy is derived in reference [7],

$$\left\langle 2T - \sum_{i=1}^{N} \sum_{j=1}^{3} x_{ij} \frac{\partial V}{\partial x_{ij}} \right\rangle_e = C/\beta, \tag{43}$$

where T is the kinetic energy and V is the potential energy, C is an integration constant, β is the Boltzmann constant, the subscript e denotes ensemble average. But the Virial theorem under the mixed state case including coordinates-momentum couplings in Hamiltonians is not discussed yet. The above discussion is about the concrete form of Virial theorem which is suitable for pure states including coordinates-momentum couplings in Hamiltonians. Now we extend the pure state case to mixed state case. It is interesting to find that the results under the mixed state case are similar with the pure state case.

Case 1: When the coordinate-momentum is

$$H_1=\sum_{i=1}^{n}\left(\frac{P_i^2}{2m}+\frac{1}{2}m\omega^2Q_i^2\right)+\lambda\left(\prod_{i=1}^{n}P_i+\prod_{i=1}^{n}Q_i\right),$$

we have

$$\left\langle\frac{d}{dt}\left(\sum_{i=1}^{n}P_iQ_i\right)\right\rangle_e=\left\langle-i\left[\sum_{i=1}^{n}P_iQ_i,H_1\right]\right\rangle_e=0, \tag{44}$$

so we conclude

$$\left\langle\sum_{i=1}^{n}\frac{P_i^2}{m}+2\lambda\prod_{i=1}^{n}P_i\right\rangle_e=\left\langle\sum_{i=1}^{n}m\omega^2Q_i^2+2\lambda\prod_{i=1}^{n}Q_i\right\rangle_e. \tag{45}$$

This is a non-trivial generalization of the Virial theorem for H_1.

Case 2: When the N-mode Hamiltonian is

$$H_2=\sum_{i=1}^{n}\left(\frac{P_i^2}{2m}+\frac{1}{2}m\omega^2Q_i^2\right)+\lambda\left(\sum_{i=1}^{n-1}Q_iP_{i+1}+Q_nP_1\right),$$

in which the coordinates-momenta are cross coupled. Owing to

$$\left\langle\left[\prod_{i=1}^{n}Q_i,H_2\right]\right\rangle=\left\langle\left(\prod_{i=1}^{n}Q_i\right)H_2\right\rangle-\left\langle H_2\prod_{i=1}^{n}Q_i\right\rangle=0, \tag{46}$$

$$\begin{aligned}\left\langle\left(\prod_{i=1}^{n}Q_i\right)H_2\right\rangle&=\frac{\mathrm{Tr}(\rho(\prod_{i=1}^{n}Q_i)H_2)}{\mathrm{Tr}\,\rho}=\frac{1}{\mathrm{Tr}\,\rho}\mathrm{Tr}\left(\sum_j|j\rangle\langle j|e^{-\beta H_2}\left(\prod_{i=1}^{n}Q_i\right)H_2\right)\\&=\frac{1}{\mathrm{Tr}\,\rho}\sum_j e^{-\beta E_j}\langle j|\prod_{i=1}^{n}Q_i|j\rangle,\end{aligned} \tag{47}$$

and

$$\left\langle H_2\prod_{i=1}^{n}Q_i\right\rangle=\frac{1}{\mathrm{Tr}\,\rho}\sum_j e^{-\beta E_j}\langle j|\prod_{i=1}^{n}Q_i|j\rangle, \tag{48}$$

then

$$\left\langle\frac{d}{dt}\left(\prod_{i=1}^{n}Q_i\right)\right\rangle_e=-i\left\langle\left[\prod_{i=1}^{n}Q_i,H_2\right]\right\rangle_e=0. \tag{49}$$

Combing (23), we see

$$\left\langle\left(\sum_{i=1}^{n-1}Q_iP_{i+1}+Q_nP_1\right)\right\rangle_e={}_e\langle\Psi|\frac{\partial H_2}{\partial\lambda}|\Psi\rangle_e=-\lambda m\left\langle\sum_{i=1}^{n}Q_i^2\right\rangle_e=\frac{\partial\overline{E_n}}{\partial\lambda}. \tag{50}$$

On the other hand, from (27) and

$$\left\langle \frac{d}{dt}\left(\prod_{i=1}^{n} P_i\right)\right\rangle_e = -i\left\langle\left[\prod_{i=1}^{n} P_i, H_2\right]\right\rangle_e = 0, \tag{51}$$

we have

$$\frac{\partial \overline{E_n}}{\partial \lambda} = \left\langle\left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1\right)\right\rangle_e = -\frac{\lambda}{m\omega^2}\left\langle\sum_{i=1}^{n} P_i^2\right\rangle_e = -\lambda m\left\langle\sum_{i=1}^{n} Q_i^2\right\rangle_e \tag{52}$$

so in this case we still have $m\omega^2\langle\sum_{i=1}^{n} Q_i^2\rangle_e = \frac{1}{m}\langle\sum_{i=1}^{n} P_i^2\rangle_e$. The ensemble average value of total energy

$$\langle H_2\rangle_e = \left\langle\sum_{i=1}^{n}\frac{P_i^2}{m} + \lambda\left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1\right)\right\rangle_e = \left\langle\sum_{i=1}^{n}\frac{\omega^2-\lambda^2}{m\omega^2} P_i^2\right\rangle_e = \overline{E_n}. \tag{53}$$

Thus the contribution arising from $\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1$ is,

$$\left\langle\left(\sum_{i=1}^{n-1} Q_i P_{i+1} + Q_n P_1\right)\right\rangle_e = -\frac{\lambda}{\omega^2-\lambda^2}\overline{E}. \tag{54}$$

From (52), we also have

$$\overline{E_n} = -m\int \lambda\left\langle\sum_{i=1}^{n} Q_i^2\right\rangle_e d\lambda + C. \tag{55}$$

Case 3: The Hamiltonian is

$$H_3 = \sum_{i=1}^{n}\left(\frac{P_i^2}{2m} + \frac{1}{2}m\omega^2 Q_i^2\right) + f\sum_{i=1}^{n}(P_i Q_i + Q_i P_i).$$

Owing to

$$\left\langle\left[\sum_{i=1}^{n} P_i^2, H_3\right]\right\rangle_e = \left\langle\left(\sum_{i=1}^{n} P_i^2\right) H_3\right\rangle_e - \left\langle H_3\sum_{i=1}^{n} P_i^2\right\rangle_e = 0, \tag{56}$$

$$\begin{aligned}\left\langle\left(\sum_{i=1}^{n} P_i^2\right) H_3\right\rangle_e &= \frac{\mathrm{Tr}(\rho(\sum_{i=1}^{n} P_i^2) H_3)}{\mathrm{Tr}\,\rho} = \frac{1}{\mathrm{Tr}\,\rho}\mathrm{Tr}\left(\sum_j |j\rangle\langle j| e^{-\beta H_3}\sum_{i=1}^{n} P_i^2 H_1\right)\\ &= \frac{1}{\mathrm{Tr}\,\rho}\sum_j \langle j| e^{-\beta H_3}\sum_{i=1}^{n} P_i^2 H_3|j\rangle\\ &= \frac{1}{\mathrm{Tr}\,\rho}\sum_j e^{-\beta E_j} E_j\langle j|\sum_{i=1}^{n} P_i^2|j\rangle,\end{aligned} \tag{57}$$

and

$$\left\langle H_3\sum_{i=1}^{n} P_i^2\right\rangle_e = \frac{1}{\mathrm{Tr}\,\rho}\sum_j \langle j| e^{-\beta H_3} H_3\sum_{i=1}^{n} P_i^2|j\rangle = \frac{1}{\mathrm{Tr}\,\rho}\sum_j e^{-\beta E_j} E_j\langle j|\sum_{i=1}^{n} P_i^2|j\rangle, \tag{58}$$

we see

$$\left\langle \frac{d\sum_{i=1}^{n} P_i^2}{dt} \right\rangle_e = -i\left\langle \left[\sum_{i=1}^{n} P_i^2, H_3 \right] \right\rangle_e = 0,$$
$$\left\langle \frac{d\sum_{i=1}^{n} Q_i^2}{dt} \right\rangle_e = -i\left\langle \left[\sum_{i=1}^{n} Q_i^2, H_3 \right] \right\rangle_e = 0, \tag{59}$$

combining (36) and (37), we have

$$\left\langle -m\omega^2 \sum_{i=1}^{n} (P_i Q_i + Q_i P_i) \right\rangle_e - \left\langle 4f \sum_{i=1}^{n} P_i^2 \right\rangle_e = 0, \tag{60}$$

and

$$\left\langle \frac{1}{m} \sum_{i=1}^{n} (P_i Q_i + Q_i P_i) \right\rangle_e + \left\langle 4f \sum_{i=1}^{n} P_i^2 \right\rangle_e = 0, \tag{61}$$

it then follows

$$\left\langle \sum_{i=1}^{n} (P_i Q_i + Q_i P_i) \right\rangle_e = -\frac{4f}{m\omega^2} \left\langle \sum_{i=1}^{n} P_i^2 \right\rangle_e = -4mf \left\langle \sum_{i=1}^{n} Q_i^2 \right\rangle_e, \tag{62}$$

still we see $m\omega^2 \ \langle \sum_{i=1}^{n} Q_i^2 \rangle_e = \frac{1}{m} \langle \sum_{i=1}^{n} P_i^2 \rangle_e$. The ensemble average value of total energy is

$$\langle H_3 \rangle_e = \left\langle \sum_{i=1}^{n} \left(\frac{P_i^2}{2m} + \frac{1}{2} m\omega^2 Q_i^2 \right) + f \sum_{i=1}^{n} (P_i Q_i + Q_i P_i) \right\rangle_e$$
$$= \overline{E_n} = \frac{\omega^2 - 4f^2}{m\omega^2} \left\langle \sum_{i=1}^{n} P_i^2 \right\rangle_e, \tag{63}$$

so

$$\left\langle \sum_{i=1}^{n} \left(\frac{P_i^2}{2m} \right) \right\rangle_e = \frac{\omega^2}{2(\omega^2 - 4f^2)} \overline{E}. \tag{64}$$

Thus the contribution from the coordinate-momentum coupling term is

$$\left\langle f \sum_{i=1}^{n} (P_i Q_i + Q_i P_i) \right\rangle_e = -\frac{8f^2}{\omega^2} \left\langle \sum_{i=1}^{n} \frac{P_i^2}{2m} \right\rangle_e = \frac{-4f^2}{(\omega^2 - 4f^2)} \overline{E_n}. \tag{65}$$

We find that the result is similar to the pure state case.

4 Conclusion

In summary, to know the energy contribution arising from the coordinates-momentum coupling terms in Hamiltonians, we should select some operators whose Heisenberg equation of motion can generate all the terms involved in the Hamiltonians, then by virtue of the

Feynman-Hellmann theorem we can derive their contribution to the energy eigenvalues of the Hamiltonian. The mixed state case is also discussed in which the results are similar to the pure state case.

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