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Deriving Energy-Gap of Some Hamiltonians with Kinetic Coupling by the Invariant Eigen-Operator Method

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Abstract We begin with proposing a unitary operator responsible for diagonalizing the Hamiltonian with kinetic couplings in particle physics to get a new form of Hamiltonian which has no coupling terms. By virtue of the invariant eigen-operator (IEO) method we search for the invariant eigen-operators for the new Hamiltonian. In this way the energy-gap of the Hamiltonians can be naturally obtained. This method may be generalized to N-mode Hamiltonian with kinetic couplings case.

Keywords Unitary operator · The invariant eigen-operator · Coupling terms

1 Introduction

It is well known the internal coordinates are frequently adopted in theoretical molecular physics [1], and consequently there naturally arise kinetic energy coupling terms in the dynamic vibrational Hamiltonian describing the molecules [2]. The kinetic energy coupling in one-dimensional diatomic systems is treated in the representation based on the eigenvectors of two particles' relative position and total momentum [3–5]. Later, a method of linear change of variables was suggested, which seems effective to decouple the kinetic energy operator in the two-body Hamiltonian [6]. In [7], the authors solved some three-body problems regarding molecular vibrational dynamics. A interesting question thus naturally arises: is it possible to solve such Hamiltonians with kinetic coupling by the invariant eigen-operator method? If yes, it will greatly facilitates the calculations of the problem.

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The work is arranged as follows: in Sect. 2, the idea of IEO will be briefly recapitulated, in Sect. 3, we will we employ the IEO method to derive the energy-gap for a type of two-particle Hamiltonian with kinetic coupling, in Sect. 4 we consider a three-particle Hamiltonian with kinetic coupling. This work is useful for deriving energy-gap of some Hamiltonians with kinetic coupling.

2 Invariant Eigen-Operator Method

We usually set up Schrödinger equation [7] to solve quantum mechanical dynamic problems. When Hamiltonian $\hat{H}$ does not include time, the solution of stationary Schrödinger equation $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$ can straightforwardly depict system energy spectra and eigenstates [8]. However, only very limited Hamiltonians can be solved analytically. As important as the Schrödinger equation there is the Heisenberg equation [9]

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

but (1) is seldom used to directly solve energy spectrum problem. In [10, 11] we have developed the idea of stationary Schrödinger equation to so-called invariant eigen-operator equation, i.e. we construct the following equation

$$\left(i\frac{d}{dt}\right)^n \hat{O}_e = \big[\ldots\big[\big[\hat{O}_e, \hat{H}\big], \hat{H}\big]\ldots, \hat{H}\big] = \lambda \hat{O}_e \tag{2}$$

to derive energy-level gap of dynamic systems. In (2), $\hat{O}_e$ is named invariant eigen-operator since it satisfies the eigenvector-like equation. The essence of this method is based on the observation of Schrödinger operator $i\frac{d}{dt} \longleftrightarrow \hat{H}$ (the energy operator), $(i\frac{d}{dt})^n \longleftrightarrow \hat{H}^n$, so (2) can be viewed as an eigen-operator equation with λ being the eigenvalue of $(i\frac{d}{dt})^n$. Therefore from (2) we know that the energy gap is $\sqrt[n]{\lambda}$. By virtue of this method, we have directly and conveniently obtained energy levels of certain dynamic systems.

3 Energy-Gap of Two-Particle Hamiltonian with Kinetic Coupling

We consider a two-particle Hamiltonian with kinetic coupling

$$H_1 = \omega(a^\dagger a + b^\dagger b) + k(a^\dagger b^\dagger + ab) + \frac{g}{(X_1 - X_2)^2}, \tag{3}$$

where ω, k and g are real parameters.

Now we use a two-mode squeezed transformation to derive the energy-gap for the Hamiltonian in (3). We begin with proposing a two-mode squeezed operator for diagonalizing H in (3) having the form

$$S_2 = \exp(a^\dagger b^\dagger \tanh\lambda)\exp[(a^\dagger a + b^\dagger b + 1)In\,\mathrm{sech}\,\lambda]\exp(-ab\tanh\lambda). \tag{4}$$

Using the operator formula

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \cdots, \tag{5}$$

and

$$X_i = \frac{a_i + a_i^\dagger}{\sqrt{2}}, \quad i = 1, 2 \tag{6}$$

we have

$$\begin{aligned} S_2 a S_2^{-1} &= a\cosh\lambda - b^\dagger \sinh\lambda, \qquad & S_2 b S_2^{-1} &= b\cosh\lambda - a^\dagger \sinh\lambda, \\ S_2 a^\dagger S_2^{-1} &= a^\dagger \cosh\lambda - b\sinh\lambda, \qquad & S_2 b^\dagger S_2^{-1} &= b^\dagger \cosh\lambda - a\sinh\lambda. \end{aligned} \tag{7}$$

From (6), (7) and (3), we get

$$\begin{aligned} H_1' &\equiv S_2 H_1 S_2^{-1} \\ &= (a^\dagger a + b^\dagger b)[\omega(1 + 2\sinh^2\lambda) - k\sinh 2\lambda] \\ &\quad - (a^\dagger b^\dagger + ab)[\omega\sinh 2\lambda - k(1 + 2\sinh^2\lambda)] + \frac{g}{(\cosh\lambda - \sinh\lambda)^2 (X_1 - X_2)^2} \\ &\quad + 2\omega\sinh^2\lambda - k\sinh 2\lambda. \end{aligned} \tag{8}$$

In the case $\omega\sinh 2\lambda = k(1 + 2\sinh^2\lambda)$, (8) can be changed into

$$H_1' = K(a^\dagger a + b^\dagger b) + \frac{G}{(X_1 - X_2)^2} + C, \tag{9}$$

where

$$\begin{aligned} K &= \omega(1 + 2\sinh^2\lambda) - k\sinh 2\lambda, \qquad G = \frac{g}{(\cosh\lambda - \sinh\lambda)^2}, \\ C &= 2\omega\sinh^2\lambda - k\sinh 2\lambda. \end{aligned}$$

It is remarkable that H_1' has no coupling terms, and if $|E\rangle$ is an eigenvector of H_1', $S_2 H_1 S_2^{-1}|E\rangle$ is the eigenvector of H with the same energy eigenvalue.

For

$$\begin{aligned} &\left[\sum_i P_i^2, \frac{1}{(X_1 - X_2)^2}\right] \\ &\quad = -i\sum_i P_i \frac{\partial}{\partial X_i}\frac{1}{(X_1 - X_2)^2} - i\sum_i \frac{\partial}{\partial X_i}\frac{1}{(X_1 - X_2)^2} P_i \\ &\quad = 2i(P_1 - P_2)\frac{1}{(X_1 - X_2)^3} + 2i\frac{1}{(X_1 - X_2)^3}(P_1 - P_2), \end{aligned} \tag{10}$$

we have

$$\begin{aligned} &\left[\frac{1}{2}\sum_i a_i^2, \frac{1}{(X_1 - X_2)^2}\right] \\ &\quad = -\frac{1}{4}\left[\sum_i P_i^2, \frac{1}{(X_1 - X_2)^2}\right] + \frac{i}{4}\left[\sum_i (X_i P_i + P_i X_i), \frac{1}{(X_1 - X_2)^2}\right] \\ &\quad = -i\left[(P_1 - P_2)\frac{1}{(X_1 - X_2)^3} + \frac{1}{(X_1 - X_2)^3}(P_1 - P_2)\right] - \frac{2}{(X_1 - X_2)^2}, \end{aligned} \tag{11}$$

and

$$\begin{aligned}&\left[\sum_i a_i^\dagger a_i, \frac{1}{(X_1-X_2)^2}\right]\\&=\frac{1}{2}\left[\sum_i P_i^2, \frac{1}{(X_1-X_2)^2}\right]\\&=i\left[(P_1-P_2)\frac{1}{(X_1-X_2)^3}+\frac{1}{(X_1-X_2)^3}(P_1-P_2)\right].\end{aligned}\tag{12}$$

Assuming the invariant eigen-operator of the Hamiltonian in (9) be

$$\hat{O}_1=(a^2+b^2)-\frac{G}{K}\frac{1}{(X_1-X_2)^2},\tag{13}$$

we have

$$\begin{aligned}[\hat{O}_1, H_1']&=K\left[(a^2+b^2), K(a^\dagger a+b^\dagger b)\right]+G\left[(a^2+b^2), \frac{1}{(X_1-X_2)^2}\right]\\&\quad+G\left[(a^\dagger a+b^\dagger b), \frac{1}{(X_1-X_2)^2}\right]\\&=2K(a^2+b^2)-\frac{2G}{(X_1-X_2)^2}=2K\hat{O}_1.\end{aligned}\tag{14}$$

According (2), we can write down the energy-gap of H_1' (or H_1):

$$\Delta E_1=2K=2[\omega(1+2\sinh^2\lambda)-k\sinh 2\lambda].\tag{15}$$

4 Energy-Gap of Three-Particle Hamiltonian with Kinetic Coupling

We consider a triatomic molecule model with the kinetic coupling terms as the following:

$$H_2=\sum_{i=1}^{3}\frac{P_i^2}{2m}+kP_1P_2+lP_1P_3+lP_2P_3+V_1(X_2-X_1)+V_2(X_3-X_{12}),\tag{16}$$

where $X_{12}=(X_1+X_2)/2$ is the center-of-mass of particles 1 and 2, which have the same mass. V_1 and V_2 are arbitrary functions about (X_2-X_1) and (X_3-X_{12}), respectable. k and l are the coupling parameters.

We give a unitary operator responsible for diagonalizing H_2 in (16) having the form

$$U(A)=\sqrt{\det A}\int|Ap\rangle\langle p|dp,\tag{17}$$

where $|P\rangle=|p_1, p_2, p_3\rangle$ is the three-mode momentum eigenstate, with $P_i|p\rangle=p_i|p\rangle$, A is a 3×3 matrix,

$$A=\begin{bmatrix}-1 & -1/2 & \eta v\\ 1 & -1/2 & \eta v\\ 0 & 1 & v\end{bmatrix},$$

$$\eta = \frac{m^{-1} - l}{m^{-1} + k - 2l}, \quad v \neq 0, \tag{18}$$

$$A^{-1} = \frac{1}{(2\eta + 1)v} \begin{bmatrix} -(\eta + \frac{1}{2})v & (\eta + \frac{1}{2})v & 0 \\ -v & -v & 2\eta v \\ 1 & 1 & 1 \end{bmatrix}. \tag{19}$$

In (18) v can be an arbitrary number except zero, and

$$\det(A) = (2\eta + 1)v = \frac{3m^{-1} - 4l + k}{m^{-1} + k - 2l} v \neq 0. \tag{20}$$

This unitary operator U is v-dependent.

From $\langle p_i | p_j \rangle = \delta(p_i - p_j)\delta_{ij}$, we can easily prove that $UU^\dagger = U^\dagger U = 1$, i.e.,

$$UU^\dagger = \det A \iint |Ap\rangle\langle p|p'\rangle\langle Ap'|dpdp' = 1. \tag{21}$$

Under U transformation, P and X transform as

$$U^\dagger P U = AP, \qquad U^\dagger X U = \tilde{A}^{-1} X, \tag{22}$$

where $\tilde{A}$ is the transposition of A.

Moreover, from

$$\begin{aligned} U(A)U(A^{-1}) &= U(A).\sqrt{\det A^{-1}} \int |A^{-1}p\rangle\langle p|dp \iint |Ap\rangle\delta(p - A^{-1}p')\langle p'|dpdp' \\ &= \int |AA^{-1}p'\rangle\langle p'|dp' = 1, \end{aligned} \tag{23}$$

we can derive

$$U^\dagger(A) = U(A^{-1}). \tag{24}$$

As a result of (22) and (24) we have

$$UPU^\dagger = A^{-1}P, \qquad UXU^\dagger = \tilde{A}X. \tag{25}$$

Performing the U transformation on H, as a result of (18), (19), and (22), we obtain

$$U^\dagger H_2 U = \sum_{i=1}^{3} \lambda_i P_i^2 + V_1(X_1) + V_2(X_2) \equiv H_2', \tag{26}$$

where

$$\begin{aligned} \lambda_1 &= m^{-1} - k, \\ \lambda_2 &= \frac{3}{4m} + \frac{1}{4}k - l, \\ \lambda_3 &= \Lambda v^2, \\ \Lambda &= \left(\frac{m^{-1} - l}{m^{-1} + k - 2l}\right)^2 \left(\frac{1}{m} + k\right) + \frac{1}{2m} + 2l\frac{m^{-1} - l}{m^{-1} + k - 2l}. \end{aligned}$$

It is remarkable that H_2' has no coupling terms.

Here we examine the case when

$$V_1(X_1) = \lambda_2 X_1^2, \qquad V_2(X_2) = \lambda_1 X_2^2. \tag{27}$$

Substituting (27) into (26), we have

$$H_2'' = \sum_{i=1}^{3} \lambda_i P_i^2 + \lambda_2 X_1^2 + \lambda_1 X_2^2. \tag{28}$$

Assuming the invariant eigen-operator of the Hamiltonian in (28) to be

$$\hat{O}_2 = X_1 + X_2, \tag{29}$$

we have

$$[\hat{O}_2, H_2''] = 2i\lambda_1 P_1 + 2i\lambda_2 P_2, \tag{30}$$

and

$$[[\hat{O}_2, H_2''], H_2''] = 4\lambda_1\lambda_2(X_1 + X_2). \tag{31}$$

According to (2), we know that the energy-level gap of H_2'' is

$$\Delta E_1 = 2\sqrt{\lambda_1\lambda_2}. \tag{32}$$

In summary, we begin with proposing a unitary operator responsible for diagonalizing the Hamiltonians with kinetic coupling terms, then by virtue of the IEO method we can derive the energy-gap of the Hamiltonians. This method may be generalized to the N-mode case and will be useful for analyzing both the squeezing and entangling mechanisms.

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