

Common eigenkets of three-particle compatible observables

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We give common eigenkets of three compatible observables $\{P_1 + P_2 + P_3, (\mu_2 Q_2 + \mu_3 Q_3)/(\mu_2 + \mu_3) - Q_1, Q_3 - Q_2\}$, which are composed of three particles' coordinate Q_i and momentum P_i , where $\mu_i = m_i/(m_1 + m_2 + m_3)$. This set of operators are so-called Jacobi coordinates and momenta. By compatible we mean such observables can be simultaneously determined. Using the technique of integration within an ordered product of operators, we prove that the common eigenkets are complete and orthonormal, and hereby qualified for making up a representation. Applying this representation to solving some new three-body problems is also shown. [S1050-2947(98)09604-8]

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I. INTRODUCTION

In Ref. [1] the explicit form of the common eigenkets of two particles' total momentum $P_1 + P_2$ and relative position $Q_1 - Q_2$ is constructed in the two-mode Fock space. It was Einstein, Podolsky, and Rosen [2] who first used $[P_1 + P_2, Q_1 - Q_2] = 0$ to challenge that the quantum-mechanical state vector is incomplete. Although the experimental conformation that studies the correlated systems and the significance on the outcome of a second, noncausally connected measurement on the results of a first measurement is fully in accord with quantum mechanics, this fact does not diminish interest in properties of compatible operators and their eigenkets [3] and in entangled states [4] in quantum optics measurement.

The purpose of this work is to construct eigenvectors for a set of three-particle compatible observables

$$\{P, (\mu_2 Q_2 + \mu_3 Q_3)/(\mu_2 + \mu_3) - Q_1, Q_3 - Q_2\},$$

where $P = P_1 + P_2 + P_3$ is the total momentum, $(\mu_2 Q_2 + \mu_3 Q_3)/(\mu_2 + \mu_3) - Q_1$ is the relative position between particle 1 and the center-of-mass of particle 2 and 3 (so-called Jacobi coordinates), $\mu_i = m_i/M$, $i = 1, 2, 3$, $M = m_1 + m_2 + m_3$. As

$$\left[P, \frac{\mu_2 Q_2 + \mu_3 Q_3}{\mu_2 + \mu_3} - Q_1 \right] = 0, \quad [P, Q_3 - Q_2] = 0, \quad (1)$$

we are challenged to search for the common eigenvectors $|p, \chi_2, \chi_3\rangle$ of these three compatible observables. By virtue of the technique of integration within an ordered product (IWOP) of operators [5], we show that $|p, \chi_2, \chi_3\rangle$ makes a complete representation. Thus they can be used for solving some new three-body dynamic problems.

II. COMMON EIGENKETS OF THE THREE COMPATIBLE OBSERVABLES

We begin with introducing the three-mode Fock space spanned by $|l, m, n\rangle = (a_1^{+l} a_2^{+m} a_3^{+n} / \sqrt{l!m!n!})|000\rangle$, where $[a_i, a_j^+] = \delta_{ij}$, $|000\rangle$ is the ground state, and a_i and a_i^+ are related to Q_i and P_i by

$$Q_i = \frac{a_i + a_i^+}{\sqrt{2}}, \quad P_i = \frac{a_i - a_i^+}{i\sqrt{2}}, \quad [a_i, a_j^+] = \delta_{ij}. \quad (2)$$

We shall prove that the common eigenkets of $\{P, (\mu_2 Q_2 + \mu_3 Q_3)/(\mu_2 + \mu_3) - Q_1, Q_3 - Q_2\}$, denoted by $|p, \chi_2, \chi_3\rangle$, are given in three-mode Fock space by

$$\begin{aligned} |p, \chi_2, \chi_3\rangle = & \frac{\pi^{-3/4}}{\sqrt{3}} \exp \left\{ -\frac{(a_1^+ + a_2^+ + a_3^+)^2}{2} \right. \\ & + \frac{(a_1^+ + a_2^+ + a_3^+)^2}{3} + \frac{\sqrt{2}}{3} \left(ip - 2\chi_2 \right. \\ & - \frac{\mu_2 - \mu_3}{\mu_2 + \mu_3} \chi_3 \left. \right) a_1^+ + \frac{\sqrt{2}}{3} \left(ip + \chi_2 \right. \\ & - \frac{\mu_2 + 2\mu_3}{\mu_2 + \mu_3} \chi_3 \left. \right) a_2^+ + \frac{\sqrt{2}}{3} \left(ip + \chi_2 \right. \\ & + \frac{2\mu_2 + \mu_3}{\mu_2 + \mu_3} \chi_3 \left. \right) a_3^+ - \frac{p^2}{6} - \frac{\chi_2^2}{3} \\ & - \frac{(\mu_2^2 + \mu_3^2 + \mu_2 \mu_3) \chi_3^2}{3(\mu_2 + \mu_3)^2} - \frac{(\mu_2 - \mu_3) \chi_2 \chi_3}{3(\mu_2 + \mu_3)} \\ & \left. + i \frac{p}{3} \left[(1 - 3\mu_1) \chi_2 - \frac{\mu_2 - \mu_3}{\mu_2 + \mu_3} \chi_3 \right] \right\} |000\rangle. \end{aligned} \quad (3)$$

In fact, acting a_i on $|p, \chi_2, \chi_3\rangle$ we have

$$a_1|p, \chi_2, \chi_3\rangle = \left[-a_1^+ + \frac{2(a_1^+ + a_2^+ + a_3^+)}{3} + \frac{\sqrt{2}}{3} \left(ip - 2\chi_2 - \frac{\mu_2 - \mu_3}{\mu_2 + \mu_3} \chi_3 \right) \right] |p, \chi_2, \chi_3\rangle, \quad (4)$$

$$a_2|p, \chi_2, \chi_3\rangle = \left[-a_2^+ + \frac{2(a_1^+ + a_2^+ + a_3^+)}{3} + \frac{\sqrt{2}}{3} \left(ip + \chi_2 - \frac{\mu_2 + 2\mu_3}{\mu_2 + \mu_3} \chi_3 \right) \right] |p, \chi_2, \chi_3\rangle, \quad (5)$$

$$a_3|p, \chi_2, \chi_3\rangle = \left[-a_3^+ + \frac{2(a_1^+ + a_2^+ + a_3^+)}{3} + \frac{\sqrt{2}}{3} \left(ip + \chi_2 + \frac{2\mu_2 + \mu_3}{\mu_2 + \mu_3} \chi_3 \right) \right] |p, \chi_2, \chi_3\rangle. \quad (6)$$

The sum of Eqs. (4)–(6) leads to

$$P|p, \chi_2, \chi_3\rangle = p|p, \chi_2, \chi_3\rangle. \quad (7)$$

Further, $\{[\mu_2 \times \text{Eq. (5)} + \mu_3 \times \text{Eq. (6)}] / (\mu_2 + \mu_3) - \text{Eq. (4)}\}$ shows

$$[(\mu_2 Q_2 + \mu_3 Q_3) / (\mu_2 + \mu_3) - Q_1] |p, \chi_2, \chi_3\rangle = \chi_2 |p, \chi_2, \chi_3\rangle, \quad (8)$$

while the subtraction of Eq. (5) from Eq. (6) yields

$$(Q_3 - Q_2) |p, \chi_2, \chi_3\rangle = \chi_3 |p, \chi_2, \chi_3\rangle. \quad (9)$$

Thus we know $|p, \chi_2, \chi_3\rangle$ is the eigenkets we required.

III. THE COMPLETENESS RELATION OF $|p, \chi_2, \chi_3\rangle$

We now examine if $|p, \chi_2, \chi_3\rangle$ satisfies a completeness relation. By virtue of IWOP and the normal ordering form of the three-mode vacuum projector,

$$|000\rangle\langle 000| = : \exp(-a_1^+ a_1 - a_2^+ a_2 - a_3^+ a_3) : , \quad (10)$$

we can easily perform the following integration:

$$\begin{aligned} \int \int \int_{-\infty}^{\infty} dp \, d\chi_2 d\chi_3 |p, \chi_2, \chi_3\rangle \langle p, \chi_2, \chi_3| &= \int \int \int_{-\infty}^{\infty} dp \, d\chi_2 d\chi_3 \frac{\pi^{-3/2}}{3} : \exp \left\{ -\frac{p^2}{3} - \frac{2\chi_2^2}{3} - \frac{2(\mu_2^2 + \mu_3^2 + \mu_2\mu_3)\chi_3^2}{3(\mu_2 + \mu_3)^2} \right. \\ &+ \frac{2(\mu_3 - \mu_2)\chi_2\chi_3}{3(\mu_2 + \mu_3)} + \frac{i\sqrt{2}}{3} [(a_1^+ - a_1) + (a_2^+ - a_2) + (a_3^+ - a_3)]p \\ &+ \frac{\sqrt{2}}{3} [-2(a_1^+ + a_1) + (a_2^+ + a_2) + (a_3^+ + a_3)]\chi_2 + \frac{\sqrt{2}}{3(\mu_2 + \mu_3)} [(\mu_3 - \mu_2) \\ &\times (a_1^+ + a_1) - (\mu_2 + 2\mu_3)(a_2^+ + a_2) + (2\mu_2 + \mu_3)(a_3^+ + a_3)]\chi_3 \\ &- \frac{a_1^{+2} + a_2^{+2} + a_3^{+2} + a_1^2 + a_2^2 + a_3^2}{2} + \frac{(a_1^+ + a_2^+ + a_3^+)^2 + (a_1 + a_2 + a_3)^2}{3} \\ &\left. - a_1^+ a_1 - a_2^+ a_2 - a_3^+ a_3 \right\} : = 1. \end{aligned} \quad (11)$$

Using Eqs. (7)–(9) we can also calculate

$$\begin{aligned} \langle p', \chi_2', \chi_3' | P | p, \chi_2, \chi_3 \rangle &= p' \langle p', \chi_2', \chi_3' | p, \chi_2, \chi_3 \rangle \\ &= p \langle p', \chi_2', \chi_3' | p, \chi_2, \chi_3 \rangle, \end{aligned} \quad (12)$$

$$\begin{aligned} \langle p', \chi_2', \chi_3' | [(\mu_2 Q_2 + \mu_3 Q_3) / (\mu_2 + \mu_3) - Q_1] | p, \chi_2, \chi_3 \rangle \\ = \chi_2' \langle p', \chi_2', \chi_3' | p, \chi_2, \chi_3 \rangle = \chi_2 \langle p', \chi_2', \chi_3' | p, \chi_2, \chi_3 \rangle, \end{aligned}$$

$$\begin{aligned} \langle p', \chi_2', \chi_3' | (Q_3 - Q_2) | p, \chi_2, \chi_3 \rangle &= \chi_3' \langle p', \chi_2', \chi_3' | p, \chi_2, \chi_3 \rangle \\ &= \chi_3 \langle p', \chi_2', \chi_3' | p, \chi_2, \chi_3 \rangle, \end{aligned}$$

which tell us that the overlap

$$\langle p', \chi_2', \chi_3' | p, \chi_2, \chi_3 \rangle = \delta(p' - p) \delta(\chi_2' - \chi_2) \delta(\chi_3' - \chi_3), \quad (13)$$

indicating that $|p, \chi_2, \chi_3\rangle$ are orthonormal.

From Eqs. (11) and (13) we see that $|p, \chi_2, \chi_3\rangle$ are qualified for making up a representation.

IV. SCHRÖDINGER EQUATION FOR A THREE-BODY SYSTEM WITH KINETIC COUPLINGS IN THE $\langle p, \chi_2, \chi_3 |$ REPRESENTATION

We now write the Schrödinger equation for a three-body system with kinetic couplings in the $\langle p, \chi_2, \chi_3 |$ representation. The three-body dynamic Hamiltonian that we deal with here is

$$H = \sum_{i=1}^3 \frac{p_i^2}{2m_i} + k_{12}P_1P_2 + k_{13}P_1P_3 + k_{23}P_2P_3 + V_2 \left(\frac{\mu_2 Q_2 + \mu_3 Q_3}{\mu_2 + \mu_3} - Q_1 \right) + V_3(Q_3 - Q_2), \quad (14)$$

where potentials V_2 and V_3 depend only on the Jacobi coordinates. P_1P_2 , P_1P_3 , and P_2P_3 are kinetic coupling energies, which often exist in a polyatomic molecule when the molecular vibration is considered [6].

Let

$$P_R = \mu_1(P_2 + P_3) - (\mu_2 + \mu_3)P_1, \\ P_r = (\mu_2P_3 - \mu_3P_2)/(\mu_2 + \mu_3), \quad (15)$$

where P_R (P_r) is the mass-weighted relative momentum between particle 2+3 and particle 1 (between particle 2 and particle 3). Then it is easy to see that H can be rewritten as

$$H = \frac{p^2}{2M} + \frac{P_R^2}{2m_R} + \frac{P_r^2}{2m_r} + \sum_{i<j} k_{ij}P_iP_j + V_2 \left(\frac{\mu_2 Q_2 + \mu_3 Q_3}{\mu_2 + \mu_3} - Q_1 \right) + V_3(Q_3 - Q_2), \quad (16)$$

where

$$m_R = m_1(m_2 + m_3)/M, \quad (17)$$

$$m_r = m_2m_3/(m_2 + m_3). \quad (18)$$

m_R (m_r) is the reduced mass of particle 2+3 and particle 1 (particle 2 and particle 3).

From Eqs. (2) and (3) it is not difficult to derive P_i 's representation in $\langle p, \chi_2, \chi_3 |$ basis, i.e.,

$$\langle p, \chi_2, \chi_3 | P_1 = \left(\mu_1 p + i \frac{\partial}{\partial \chi_2} \right) \langle p, \chi_2, \chi_3 |, \quad (19)$$

$$\langle p, \chi_2, \chi_3 | P_2 = \left(\mu_2 p - i \frac{\mu_2}{\mu_2 + \mu_3} \frac{\partial}{\partial \chi_2} + i \frac{\partial}{\partial \chi_3} \right) \langle p, \chi_2, \chi_3 |, \quad (20)$$

$$\langle p, \chi_2, \chi_3 | P_3 = \left(\mu_3 p - i \frac{\mu_3}{\mu_2 + \mu_3} \frac{\partial}{\partial \chi_2} - i \frac{\partial}{\partial \chi_3} \right) \langle p, \chi_2, \chi_3 |. \quad (21)$$

Combining Eqs. (19)–(21) and using Eq. (15) we find that

$$\langle p, \chi_2, \chi_3 | P = p \langle p, \chi_2, \chi_3 |,$$

$$\langle p, \chi_2, \chi_3 | P_R = -i \frac{\partial}{\partial \chi_2} \langle p, \chi_2, \chi_3 |,$$

$$\langle p, \chi_2, \chi_3 | P_r = -i \frac{\partial}{\partial \chi_3} \langle p, \chi_2, \chi_3 |. \quad (22)$$

As a result of Eqs. (8), (9), (16), and (19)–(22), sandwiching H between $\langle p, \chi_2, \chi_3 |$ and H 's eigenstate $|E_n\rangle$, we obtain

$$\begin{aligned} \langle p, \chi_2, \chi_3 | H | E_n \rangle = E_n \langle p, \chi_2, \chi_3 | E_n \rangle = & \left\{ \left(\frac{1}{2M} + k_{12}\mu_1\mu_2 + k_{13}\mu_1\mu_3 + k_{23}\mu_2\mu_3 \right) p^2 - \left(\frac{1}{2m_r} - k_{23} \right) \frac{2}{\partial \chi_3^2} \left[\frac{1}{2m_R} \right. \right. \\ & + k_{23} \frac{\mu_2\mu_3}{(\mu_2 + \mu_3)^2} - k_{12} \frac{\mu_2}{\mu_2 + \mu_3} - k_{13} \frac{\mu_3}{\mu_2 + \mu_3} \left. \right] \frac{\partial^2}{\partial \chi_2^2} - i \left[(k_{12}\mu_2 + k_{13}\mu_3) \frac{2\mu_1 - 1}{\mu_2 + \mu_3} + 2k_{23} \frac{\mu_2\mu_3}{\mu_2 + \mu_3} \right] \\ & \times p \frac{\partial}{\partial \chi_2} - i [(k_{13} - k_{12})\mu_1 + k_{23}(\mu_2 - \mu_3)] p \frac{\partial}{\partial \chi_3} - \left(k_{12} - k_{13} + k_{23} \frac{\mu_2 - \mu_3}{\mu_2 + \mu_3} \right) \frac{\partial^2}{\partial \chi_2 \partial \chi_3} \\ & \left. + V_2(\chi_2) + V_3(\chi_3) \right\} \langle p, \chi_2, \chi_3 | E_n \rangle. \quad (23) \end{aligned}$$

$\langle p, \chi_2, \chi_3 | E_n \rangle \equiv \varphi_n$ is the wave function. Equation (23) is the Schrödinger equation in the $\langle p, \chi_2, \chi_3 |$ representation.

V. SOLUTION TO EQ. (23) FOR THE CASE WHEN $m_2 = m_3$ AND $k_{12} = k_{13}$

In this section we provide a concrete example of how to solve Eq. (23) for $m_2 = m_3$ and $k_{12} = k_{13}$. In this case, Eq. (23) is reduced to

$$\begin{aligned} \lambda_2 \frac{\partial^2}{\partial \chi_2^2} \varphi_n + i \zeta_2 p \frac{\partial}{\partial \chi_2} \varphi_n + \lambda_3 \frac{\partial^2}{\partial \chi_3^2} \varphi_n + [E_n - \lambda p^2 \\ - V_2(\chi_2) - V_3(\chi_3)] \varphi_n = 0, \quad (24) \end{aligned}$$

where

$$\lambda = \frac{1}{2M} + 2K \frac{m_1 m}{M^2} + k \frac{m^2}{M^2}, \quad (25)$$

$$\lambda_2 = \frac{1}{2m_1} + \frac{1}{4m} + \frac{k}{4} - K, \quad \lambda_3 = \frac{1}{m} - k,$$

$$\zeta_2 = \frac{(m_1 - 2m)K + mk}{M}, \quad m_2 = m_3 \equiv m,$$

$$k_{12} = k_{13} \equiv K, \quad k_{23} \equiv k.$$

To solve this differential equation we make the ansatz

$$\varphi_n = \exp\left(-i \frac{\zeta_2}{2\lambda_2} p\chi_2\right) \psi_n. \quad (26)$$

After substituting Eq. (26) into Eq. (24), we obtain the following equation for ψ_n :

$$\lambda_2 \frac{\partial^2}{\partial \chi_2^2} \psi_n + \lambda_3 \frac{\partial^2}{\partial \chi_3^2} \psi_n + [E_n - \lambda' p^2 - V_2(\chi_2) - V_3(\chi_3)] \psi_n = 0, \quad (27)$$

where

$$\lambda' = [(m_1 m)^{-1} + k m_1^{-1} - 2K^2] / [2(m^{-1} + 2m_1^{-1} + k - 4K)] = \lambda - \zeta_2^2 / 4\lambda_2. \quad (28)$$

Thus we see that once we have worked in the $\langle p, \chi_2, \chi_3 |$ representation, the complicated dynamic problem of three-coupled particles can be simplified as two independent one-variable differential equations, including another variable p as a parameter. It then follows that

$$E_n = \lambda' p^2 + E_{n_2} + E_{n_3}, \quad (29)$$

where E_{n_j} ($j=2,3$) is the energy eigenvalue of the equation

$$\lambda_j \frac{\partial^2}{\partial \chi_j^2} \psi_{n_j}(\chi_j) + [E_{n_j} - V_j(\chi_j)] \psi_{n_j}(\chi_j) = 0, \quad (30)$$

and the wave function

$$\varphi_n = \exp(-i(\zeta_2/2\lambda_2)p\chi_2) \psi_{n_2} \psi_{n_3}. \quad (31)$$

In particular, when V_j ($j=2,3$) in Eq. (16) is the harmonic potential, which is the simplest molecular vibrational model, i.e.,

$$V_2\left(\frac{Q_2 + Q_3}{2} - Q_1\right) = \frac{1}{2} D_2^2 \left(\frac{Q_2 + Q_3}{2} - Q_1\right)^2;$$

$$V_3(Q_3 - Q_2) = \frac{1}{2} D_3^2 (Q_3 - Q_2)^2, \quad (32)$$

where D_j ($j=2,3$) is the spring constant. Since the energy level of the one-dimensional harmonic oscillator is well known, we can directly write down the energy level of Eq. (30) as $E_{n_j} = (n_j + \frac{1}{2}) \sqrt{2\lambda_j} D_j$, thus Eq. (29) becomes

$$E_n = \sqrt{m_1^{-1} + (2m)^{-1} + 2^{-1}k - 2KD_2} (n_2 + \frac{1}{2})$$

$$+ \sqrt{2m^{-1} - 2k} D_3 (n_3 + \frac{1}{2})$$

$$+ \frac{(m_1 m)^{-1} + k m_1^{-1} - 2K^2}{2(m^{-1} + 2m_1^{-1} + k - 4K)} p^2. \quad (33)$$

In conclusion, by establishing the $\langle p, \chi_2, \chi_3 |$ representation, we provide a convenient approach for solving some dynamic problems of three-body systems.

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