Unitary operator for an arbitrary number of coupled identical oscillators

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In view of a recent paper [F. Michelot, Phys. Rev. A **45**, 4271 (1992)] tackling the Hamiltonian of an arbitrary number of harmonically coupled oscillators, we present a coordinate representation of the unitary operator that can diagonalize the Hamiltonian. The normally ordered form of the unitary operator, which manifestly connects two Fock spaces associated with the uncoupled and coupled oscillators, is also derived by virtue of the technique of integration within an ordered product of operators.

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I. INTRODUCTION

The coupled-oscillator model can describe some interactions in atomic, molecular, and nuclear physics [1]; as a result, in Ref. [2] the solution for four harmonically coupled identical oscillators has been found through a unitary transformation approach. The coordinate representation of the corresponding unitary operator is identified and its normally ordered form is derived by virtue of the technique of integration within an ordered product (IWOP) of operators [3,4]. The normally ordered unitary operator can transform, in a straightforward way, the Fock space of four uncoupled oscillators into the space in which the Hamiltonian of four coupled oscillators is diagonalized. Generalizing the work [2], Michelot [5] proposed a solution to the problem of solving the Schrödinger equation for an arbitrary number of identical one-dimensional, harmonically coupled oscillators whose Hamiltonian is

$$H=\sum_{i=1}^{d}\left[\frac{\hat{P}_i^2}{2m}+\tfrac{1}{2}m\omega^2\hat{x}_i^{\,2}\right]+\frac{k}{4}\sum_{k,j=1}^{d}(\hat{x}_i-\hat{x}_j)^2 . \quad (1)$$

He also considered the relation between the two Fock spaces of coupled and uncoupled oscillators by using the Lie-algebraic techniques and the permutational symmetry of the problem. However, Mechelot only gave the operator, in his notation ${}^{(0)}U$, to relate the vacuum states of these two Fock spaces. The form of ${}^{(0)}U$ is not unitary; in other words, this ${}^{(0)}U$ cannot relate the excitation states of these two Fock spaces. In the present work, we show that the normally ordered unitary operator U connecting the two Fock spaces can be easily derived by the IWOP technique. Our work is arranged as follows. In Sec. II, we identify U with its coordinate representation and then prove its unitarity. In Sec. III, we employ the IWOP technique to derive U's normal product form, with which we prove that this U indeed connects the two Fock spaces. In Sec. IV, we analyze U in more detail to find a new boson realization for su(1,1) Lie algebra.

II. COORDINATE REPRESENTATION OF U

We begin by identifying U with the following x-representation for $d\geq 3$,

$$U=\left[\frac{\omega}{\varpi}\right]^{(d-1)/4}\int_{-\infty}^{\infty}d^d\mathbf{x}|u\mathbf{x}\rangle\langle\mathbf{x}| , \quad (2)$$

where $(\omega/\varpi)^{(d-1)/4}$ is a normalization coefficient anticipating the unitarity of U, as we shall see later, $|\mathbf{x}\rangle$ is the coordinate eigenstate

$$|\mathbf{x}\rangle=\left|\begin{pmatrix}x_1\\x_2\\\vdots\\x_d\end{pmatrix}\right\rangle=|x_1\ \ x_2\cdots x_d\rangle$$
$$=|x_1\rangle|x_2\rangle\cdots|x_d\rangle , \quad (3)$$

and u is a $d\times d$ matrix given by (4). Let us explain the matrix in more detail. The symbols $X(\Delta)$ represent $-[(d-1)(d-2)]^{-1/2}\gamma$ $(-[d(d-1)]^{-1/2}\gamma)$ respectively, the elements in the first column are all $d^{-1/2}$, the elements below the center diagonal except for the first column are all zero, and the new frequency $\varpi=(\omega^2+kd/m)^{1/2}$ is as Ref. [5] defines. In the Fock space spanned by the eigenvectors of the uncoupled oscillators, the state $|\mathbf{x}\rangle$ is expressed as in Eq. (5).

$$u=\begin{pmatrix} d^{-1/2} & -\sqrt{\tfrac{1}{2}}\gamma & -\sqrt{\tfrac{1}{6}}\gamma & -\sqrt{\tfrac{1}{12}}\gamma & \cdots & -\left[\frac{1}{(d-1)(d-2)}\right]^{1/2}\gamma & -\left[\frac{1}{d(d-1)}\right]^{1/2}\gamma \\ d^{-1/2} & \sqrt{\tfrac{1}{2}}\gamma & -\sqrt{\tfrac{1}{6}}\gamma & -\sqrt{\tfrac{1}{12}}\gamma & \cdots & -\left[\frac{1}{(d-1)(d-2)}\right]^{1/2}\gamma & -\left[\frac{1}{d(d-1)}\right]^{1/2}\gamma \\ d^{-1/2} & 0 & \sqrt{\tfrac{2}{3}}\gamma & -\sqrt{\tfrac{1}{12}}\gamma & \cdots & X & \Delta \\ d^{-1/2} & 0 & 0 & \sqrt{\tfrac{3}{4}}\gamma & \cdots & X & \Delta \\ \vdots & \vdots & & & & \vdots & \vdots \\ & & & & & X & \Delta \\ d^{-1/2} & 0 & & & & \left[\frac{d-2}{d-1}\right]^{1/2}\gamma & -\left[\frac{1}{d(d-1)}\right]^{1/2}\gamma \\ d^{-1/2} & 0 & 0 & 0 & & 0 & \left[\frac{d-1}{d}\right]^{1/2}\gamma \end{pmatrix},$$

$$\gamma\equiv\left[\frac{\omega}{\varpi}\right]^{1/2}. \tag{4}$$

$$|\mathbf{x}\rangle=\left[\frac{m\omega}{\pi\hbar}\right]^{d/4}\prod_i^d \exp\left[-\frac{m\omega}{2\hbar}x_i^2+\left[\frac{2m\omega}{\hbar}\right]^{1/2}x_i a_i^\dagger-\tfrac{1}{2}a_i^{\dagger 2}\right]|0\rangle\ , \tag{5}$$

where $|0\rangle$ is the vacuum state, and a_i and $a_i^\dagger$ are related to $\hat{x}_i$ and $\hat{P}_i$ by

$$\hat{x}_i=\left[\frac{\hbar}{2m\omega}\right]^{1/2}(a_i+a_i^\dagger),\quad \hat{P}_i=\left[\frac{m\omega\hbar}{2}\right]^{1/2}\frac{a_i-a_i^\dagger}{i}\ . \tag{6}$$

To prove the unitarity of U, we first calculate the determinant of u by taking advantage of the fact that if a matrix B is obtained from A by adding a multiple of one row (column) to another, then $\det B=\det A$. The result is

$$\det u=(-1)^d\sqrt{d}\left[-\left[\frac{d-1}{d}\right]^{1/2}\gamma\right]\left[-\left[\frac{d-2}{d-1}\right]^{1/2}\gamma\right]\cdots(-\sqrt{\tfrac{3}{4}}\gamma)(-\sqrt{\tfrac{2}{3}}\gamma)\sqrt{\tfrac{1}{2}}\gamma=\gamma^{d-1}=\left[\frac{\omega}{\varpi}\right]^{(d-1)/2}. \tag{7}$$

Then we use the orthonormal property $\langle x_i'|x_i\rangle=\delta(x_i'-x_i)$ to calculate

$$UU^\dagger=\left[\frac{\omega}{\varpi}\right]^{(d-1)/2}\int d^d\mathbf{x}|u\mathbf{x}\rangle\langle u\mathbf{x}|=1\ , \tag{8}$$

because the Jacobian of the integration variables' transformation is just $|\det u|=(\omega/\varpi)^{(d-1)/2}$. As one can see from Ref. [2], the coordinate representation of the unitary operator can provide us with a convenient way to calculate the wave functions for H. Here, instead of doing that, we give the normal product form of U to explain why this U, defined by Eq. (2), can diagonalize the Hamiltonian.

III. THE NORMAL PRODUCT FORM OF U

Using (3)–(5) and the normal product form of $|0\rangle\langle 0|$

$$|0\rangle\langle 0|=:\exp\left[-\sum_{i=1}^d a_i^\dagger a_i\right]:, \tag{9}$$

as well as the IWOP, we are able to perform the integration (2) [note that all the bilinear terms $x_i x_j$ $(i\neq j)$ cancel each other in the state $|u\mathbf{x}\rangle$ when expressed according to (5)]:

$$U=\left[\frac{\omega}{\varpi}\right]^{(d-1)/4}:\int_{-\infty}^{\infty}dx_1\frac{1}{\sqrt{\pi}}\exp\left\{-x_1^2+\sqrt{2}x_1\left[d^{-1/2}\left[\sum_{i=1}^d a_i^\dagger\right]+a_1\right]\right\}$$
$$\times\int_{-\infty}^{\infty}dx_2\frac{1}{\sqrt{\pi}}\exp\left\{-\frac{x_2^2}{2}\left[1+\frac{\omega}{\varpi}\right]+\sqrt{2}x_2\left[\left[\frac{\omega}{2\varpi}\right]^{1/2}(a_2^\dagger-a_1^\dagger)+a_2\right]\right\}$$
$$\times\int_{-\infty}^{\infty}dx_3\frac{1}{\sqrt{\pi}}\exp\left\{-\frac{x_3^2}{2}\left[1+\frac{\omega}{\varpi}\right]+\sqrt{2}x_3\left[\left[\frac{2\omega}{3\varpi}\right]^{1/2}\left[a_3^\dagger-\frac{a_1^\dagger+a_2^\dagger}{2}\right]+a_3\right]\right\}\cdots$$

$$\times \int_{-\infty}^{\infty} dx_d \frac{1}{\sqrt{\pi}} \exp\left\{ -\frac{x_d^2}{2}\left[1+\frac{\omega}{\varpi}\right] + \sqrt{2}x_d \left[\left[\frac{(d-1)\omega}{d\varpi}\right]^{1/2} \left[a_d^\dagger - \frac{1}{d-1}\sum_{i=1}^{d-1} a_i^\dagger\right] + a_d \right] - \frac{1}{2}\sum_{i=1}^{d}(a_i+a_i^\dagger)^2 \right\}:$$

$$= \left[\frac{4\varpi\omega}{(\varpi+\omega)^2}\right]^{(d-1)/4} :\exp\left[\tfrac{1}{2}\left[d^{-1/2}\left[\sum_{i=1}^{d} a_i^\dagger\right] + a_1\right]^2 + \frac{\varpi}{\varpi+\omega}\left\{ \left[\left[\frac{\omega}{2\varpi}\right]^{1/2}(a_2^\dagger - a_1^\dagger) + a_2\right]^2 \right.\right.$$

$$+ \left[\left[\frac{2\omega}{3\varpi}\right]^{1/2}\left[a_3^\dagger - \frac{a_1^\dagger + a_2^\dagger}{2}\right] + a_3\right]^2 + \cdots$$

$$\left. + \left[\left[\frac{(d-1)\omega}{d\varpi}\right]^{1/2}\left[a_d^\dagger - \frac{1}{d-1}\sum_{i=1}^{d-1} a_i^\dagger\right] + a_d\right]^2 \right\}$$

$$\left. - \frac{1}{2}\sum_{i=1}^{d}(a_i^\dagger + a_i)^2 \right]:$$

$$= W_1 W_2 W_3 \ , \tag{10}$$

where

$$W_1 \equiv \left[\frac{4\varpi\omega}{(\varpi+\omega)^2}\right]^{(d-1)/4} \exp\left[\frac{\omega-\varpi}{d(\varpi+\omega)}\left[\frac{d-1}{2}\sum_{i=1}^{d} a_i^{\dagger 2} - \sum_{i,j=1}^{d}{}' a_i^\dagger a_j^\dagger\right]\right] , \tag{11}$$

$$W_2 \equiv :\exp[(a_1^\dagger \ a_2^\dagger \ \cdots a_d^\dagger)(F - \mathbb{1})(a_1 \ a_2 \ \cdots \ a_d)^T]: , \quad (T \text{ means transpose operation}) \tag{12}$$

$$W_3 \equiv \exp\left[\frac{\varpi-\omega}{2(\varpi+\omega)}\sum_{i=2}^{d} a_i^2\right]$$

with $\mathbb{1}$ being the $d \times d$ unit matrix and $\sum'$ indicating that the summation is restricted to $i<j$. In Eq. (12), F is also a $d \times d$ matrix that possesses the same structure as (4), except γ in (4) is now replaced by λ, e.g.,

$$F \equiv \begin{bmatrix} d^{-1/2} & -\sqrt{\tfrac{1}{2}}\lambda & -\sqrt{\tfrac{1}{6}}\lambda & \cdots & \cdots & -\left[\dfrac{1}{d(d-1)}\right]^{1/2}\lambda \\ d^{-1/2} & \sqrt{\tfrac{1}{2}}\lambda & -\sqrt{\tfrac{1}{6}}\lambda & & & -\left[\dfrac{1}{d(d-1)}\right]^{1/2}\lambda \\ d^{-1/2} & 0 & \sqrt{\tfrac{2}{3}}\lambda & & & \vdots \\ \vdots & & 0 & & & \\ \vdots & & & & & \vdots \\ d^{-1/2} & & & & & \left[\dfrac{d-1}{d}\right]^{1/2}\lambda \end{bmatrix} , \quad \lambda \equiv \frac{2\sqrt{\varpi\omega}}{\varpi+\omega} . \tag{13}$$

Following the same procedures as used in deriving Eqs. (3.1)–(3.9) of Ref. [2], we obtain the transformation property of $a_r^\dagger$ $(1<r\le d)$ and $a_1^\dagger$ under the U transformation, e.g.,

$$Ua_r^\dagger U^{-1} = \frac{\varpi+\omega}{2\sqrt{\varpi\omega}}\left[\frac{r-1}{r}\right]^{1/2}\left[a_r^\dagger - \frac{1}{r-1}\sum_{i=1}^{r-1} a_i^\dagger\right] + \frac{\varpi-\omega}{2\sqrt{\varpi\omega}}\left[\frac{r-1}{r}\right]^{1/2}\left[a_r - \frac{1}{r-1}\sum_{i=1}^{r-1} a_i\right]$$

$$\equiv b_{r-1}^\dagger \ , \tag{14}$$

$$Ua_1^\dagger U^{-1} = d^{-1/2}\sum_{i=1}^{d} a_i^\dagger \equiv b_d^\dagger \ . \tag{15}$$

Note that our $b_d^\dagger$ and $-b_{r-1}^\dagger$ have the same expressions as Eq. (5.1) of Ref. [5]. Operating the normally ordered U on the vacuum state of the uncoupled oscillators gives

$$U|0\rangle = W_1|0\rangle \ . \tag{16}$$

It is not strange to see that our W_1 is the same as Eq. (5.18) of Ref. [5], except for a minus sign difference in their exponents, because from the transformed operators b_{r-1} and b_d we can define the Jacobian coordinates as

$$\hat{X}_{r-1}=\left[\frac{\hbar}{2m\varpi}\right]^{1/2}(b_{r-1}+b_{r-1}^{\dagger})=\left[\frac{\hbar}{2m\varpi}\right]^{1/2}\left[\frac{\varpi}{\omega}\right]^{1/2}\left[\frac{r-1}{r}\right]^{1/2}\left[a_r+a_r^{\dagger}-\frac{1}{r-1}\sum_{i=1}^{r-1}(a_i+a_i^{\dagger})\right]$$

$$=\left[\frac{r-1}{r}\right]^{1/2}\hat{x}_r-\frac{1}{\sqrt{r(r-1)}}\sum_{i=1}^{r-1}\hat{x}_i\ , \qquad (17)$$

$$\hat{X}_d=\left[\frac{\hbar}{2m\omega}\right]^{1/2}(b_d+b_d^{\dagger})=d^{-1/2}\sum_{i=1}^{d}\hat{x}_i\ . \qquad (18)$$

Equation (17) differs from the definition of Ref. [5] [see Eq. (3.2) of Ref. [5] by a minus sign. Nevertheless, this difference does not affect the result of using our U to diagonalize the Hamiltonian. In our new coordinate system of $\hat{X}_{r-1}$ and $\hat{X}_d$, the Hamiltonian is also diagonalized as (3.9) of Ref. [5].

IV. NEW BOSON REALIZATION OF su(1,1) GENERATORS INVOLVED IN U

From Eqs. (10)–(13), we see that U is a rather complicated unitary transformation that includes frequency-jump-related squeezing. Thus we need to analyze Eq. (11) in more detail. Taking $d=4$, for example, let us denote the operator in the exponential of W_1 as $R^{\dagger}$:

$$\frac{3}{2}\sum_{i=1}^{4}a_i^{\dagger 2}-\sum_{i,j=1}^{4}{}' a_i^{\dagger}a_j^{\dagger}=R^{\dagger}\ . \qquad (19)$$

Using the commutator $[a_i,a_j^{\dagger}]=\delta_{i,j}$, we calculate

$$\left[\frac{R}{4},\frac{R^{\dagger}}{4}\right]=\frac{1}{4}\left[3\sum_{i=1}^{4}a_i^{\dagger}a_i-(a_2^{\dagger}+a_3^{\dagger}+a_4^{\dagger})a_1-(a_1^{\dagger}+a_3^{\dagger}+a_4^{\dagger})a_2-(a_1^{\dagger}+a_2^{\dagger}+a_4^{\dagger})a_3-(a_1^{\dagger}+a_2^{\dagger}+a_3^{\dagger})a_4+6\right]\equiv 2J\ . \qquad (20)$$

It then follows

$$\left[\frac{R}{4},J\right]=\frac{R}{4},\quad \left[\frac{R^{\dagger}}{4},J\right]=-\frac{R^{\dagger}}{4},\quad J^{\dagger}=J\ , \qquad (21)$$

which shows that $R/4$, $R^{\dagger}/4$, and J make up a su(1,1) Lie algebra. In other words, they are a new boson realization of su(1,1). Further, it is not difficult to know that $U(d=4)$ can be decomposed as a product of a su(1,1) transformation $\exp[\frac{1}{4}(R^{\dagger}-R)\ln\gamma]$ and a rotation operator (this can be generalized to $d>4$ cases). Our analysis is consistent with the observation that the Hamiltonian in Eq. (1) has a dynamical algebra isomorphic with su(1,1).

In summary, we have presented the coordinate representation and normally ordered form of the unitary operator for diagonalizing the Hamiltonian. The IWOP technique plays an essential role to normally order the structure of U, which reduces Michelot's ${}^{(0)}U$ when it operates on the vacuum state of the uncoupled oscillators. Equation (2) tells us how this U is constructed in terms of a simple mapping of the classical transformation to quantum-mechanical Hilbert space in Dirac's coordinate representation. The explicit expression of U is useful. For example, if we want to calculate that density matrix $\langle \mathbf{x}'|\exp(-\beta H)|\mathbf{x}\rangle\equiv\rho_{\mathbf{x}'\mathbf{x}}$, where β is Boltzmann's constant, we can rewrite it as $\rho_{\mathbf{x}'\mathbf{x}}=\langle \mathbf{x}'|U\exp(-\beta\mathcal{H})U^{-1}|\mathbf{x}\rangle$, where $\mathcal{H}$ is d-independent harmonic oscillators, e.g.,

$$\mathcal{H}=\left[\omega(a_1^{\dagger}a_1+\tfrac{1}{2})+\varpi\left[\sum_{r=2}^{d}a_r^{\dagger}a_r+\frac{d-1}{2}\right]\right]\hbar\ .$$

The coordinate representation of U and the orthonormal relation $\langle x_i|x_j\rangle=\delta(x_i-x_j)$ then make the calculation very easy, which again shows that solving the dynamics for a given Hamiltonian is equivalent to finding its diagonalizable unitary operator [6].

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