Solution for an arbitrary number of coupled identical oscillators

F. Michelot
Laboratoire de Spectronomie Moléculaire et Instrumentation Laser, Université de Bourgogne, 6 Boulevard Gabriel, 21000 Dijon, France
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We propose a solution to the problem of solving the Schrödinger equation for an arbitrary number of identical one-dimensional harmonically coupled oscillators raised by Fan Hong-yi [Phys. Rev. A **42**, 4377 (1990)]. The relationship between the Fock spaces associated with the uncoupled and coupled oscillators is given as well as the coordinate representation of the eigenstates. In view of further applications, the Lie algebraic properties of the model are examined, and the generalization to three spatial dimensions is made.

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I. INTRODUCTION

Many problems in molecular, atomic, and nuclear physics rely upon the solution of Schrödinger-type equations for coupled harmonic oscillators. In particular, in a recent paper [1] a solution for four harmonically coupled identical oscillators was proposed and the generalization to the case of an arbitrary number of oscillators left as a challenge for the future.

In this paper we show that the solution can be obtained through only one simple, clearly defined, coordinate transformation. The computations can be made entirely in two Fock spaces; but the connection with Schrödinger-type representations is also given. In view of further applications, we indicate how the use of Lie algebraic techniques and of the permutational symmetry of the problem allows us to classify the degenerate eigenstates. Also, the straightforward generalization to three spatial dimensions is established.

Although the problem treated here is very different from the one considered by Kramer and Moshinsky [2] in their study of the dynamics of an n-nucleon system, their approach was quite useful to us and should be borne in mind for applications to specific physical problems.

II. THE HAMILTONIAN

Let d be the number of coupled oscillators; then the extension of the previously considered Hamiltonian [1] is

$$H=\sum_{i=1}^{d}\left[\frac{p_i^2}{2m}+\tfrac{1}{2}m\omega^2 x_i^2\right]+\frac{k}{4}\sum_{i,j=1}^{d}(x_i-x_j)^2 =H_0+H' , \tag{2.1}$$

where H_0 is the Hamiltonian for d identical one-dimensional harmonic oscillators (HO) or equivalently for a d-dimensional isotropic harmonic oscillator (IHO). Both H_0 and H' can be expressed in terms of the usual dimensionless annihilation and creation operators

$$a_j=\left[\frac{m\omega}{2\hbar}\right]^{1/2}x_j+i\left[\frac{1}{2m\omega\hbar}\right]^{1/2}p_j ,$$
$$a_j^\dagger=\left[\frac{m\omega}{2\hbar}\right]^{1/2}x_j-i\left[\frac{1}{2m\omega\hbar}\right]^{1/2}p_j , \tag{2.2}$$

which satisfy

$$[a_i,a_j]=[a_i^\dagger,a_j^\dagger]=0,\quad [a_i,a_j^\dagger]=\delta_{ij} . \tag{2.3}$$

We then have

$$H=a_0 I+b_0\sum_{i=1}^{d}a_i^\dagger a_i+c_0{\sum_{i,j=1}^{d}}'(a_i^\dagger a_j+a_j^\dagger a_i) +d_0\sum_{i=1}^{d}(a_i^{\dagger 2}+a_i^2)+c_0{\sum_{i,j=1}^{d}}'(a_i^\dagger a_j^\dagger+a_i a_j) , \tag{2.4}$$

where I is the identity operator and $\sum'$ means that the summation is made with the condition $i<j$; also for convenience we set

$$a_0=\frac{\hbar\omega d}{2}+\frac{k\hbar(d-1)}{4m\omega},\quad b_0=\frac{2a_0}{d} ,$$
$$c_0=-\frac{k\hbar}{2m\omega},\quad d_0=\frac{k\hbar(d-1)}{4m\omega} . \tag{2.5}$$

At this point it is important to note that H is obviously invariant in the permutation group S_d of the "particle" indices. Also a basis for the Hilbert space of states $\mathcal{H}$ is given by the eigenstates of H_0,

$$|n_1,\ldots,n_d\rangle=\prod_{i=1}^{d}|n_i\rangle=\prod_{i=1}^{d}(n_i!)^{-1/2}{a_i^\dagger}^{n_i}|o_i\rangle . \tag{2.6}$$

Likewise we could use the "x representation"

$$|x_1,\ldots,x_d\rangle=\prod_{i=1}^{d}|x_i\rangle , \tag{2.7}$$

both bases being related by

$$\langle x_i,\ldots,x_d|n_1,\ldots,n_d\rangle=\prod_{i=1}^{d}\varphi_{n_i}(x_i)\ , \tag{2.8}$$

where the φ_{n_i} are the usual HO eigenfunctions. In the following, when there is no ambiguity, we shall set

$$|n_1,\ldots,n_d\rangle=|n\rangle,\quad |x_1,\ldots,x_d\rangle=|x\rangle\ , \tag{2.9}$$

and the vacuum state will be denoted $|\dot{o}\rangle$, where the dot means repeated zero.

III. EIGENVALUES AND EIGENSTATES

Let Γ be the representation of S_d generated by the set $\{x_i\}$ (or $\{a_i\}$, or $\{a_i^\dagger\}$). Within a class $(1^{\nu_1}, 2^{\nu_2},\ldots,d^{\nu_d})$ of S_d, the contribution to the character is equal to the number of cycles of length one,

$$\chi^{\Gamma}(1^{\nu_1},\ldots,d^{\nu_d})=\nu_1\ .$$

The reduction of Γ is obtained by standard rules [3]

$$\Gamma=[d]+[d-1\ 1]\ . \tag{3.1}$$

This suggests that the Jacobi coordinates, as introduced in Ref. [2], should be appropriate since they are classified according to the irreducible representations of S_d. These can be written

$$\begin{aligned} X_r&=\left[\frac{1}{r(r+1)}\right]^{1/2}\sum_{i=1}^{r}x_i-\left[\frac{r}{r+1}\right]^{1/2}x_{r+1}\ ,\\ &\quad 1\le r\le d-1\\ X_d&=\left[\frac{1}{d}\right]^{1/2}\sum_{i=1}^{d}x_i\ . \end{aligned} \tag{3.2}$$

We note that

$$X_d\in[d]\ \text{ and }\ \{X_r\}\in[d-11] \tag{3.3}$$

and that these new coordinates are naturally symmetrized in the whole chain $S_d\supset S_{d-1}\supset\cdots\supset S_2$. If we set

$$x=\begin{bmatrix}x_1\\ \vdots\\ x_d\end{bmatrix},\quad X=\begin{bmatrix}X_1\\ \vdots\\ X_d\end{bmatrix}\ , \tag{3.4}$$

Eq. (3.2) can be written

$$X=Ax\ , \tag{3.5}$$

A being an orthogonal $d\times d$ matrix. Then the transformation law for the conjugate momenta is

$$p_x=A^{t}P_X=A^{-1}P_X\ , \tag{3.6}$$

with

$$p_x=\begin{bmatrix}p_1\\ \vdots\\ p_d\end{bmatrix},\quad P_X=\begin{bmatrix}P_1\\ \vdots\\ P_d\end{bmatrix}\ ,$$

and

$$p_j=\frac{\hbar}{i}\frac{\partial}{\partial x_j},\quad P_s=\frac{\hbar}{i}\frac{\partial}{\partial X_s}\ .$$

Straightforward computations with the preceding relations lead to

$$H_0=\sum_{r=1}^{d}\frac{P_r^2}{2m}+\tfrac{1}{2}m\omega^2X_r^2\ , \tag{3.7}$$

and

$$H'=\frac{kd}{2}\sum_{r=1}^{d-1}X_r^2\ . \tag{3.8}$$

Thus

$$\begin{aligned} H&=\sum_{r=1}^{d-1}\left[\frac{P_r^2}{2m}+\tfrac{1}{2}m\bar{\omega}^2X_r^2\right]+\frac{P_d^2}{2m}+\tfrac{1}{2}m\omega^2X_d^2\\ &=H_1+H_2\ . \end{aligned} \tag{3.9}$$

In the new coordinate system H is the Hamiltonian of two uncoupled IHO, one of dimension $d-1$ with frequencies

$$\bar{\omega}=\left[\omega^2+\frac{dk}{m}\right]^{1/2} \tag{3.10}$$

in each dimension, the other being one dimensional and of frequency ω.

The transformation (3.2) being orthogonal, we necessarily have for the Jacobi coordinates operators and their conjuguate momenta

$$[X_s,P_{s'}]=i\hbar\delta_{ss'},\quad s,s'=1,\ldots,d\ . \tag{3.11}$$

Thus, new dimensionless annihilation and creation operators can be defined by standard rules

$$\begin{aligned} b_r&=\left[\frac{m\bar{\omega}}{2\hbar}\right]^{1/2}X_r+i\left[\frac{1}{2m\bar{\omega}\hbar}\right]^{1/2}P_r,\quad 1\le r\le d-1\\ b_r^\dagger&=\left[\frac{m\bar{\omega}}{2\hbar}\right]^{1/2}X_r-i\left[\frac{1}{2m\bar{\omega}\hbar}\right]^{1/2}P_r\ ,\\ b_d&=\left[\frac{m\omega}{2\hbar}\right]^{1/2}X_d+i\left[\frac{1}{2m\omega\hbar}\right]^{1/2}P_d\ ,\\ b_d^\dagger&=\left[\frac{m\omega}{2\hbar}\right]^{1/2}X_d-i\left[\frac{1}{2m\omega\hbar}\right]^{1/2}P_d\ . \end{aligned} \tag{3.12}$$

So the Hamiltonian (3.9) becomes

$$H=\hbar\bar{\omega}\left[\bar{N}+\frac{d-1}{2}\right]+\hbar\omega(\bar{N}_d+\tfrac{1}{2})\ , \tag{3.13}$$

where the new number operators are defined by

$$\bar{N}_d=b_d^\dagger b_d,\quad \bar{N}=\sum_{r=1}^{d-1}b_r^\dagger b_r=\sum_{r=1}^{d-1}\bar{n}_r\ . \tag{3.14}$$

The new Fock space is spanned by the eigenstates of H

$$|\bar{n}_1,\ldots,\bar{n}_{d-1},\bar{n}_d\rangle=|\bar{n},\bar{n}_d\rangle = \prod_{s=1}^{d}(\bar{n}_s!)^{-1/2}b_s^{\dagger\bar{n}_s}|\bar{o}_s\rangle\ . \quad (3.15)$$

The eigenvalues are given by

$$E_{\bar{n},\bar{n}_d}=\hbar\bar{\omega}\left[\bar{n}+\frac{d-1}{2}\right]+\hbar\omega(\bar{n}_d+\tfrac{1}{2})\ , \quad (3.16)$$

where we set $\bar{n}=\sum_{r=1}^{d-1}\bar{n}_r$.

IV. THE EIGENFUNCTIONS

First we note that the "X representation" is completely determined

$$|X_1,\ldots,X_d\rangle=\prod_{s=1}^{d}|X_s\rangle$$

and

$$\langle X_1,\ldots,X_d|\bar{n}_1,\ldots,\bar{n}_d\rangle=\prod_{s=1}^{d}\varphi_{\bar{n}_s}(X_s)=\varphi_{\bar{n}}(X)\ , \quad (4.1)$$

where the $\varphi_{\bar{n}_s}(X_s)$ are the usual HO eigenfunctions,

$$\varphi_{\bar{n}_r}(X_r)=\left[\frac{m\bar{\omega}}{\pi\hbar}\right]^{1/4}(2^{\bar{n}_r}\bar{n}_r!)^{-1/2}\exp\left[\frac{-m\bar{\omega}}{2\hbar}X_r^2\right]H_{\bar{n}_r}\left[\left[\frac{m\bar{\omega}}{\hbar}\right]^{1/2}X_r\right]\quad 1\le r\le d-1$$

$$\varphi_{\bar{n}_d}(X_d)=\left[\frac{m\omega}{\pi\hbar}\right]^{1/4}(2^{\bar{n}_d}\bar{n}_d!)^{-1/2}\exp\left[\frac{-m\omega}{2\hbar}X_d^2\right]H_{\bar{n}_d}\left[\left[\frac{m\omega}{\hbar}\right]^{1/2}X_d\right]\ . \quad (4.2)$$

The $H_{\bar{n}}$ are Hermite polynomials.

The Jacobian for the transformation from the x_i to the X_s being one, the eigenfunctions

$$\varphi_{\bar{n}}(x)=\langle x_1,\ldots,x_d|\bar{n}_1,\bar{n}_2,\ldots,\bar{n}_d\rangle \quad (4.3)$$

are readily obtained from (4.1) and (4.2) with the substitution given by Eq. (3.2). As a check, one can verify that in this way the last equation of Ref. [1] is recovered (up to an unessential phase factor) by setting $d=4$ in our preceding results.

V. RELATION BETWEEN THE TWO FOCK SPACES

For most practical applications it is more interesting to work in second quantization; in addition, this allows us to see more clearly the Lie algebraic properties of the problem. The two sets of boson operators we introduced are related by

$$b_r^\dagger=\tfrac{1}{2}\left[\left[\frac{1}{r(r+1)}\right]^{1/2}[(\bar{\omega}/\omega)^{1/2}+(\omega/\bar{\omega})^{1/2}]\sum_{i=1}^{r}a_i^\dagger-\left[\frac{r}{r+1}\right]^{1/2}[(\bar{\omega}/\omega)^{1/2}+(\omega/\bar{\omega})^{1/2}]a_{r+1}^\dagger\right.$$
$$\left.+\left[\frac{1}{r(r+1)}\right]^{1/2}[(\bar{\omega}/\omega)^{1/2}-(\omega/\bar{\omega})^{1/2}]\sum_{i=1}^{r}a_i-\left[\frac{r}{r+1}\right]^{1/2}[(\bar{\omega}/\omega)^{1/2}-(\omega/\bar{\omega})^{1/2}]a_{r+1}\right]\ ,$$
$$b_d^\dagger=\left[\frac{1}{d}\right]^{1/2}\sum_{i=1}^{d}a_i^\dagger\ . \quad (5.1)$$

The corresponding equations for the annihilation operators b_r, b_d are deduced by taking the adjoint of (5.1). Then in order to relate the two Fock spaces (3.15) and (2.6) one only needs to relate the two vacuum states, respectively, defined by

$$a_i|o_i\rangle=0,\quad i=1,\ldots,d$$
$$b_s|\bar{o}_s\rangle=0,\quad s=1,\ldots,d\ . \quad (5.2)$$

The general form of the operator ${}^{(o)}U$ which connects the two vacuum sates

$$|\dot{\bar{o}}\rangle={}^{(o)}U|\dot{o}\rangle \quad (5.3)$$

can be determined with the simple following arguments. Let $\mathcal{H}_n$ denote the subspace of $\mathcal{H}$ associated with the eigenvalue $\lambda(n)=\hbar\omega(n+d/2)$ of H_0. From Eq. (2.4) it is clear that

$$H|\varphi_n\rangle=\alpha|\Psi_n\rangle+\beta|\Psi_{n+2}\rangle+\gamma|\Psi_{n-2}\rangle\ ,$$

where $|\varphi_n\rangle$ and $|\Psi_n\rangle$ belong to $\mathcal{H}_n$ and $|\Psi_{n\pm2}\rangle$ to $\mathcal{H}_{n\pm2}$. Thus H can be diagonalized by considering separately the subspaces of $\mathcal{H}$ associated with even and odd values of n: an eigenket of H is a linear superposition of kets $|\Psi_n\rangle$ with n even or odd. In particular, for the ground state $|\dot{\bar{o}}\rangle$ only even values are involved.

Moreover, the states $|\dot{o}\rangle$ and $|\dot{\bar{o}}\rangle$ are totally symmetric in S_d, i.e., of symmetry $[d]$, thus ${}^{(o)}U$ can only be a linear combination of even powers of operators invariant in S_d built from the $\{a_i^\dagger\}$. From the known symmetry properties [Eq. (3.1)] of the $\{a_i^\dagger\}$ in S_d, it is easily shown that only two operators of degree two and symmetry $[d]$ exist,

the simplest ones being

$$\sum_{i=1}^{d} a_i^{\dagger 2} \quad \text{and} \quad \sum_{i,j=1}^{d}{}' a_i^\dagger a_j^\dagger \ . \tag{5.4}$$

Thus the most general form for the operator ${}^{(o)}U$ satisfying the preceding conditions is

$${}^{(o)}U = \sum_{p,q=0}^{\infty} \gamma_{pq} \left[\sum_{i=1}^{d} a_i^{\dagger 2} \right]^p \left[\sum_{i,j=1}^{d}{}' a_i^\dagger a_j^\dagger \right]^q . \tag{5.5}$$

The complete determination of the coefficients γ_{pq} is made in three steps.

(i) Equation (5.3) implies

$$b_s|\dot{\bar{o}}\rangle = 0 = [b_s, {}^{(o)}U]|\dot{o}\rangle + U b_s|\dot{o}\rangle, \quad s=1,\ldots,d \ . \tag{5.6}$$

The computation is simplified if we choose $s=d$ [Eq. (5.1)] since then (5.6) reduces to

$$\left[\sum_{i=1}^{d} a_i, {}^{(o)}U \right] |\dot{o}\rangle = 0 \ . \tag{5.7}$$

Expanding the commutator with the known form (5.5) of ${}^{(o)}U$ leads first to a recursive relation

$$\gamma_{p,t-p} = (-1)^p \left[\frac{d-1}{2} \right]^p \frac{t!}{(t-p)!p!} \gamma_{0t} \ , \tag{5.8}$$

which allows to write (5.5)

$$\begin{aligned} {}^{(o)}U &= \sum_{t=0}^{\infty} (-1)^t \gamma_{0t} \left[\frac{d-1}{2} \sum_{i=1}^{d} a_i^{\dagger 2} - \sum_{i,j=1}^{d}{}' a_i^\dagger a_j^\dagger \right]^t \\ &= \sum_{t=0}^{\infty} (-1)^t \gamma_{0t} A^\dagger \ . \end{aligned} \tag{5.9}$$

(ii) To determine γ_{0t} it is more efficient to use

$$H|\dot{\bar{o}}\rangle = E(\bar{o})|\dot{\bar{o}}\rangle = [H, {}^{(o)}U]|\dot{o}\rangle + {}^{(o)}UH|\dot{o}\rangle \tag{5.10}$$

than (5.6) for other values of s,

$$E(\bar{o})|\dot{\bar{o}}\rangle = \left[\hbar\frac{\omega}{2} + \hbar\bar{\omega} \left[\frac{d-1}{2} \right] \right] {}^{(o)}U|\dot{o}\rangle \ . \tag{5.11}$$

The two terms on the right-hand side of (5.10) and their action on the vacuum state $|\dot{o}\rangle$ are easily determined and so we simply give the recursive relation that we obtain

$$(t+1)\gamma_{0t+1} = \lambda\gamma_{0t} + \frac{2}{d^2(t+d-1)} \left[\frac{t}{a}\gamma_{0t} - \gamma_{0t-1} \right], \quad t>0 \tag{5.12}$$

with $\lambda_{01} = \lambda\gamma_{00}$ and $\lambda = (\bar{\omega}-\omega)/d(\bar{\omega}+\omega)$, from which we readily deduce

$$\gamma_{0t} = \frac{\lambda^t}{t!}\gamma_{00}$$

and

$${}^{(o)}U = \gamma_{00} e^{-\lambda A^\dagger} \ . \tag{5.13}$$

(iii) The last coefficient is determined, up to a phase, by the normalization condition

$$\langle \dot{\bar{o}}|\dot{\bar{o}}\rangle = \langle \dot{o}|{}^{(o)}U^{\dagger(o)}U|\dot{o}\rangle = 1 \ , \tag{5.14}$$

with ${}^{(o)}U^\dagger = \gamma_{00}^* e^{-\lambda A}$

$$\langle \dot{\bar{o}}|\dot{\bar{o}}\rangle = |\gamma_{00}|^2 \sum_{t,p=0}^{\infty} (-1)^{t+p} \frac{\lambda^{t+p}}{t!p!} \langle \dot{o}|A^t A^{\dagger p}|\dot{o}\rangle \ , \tag{5.15}$$

but (5.9) implies

$$\langle \dot{o}|A^t A^{\dagger p}|\dot{o}\rangle = \langle \dot{o}|A^t A^{\dagger t}|\dot{o}\rangle \delta_{tp} \tag{5.16}$$

and

$$\begin{aligned} [A, A^{\dagger t}] = {} & \frac{d^2}{2}[td + t(2t-3)]A^{\dagger t-1} \\ & + td(d-1)A^{\dagger t-1} \sum_{i=1}^{d} a_i^\dagger a_i - tdA^{\dagger t-1} \\ & \times \sum_{i,j=1}^{d} (a_i^\dagger a_j + a_j^\dagger a_i) \ . \end{aligned} \tag{5.17}$$

With these relations we obtain

$$1 = |\gamma_{00}|^2 \sum_{t=0}^{\infty} \left[\frac{\lambda^2 d^2}{2} \right]^t \frac{1}{t!} \frac{(2t+d-3)!!}{(d-3)!!}$$

which is a convergent series since $\lambda^2 d^2 < 1$. Thus, within an arbitrary phase

$$\gamma_{00} = (1-\lambda^2 d^2)^{(d-1)/4}$$

and finally ${}^{(o)}U$ can be written

$${}^{(o)}U = \left[\frac{4\omega\bar{\omega}}{(\omega+\bar{\omega})^2} \right]^{(d-1)/4} \exp\left[\frac{\bar{\omega}-\omega}{d(\bar{\omega}+\omega)} A^\dagger \right] , \tag{5.18}$$

$A^\dagger$ being defined in (5.9). We note that in the limit $k \to 0$ (no coupling), $\bar{\omega} \to \omega$ and ${}^{(o)}U \to I$.

VI. LIE ALGEBRAIC PROPERTIES

The study of the Lie algebraic properties, considered in this section, is not of great help for the present problem since the degeneracy of the levels, when $\bar{n}$ increases, is very high as soon as $d>3$. But they are important in view of further developments in which the model Hamiltonian considered here would be a zeroth-order approximation of a more complicated system.

As it is well known [4,5] the symplectic algebra $\mathrm{sp}(2d,R)$ is of special importance for the study of d-dimensional IHO. Within our notations its $d(2d+1)$ generators can be written

$$a_i^\dagger a_j^\dagger, \ a_i a_j, \ a_i^\dagger a_j, \quad i,j=1,\ldots,d \ . \tag{6.1}$$

It admits two infinite-dimensional unitary representations which, respectively, span all the states associated with $n=\sum_i n_i$ even or odd, hence the entire space $\mathcal{H}$ of our problem. The sets

$$b_s^\dagger b_{s'}^\dagger, \ b_s b_{s'}, \ b_s^\dagger b_{s'}, \quad s,s'=1,\ldots,d \tag{6.2}$$

are also the generators of an isomorphic $\mathrm{sp}(2d,R)$ algebra; from (5.1) the two bases (6.1) and (6.2) can be related

and the coefficients of the transformation are real. Furthermore, (6.2) admits two symplectic subalgebras,

$$S_1=\mathrm{sp}(2(d-1),R),\quad S_2=\mathrm{sp}(2,R)\ ,$$

respectively, spanned by the generators (6.2) when $s,s'=1,\ldots,d-1$ and $s=s'=d$.

In addition, any element of S_1 commutes with any element of S_2. Their unitary subalgebras $\mathrm{u}(d-1)$ and $\mathrm{u}(1)$ are the degeneracy algebras of our two IHO of frequency $\bar{\omega}$ and ω. An algebraic chain for our problem is thus

$$\mathrm{sp}(2d,R)\supset\mathrm{sp}(2(d-1),R)\oplus\mathrm{sp}(2,R)\supset\mathrm{u}(d-1)\oplus\mathrm{u}(1)\ . \tag{6.3}$$

The Hamiltonian H (3.13) is a linear combination of the two linear invariants of $\mathrm{u}(d-1)$ and $\mathrm{u}(1)$ and the eigenkets (3.15) span an irreducible representation $[\bar{n}\otimes\dot{o}]$ $[\bar{\bar{n}}_d]$ of $\mathrm{u}(d-1)\oplus\mathrm{u}(1)$. One could further classify the states in the invariance groupe S_d; obviously all states $|\bar{o},\bar{\bar{n}}_d\rangle$ are of symmetry $[d]$, i.e., totally symmetric. For the other oscillator the appropriate symmetries are given by the reduction of the symmetrized Kronecker products of the $[d-1\ 1]$ irreducible representation of S_d associated with the fundamental state $|\bar{1},\bar{o}_d\rangle$. Within the zeroth-order model we have, this is not a necessary step, but it could become so if further interactions were to be added.

VII. EXTENSION TO THREE SPATIAL DIMENSIONS

We shall only briefly sketch how the extension to three spatial dimensions can be done very straightforwardly from the one-dimensional case. A natural extension of (2.1) is given by the model Hamiltonian

$$H=\sum_{i=1}^{d}\left[\frac{\mathbf{p}_i^2}{2m}+\tfrac{1}{2}m\omega^2\mathbf{r}_i^2\right]+\frac{k}{4}\sum_{i,j=1}^{d}(\mathbf{r}_i-\mathbf{r}_j)^2\ , \tag{7.1}$$

where now $r_i=(x_i,y_i,z_i)$ are the vector positions of the individual particles. The Jacobi transformation is equally well defined [2]; (3.2) can be taken in vector form. Equivalently (3.5) becomes

$$X=Ax,\quad Y=Ay,\quad Z=Az\ . \tag{7.2}$$

Instead of one, we have now three sets of boson operators

$$b_{\alpha s},b_{\beta s}^{\dagger},\quad \alpha,\beta=X,Y,Z,\quad s=1,\ldots,d\ , \tag{7.3}$$

satisfying

$$[b_{\alpha s},b_{\beta s'}^{\dagger}]=\delta_{\alpha\beta}\delta_{ss'}\ . \tag{7.4}$$

They are given for fixed α by the same equations (5.1) as in the one-dimensional case. So, without any calculation we can write

$$H=\hbar\bar{\omega}\left[\bar{\bar{N}}+3\frac{(d-1)}{2}\right]+\hbar\omega(\bar{\bar{N}}_d+\tfrac{3}{2})\ , \tag{7.5}$$

where [Eq. (3.14)]

$$\bar{\bar{N}}=\bar{N}_X+\bar{N}_Y+\bar{N}_Z,\quad \bar{\bar{N}}_d=\bar{N}_{Xd}+\bar{N}_{Yd}+\bar{N}_{Zd}\ , \tag{7.6}$$

$\bar{\omega}$ being still given by (3.10). H is now the sum of two uncoupled IHO, one of frequency $\bar{\omega}$ (respectively, ω) and dimension $3(d-1)$ (respectively, 3). The eigenvalues and eigenstates are readily obtained [Eqs. (3.15) and (3.16)]

$$E_{\bar{\bar{n}},\bar{\bar{n}}_d}=\hbar\bar{\omega}\left[\bar{\bar{n}}+\frac{3(d-1)}{2}\right]+\hbar\omega(\bar{\bar{n}}_d+\tfrac{3}{2})\ , \tag{7.7}$$

$$|\bar{\bar{n}},\bar{\bar{n}}_d\rangle=\prod_{\alpha,s}(\bar{n}_{\alpha s}!)^{-1/2}b_{\alpha s}^{\dagger\bar{n}_{\alpha s}}|\bar{o}_{\alpha s}\rangle\ , \tag{7.8}$$

where now

$$\bar{\bar{n}}=\sum_{\alpha=X,Y,Z}\bar{n}_{\alpha}=\sum_{\alpha}\sum_{r=1}^{d-1}\bar{n}_{\alpha r}\ ,$$
$$\bar{\bar{n}}_d=\sum_{\alpha=X,Y,Z}\bar{n}_{\alpha d}\ . \tag{7.9}$$

Likewise, the transformation connecting the two vacuum states is

$$|\dot{\bar{\bar{o}}}\rangle={}^{(o)}V|\dot{o}\rangle\ ,$$
$${}^{(o)}V={}^{(o)}U_x\,{}^{(o)}U_y\,{}^{(o)}U_z\ , \tag{7.10}$$

each term in the product being given by (5.18) in which $A^{\dagger}$ is replaced by $A_{\tau}^{\dagger}(\tau{:}x,y,z)$.

From an algebraic point of view there is much more freedom than in the one-dimensional case considered in Sec. VI. In addition to the S_d symmetry, the Hamiltonian (7.1) exhibits an O(3) symmetry associated with the conservation of the total angular momentum

$$\mathbf{L}=\sum_{i=1}^{d}\boldsymbol{l}_i=\sum_{i=1}^{d}\mathbf{r}_i\times\mathbf{p}_i\ . \tag{7.11}$$

From the set of boson operators (7.3) we get now a $\mathrm{sp}(6d,R)$ algebra and the subalgebras S_1 and S_2 of Sec. VI are replaced by

$$S_1'=\mathrm{sp}(6(d-1),R),\quad S_2'=\mathrm{sp}(6,R)\ .$$

We can also introduce the degeneracy algebra of (7.5) which is clearly

$$\mathrm{u}(3(d-1))\oplus\mathrm{u}(3)\ , \tag{7.12}$$

with respective generators given by

$$b_{\alpha r}^{\dagger}b_{\beta r'},\quad r,r'=1,\ldots,d-1$$
$$b_{\alpha d}^{\dagger}b_{\beta d},\quad \alpha,\beta=X,Y,Z \tag{7.13}$$

each admitting an o(3) subalgebra. Hence a possible chain is

$$\mathrm{sp}(6d,R)\supset\mathrm{sp}(6(d-1),R)\oplus\mathrm{sp}(6,R)\supset\mathrm{u}(3(d-1))\oplus\mathrm{u}(3)\supset[\mathrm{u}'(3)\oplus\mathrm{u}(d-1)]\oplus\mathrm{u}(3)\supset[\mathrm{o}'(3)\oplus\mathrm{u}(d-1)]\oplus\mathrm{o}(3)\ , \tag{7.14}$$

where the last two elements in the chain, obtained by the usual contraction process [2]

$$\sum_{r=1}^{d-1} b_{\alpha r}^{\dagger} b_{\beta r} \quad \text{and} \quad \sum_{\alpha=X,Y,Z} b_{\alpha r}^{\dagger} b_{\beta r'}$$

are, respectively, the generators of u'(3) and u($d-1$).

VIII. DISCUSSION AND CONCLUSION

We hope that our method for solving the problem of an arbitrary number of harmonically coupled oscillators will find applications in several areas of quantum physics; also the explicit realization of the transformation between the zeroth-order and the coupled bases should be useful. One interesting feature is that the appropriate degeneracy algebra is not the usual [2,5] unitary subalgebra of the initial sp($2d,R$) [or sp($6d,R$)] algebra spanned by the d-mode boson operators of the uncoupled oscillators. This comes from the mixing of annihilation and creation operators induced by the transformation to Jacobi variables as it is apparent in Eq. (5.1).

At this point we may note that in their extensive study of the correlation diagrams for rigid and nonrigid three- to six-body systems, several authors [6,7] used a Hamiltonian similar to that given by Eq. (7.1). The motion with frequency ω [Eqs. (3.13) and (7.5)] is associated with an oscillation of the center-of-mass vector, the corresponding spurious excitations of which are commonly eliminated [2,6,7]. The Hamiltonian, associated with the $3(d-1)$ remaining internal degrees of freedom, is taken as a model for an ideal nonrigid system and the starting point is the degeneracy algebra [u($3(d-1)$) in our notation] of this limiting case. The connection to the rigid limit is accomplished by introducing subalgebras associated with conservation laws inferred from the physical properties of an ideal rigid system. To some extent, our approach is complementary since it is situated higher in the dynamical chain [Eqs. (6.3) and (7.14)]. The operators lying outside the degeneracy algebra allow laddering between states of different degenerate levels; these operators are commonly associated with transition moments and their matrix elements can be easily computed either in the zeroth-order or in the coupled basis. Also our approach allows other physical interpretation of the d-mode boson operators. For instance, although the physical meaning of the dynamical variables is very different, we believe that, as suggested [8], a rather similar mechanism is involved in molecular-spectroscopy vibrational problems when one changes from external symmetry coordinates to normal coordinates. Also a possible application would be the zeroth-order treatment of stretching modes in molecules with d equivalent bonds, which are not too anharmonic, and for which algebraic models have been proposed [9–11].

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