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A Procedure for Obtaining Quantum Mechanical Transformation of Diagonalization from the Classical

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Abstract

Using as an example two coupled harmonic oscillators, a transformation to normal coordinates is made using the classical-type simultaneous diagonalization of quadratic forms, and this is then used to develop a procedure for constructing the corresponding quantum mechanical transformation to normal coordinates. The total classical transformation is nonunitary, whereas the quantum mechanical is unitary as it has to be in order to satisfy Von Neumann's theorem. Since the classical transformation has definite steps and is a very straightforward procedure, this could be a very useful procedure for constructing the quantum mechanical transformation in many models, and/or an alternative method for many models

1. *Introduction*

The harmonic oscillator is one of the most important problems in modern physics. The overriding reason for its dominant role is that complex systems can be reduced, by means of Fourier analysis, to solutions of collections of harmonic oscillators. Thus, the harmonic oscillator approximation has become one of the principal methods for studying collective excitations of many-body systems such as collections of phonons and photons, and thus, in getting a better understanding of molecular spectra, blackbody radiation, structure of nuclei, etc. Consequently, one of the most frequent and important Hamiltonians encountered in all physics is that of the harmonic oscillator, and we want to use one of these in this paper to explore forming unitary quantum mechanical transformations from nonunitary classical transformations on the same system.

Consider the case of two harmonic oscillators coupled together through their coordinates x_1 and x_2. The corresponding Hamiltonian for the system is taken to be

$$H = (p_1)^2/2m_1 + (p_2)^2/2m_2 + m_1(\omega_1)^2(x_1)^2/2 + m_2(\omega_2)^2(x_2)^2/2 + cx_1x_2 \tag{1.1}$$

where c is a constant, p refers to momentum, m refers to mass, ω to frequency, and x to position relative to equilibrium.

Our objective is to diagonalize the above Hamiltonian, thus decoupling the two oscillators. This can be done classically by using the simultaneous diagonalization of quadratic forms. It can also be done by treating p and x as quantum mechanical operators and then making a quantum mechanical transformation on these operators. Our procedure will be to use the straightforward, more-simply formed classical transformation to find the quantum mechanical transformation, which in general can be quite difficult to explicitly form.

2. *Classical Diagonalization*

To perform the simultaneous diagonalization of quadratic forms, we will essentially use the method of Friedman (1956), and write equation (1.1) in matrix form as

$$H = \tfrac{1}{2}[\tilde{\dot{x}}M\dot{x} + \tilde{x}Vx] \tag{2.1}$$

where

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad \dot{x} = \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix}, \quad M = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}, \quad V = \begin{pmatrix} m_1\omega_1^2 & c \\ c & m_2\omega_2^2 \end{pmatrix}$$

$\tilde{x}$ and $\tilde{\dot{x}}$ are the transpose matrices of x and $\dot{x}$, respectively, and $\dot{x}_1$ is the velocity of oscillator 1, $\dot{x}_2$ is the velocity of oscillator 2, $p_1 = m_1\dot{x}_1$, $p_2 = m_2\dot{x}_2$.

Now we recall a theorem from mathematical physics that in order to diagonalize two Hermitian matrices by one and the same unitary transformation, it is necessary and sufficient that they commute (Mathews & Walker, 1965a). Thus, we want to make a transformation so that M will commute with V, since in equation (2.1) they do not. So, we make a classical transformation of coordinates from the x's to a new set of coordinates, y's, by letting

$$x = Ty, \qquad \tilde{x} = \tilde{y}\tilde{T} \tag{2.2}$$

where

$$T = \begin{pmatrix} 1/(m_1)^{1/2} & 0 \\ 0 & 1/(m_2)^{1/2} \end{pmatrix}$$

Note that T is *not* a unitary matrix. Under this transformation, H in equation (2.1) becomes

$$H' = \tfrac{1}{2}[\tilde{\dot{y}}\tilde{T}MT\dot{y} + \tilde{y}\tilde{T}VTy] = \tfrac{1}{2}[\tilde{\dot{y}}\dot{y} + \tilde{y}Ry] \tag{2.3}$$

where $R = \tilde{T}VT$.

Now notice that $R = \tilde{T}VT$ is real and symmetric,

$$R = \begin{pmatrix} \omega_1^2 & c/(m_1 m_2)^{1/2} \\ c/(m_1 m_2)^{1/2} & \omega_2^2 \end{pmatrix} \tag{2.4}$$

so it is Hermitian. Then we recall that any Hermitian matrix A may be diagonalized by a unitary transformation, with the diagonal elements being real and the solutions of the secular equation $|A - \lambda I| = 0$, where λ represents the eigenvalues of this equation (Mathews & Walker, 1965b). Thus, R has two real eigenvalues λ_i and two independent, real eigenvectors u_i, i.e., $Ru_i = \lambda u_i$, where u_i is a column matrix having two elements in this case. We could denote this by writing $u_i = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$. Then, of course, this leads to the characteristic equation $|R - \lambda I| = 0$, which can be solved for the allowed values of λ, and the corresponding structure of g_1 and g_2 for each of these eigenvalues. The resulting equation is

$$\begin{vmatrix} \omega_1^2 - \lambda & c/(m_1 m_2)^{1/2} \\ c/(m_1 m_2)^{1/2} & \omega_2^2 - \lambda \end{vmatrix} = 0 \tag{2.5}$$

which gives

$$\lambda = \tfrac{1}{2}[(\omega_1^2 + \omega_2^2) \pm ((\omega_1^2 - \omega_2^2)^2 + 4c^2/m_1 m_2)^{1/2}] \tag{2.6}$$

Denote λ for the plus sign by λ_+ and for the minus sign by λ_-. Then we can find the eigenvectors corresponding to these two eigenvalues. We will call the eigenvectors, u_i, u_+ for λ_+ and u_- for λ_-.

Putting the values of λ_+ from equation (2.6) back into the characteristic equation in (2.5) and solving the two resulting equations for g_1 and g_2, we find

$$u_+ = \begin{pmatrix} (m_1 m_2)^{1/2}/2c[\omega_1^2 - \omega_2^2 + ((\omega_1^2 - \omega_2^2)^2 + 4c^2/m_1 m_2)^{1/2}] \\ 1 \end{pmatrix} \tag{2.7}$$

and the normalized value, $\hat{u}_+$, is then

$$\hat{u}_+ = 1/(1 + (m_1 m_2/4c^2)(\omega_1^2 - \omega_2^2) + (\omega_1^2 - \omega_2^2)^2 + 4c^2/m_1 m_2)^{1/2}(u_+) \tag{2.8}$$

Likewise, placing λ_- into equation (2.5) and solving the resulting equations for g_1 and g_2,

$$u_- = \begin{pmatrix} -1 \\ (m_1 m_2)^{1/2}/2c[\omega_1^2 - \omega_2^2 + ((\omega_1^2 - \omega_2^2)^2 + 4c^2/m_1 m_2)^{1/2}] \end{pmatrix} \tag{2.9}$$

and the normalized value, $\hat{u}_-$, is then

$$\hat{u}_- = 1/(1 + (m_1 m_2/4c^2)(\omega_1^2 - \omega_2^2 + ((\omega_1^2 - \omega_2^2)^2 + 4c^2/m_1 m_2)^{1/2}(u_-) \quad (2.10)$$

From $\hat{u}_+$ and $\hat{u}_-$ we can construct the unitary matrix

$$U = ((\hat{u}_+)\,(\hat{u}_-)) = \begin{pmatrix} AB & -A \\ A & AB \end{pmatrix} \quad (2.11)$$

where

$$A = 1/(1 + (m_1 m_2/4c^2)(\omega_1^2 - \omega_2^2 + ((\omega_1^2 - \omega_2^2)^2 + 4c^2/m_1 m_2)^{1/2}$$

$$B = (m_1 m_2)^{1/2}/2c[\omega_1^2 - \omega_2^2 + ((\omega_1^2 - \omega_2^2)^2 + 4c^2/m_1 m_2)^{1/2}] \quad (2.12)$$

Note that the determinant of U is 1, and $U^{-1}U = I$, and $U^{-1} = \tilde{U}^* = \tilde{U}$.

Proceeding with this classical-type diagonalization, we use U to transform $H'(y, \dot{y})$ to the diagonal form $H''(q, \dot{q})$ by letting

$$y = Uq \quad (2.13)$$

This gives

$$H'' = \tfrac{1}{2}[\tilde{\dot{q}}U^{-1}U\dot{q} + \tilde{q}U^{-1}\tilde{T}VTUq] = \tfrac{1}{2}[\tilde{\dot{q}}\dot{q} + \tilde{q}U^{-1}RUq] \quad (2.14)$$

However, as can be seen from the matrix multiplications,

$$U^{-1}RU = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \quad (2.15)$$

Consequently, the new diagonalized Hamiltonian, H'', becomes

$$H'' = \tfrac{1}{2}\dot{q}_1^2 + \tfrac{1}{2}\dot{q}_2^2 + \tfrac{1}{2}\omega_+^2 q_1^2 + \tfrac{1}{2}\omega_-^2 q_2^2 \quad (2.16)$$

where $\omega_+^2 \equiv \lambda_+$ and $\omega_-^2 \equiv \lambda_-$.

What has happened to the coordinates under this transformation? From equations (2.2) and (2.13), $x = Ty = TUq$, or

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = TU \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \quad (2.17)$$

Notice that TU is the classical transformation to diagonalized variables, and it is *not unitary*. Written out in regular equation form, we have

$$x_1 = AB/(m_1)^{1/2}q_1 - A/(m_1)^{1/2} \qquad q_2 = A/(m_1)^{1/2}(Bq_1 - q_2)$$
$$x_2 = A/(m_2)^{1/2}q_1 + AB/(m_2)^{1/2} \qquad q_2 = A/(m_2)^{1/2}(q_1 + Bq_2) \quad (2.18)$$

with A and B given in equation (2.12).

Inverting the transformation (2.17),

$$q = U^{-1}T^{-1}x \quad (2.19)$$

where

$$U^{-1} = \tilde{U}^* = \tilde{U} = \begin{pmatrix} AB & A \\ -A & AB \end{pmatrix} \tag{2.20}$$

and

$$T^{-1} = \begin{pmatrix} (m_1)^{1/2} & 0 \\ 0 & (m_2)^{1/2} \end{pmatrix} \tag{2.21}$$

Therefore,

$$\begin{aligned} q_1 &= AB(m_1)^{1/2}x_1 + A(m_2)^{1/2} \qquad x_2 = \alpha_1 x_1 + \alpha_2 x_2 \\ q_2 &= -A(m_1)^{1/2}x_1 + AB(m_2)^{1/2} \qquad x_2 = \alpha_3 x_1 - \alpha_4 x_2 \end{aligned} \tag{2.22}$$

where $\alpha_1 = AB(m_1)^{1/2}$, $\alpha_2 = A(m_2)^{1/2}$, $\alpha_3 = -A(m_1)^{1/2}$, and $\alpha_4 = AB(m_2)^{1/2}$. Note that this transformation may also be found for a simplified Hamiltonian by transforming to relative and center of mass coordinates. For example, the above H in equation (1.1) with $m_1 = m_2$ and $\omega_1 = \omega_2$ is easily done. But for a more general H, and above, it takes some good guessing and trying before the correct transformation can be found in this manner.

This classically constructed transformation is now used to see if we can find the quantum mechanical transformation to diagonalized variables.

3. *Quantum Mechanical Diagonalization*

Quantum mechanically, the coordinate and momentum operators transform like

$$q = \mathscr{S} x \mathscr{S}^{-1} = \exp(iS)\, x \exp(-iS) \tag{3.1}$$

where by construction as long as the volume of the system remains finite, $\mathscr{S}$ is a unitary operator (Von Neumann, 1931). Thus, our approach will be to use the classical transformation equation (2.19), $q = U^{-1}T^{-1}x$, to help us find the quantum mechanical operator above. Writing this out, we have

$$\begin{aligned} q_1 &= \mathscr{S} x_1 \mathscr{S}^{-1} = \alpha_1 x_1 + \alpha_2 x_2 = \alpha_1 [x_1 + (m_2)^{1/2}/B(m_1)^{1/2} x_2] \\ q_2 &= \mathscr{S} x_2 \mathscr{S}^{-1} = \alpha_3 x_1 - \alpha_4 x_2 = \alpha_3 [x_1 - B(m_2)^{1/2}/(m_1)^{1/2} x_2] \end{aligned} \tag{3.2}$$

First of all, let us use the Baker-Hausdorff expansion (Messiah, 1966a), and equation (3.2) can be written as

$$\begin{aligned} \mathscr{S} x_1 \mathscr{S}^{-1} &= x_1 + i\,[S, x_1] + i^2/2!\,[S, [S, x_1]] + \ldots, \\ \mathscr{S} x_2 \mathscr{S}^{-1} &= x_2 + i\,[S, x_2] + i^2/2!\,[S, [S, x_2]] + \ldots \end{aligned} \tag{3.3}$$

Next in order to match up the powers of the independent variables in equation (3.2), we try various trial forms for the commutators $[S, x_1]$ and $[S, x_2]$, starting with the simpler forms, linear and quadratic, and proceeding to higher orders if necessary. That is, in our example, we construct S, knowing it must produce linear commutation relation terms (since the highest-order terms of the Hamiltonian are bilinear). These steps are in an effort to find an explicit, closed form for S, similar to what Bjorken & Drell (1965) do for certain operators in quantum field theory. If we try

$$[S, x_1] = C_1(x_1 + x_2)$$
$$[S, x_2] = C_2(x_1 + x_2) \tag{3.4}$$

where C_1 and C_2 are constants to be determined, then

$$[S, [S, x_1]] = C_1(C_1 + C_2)(x_1 + x_2)$$
$$[S, [S, x_2]] = C_2(C_1 + C_2)(x_1 + x_2)$$
$$[S, [S, [S, x_1]]] = C_1(C_1 + C_2)^2 (x_1 + x_2)$$
$$[S, [S, [S, x_2]]] = C_2(C_1 + C_2)^2 (x_1 + x_2)$$

and

$$\mathcal{S} x_1 \mathcal{S}^{-1} = x_1 + [i + (i^2/2!)(C_1 + C_2) + (i^3/3!)(C_1 + C_2)^2 + \ldots] \times C_1(x_1 + x_2)$$
$$\mathcal{S} x_2 \mathcal{S}^{-1} = x_2 + [i + (i^2/2!)(C_1 + C_2) + (i^3/3!)(C_1 + C_2)^2 + \ldots] \times C_2(x_1 + x_2). \tag{3.5}$$

Letting $(C_1 + C_2) = z$, and remembering that

$$\exp(iz) = 1 + iz + (i^2/2!)z^2 + (i^3/3!)z^3 + \ldots$$

so that

$$[\exp(iz)]/z - 1/z = i + (i^2/2!)z + (i^3/3!)z^2 + \ldots$$

then

$$q_1 = \mathcal{S} x_1 \mathcal{S}^{-1} = x_1 + (\exp[i(C_1 + C_2)] - 1)(x_1 + x_2)(C_1/C_1 + C_2)$$
$$q_2 = \mathcal{S} x_2 \mathcal{S}^{-1} = x_2 + (\exp[i(C_1 + C_2)] - 1)(x_1 + x_2)(C_2/C_1 + C_2) \tag{3.6}$$

Equating the coefficients of x_1 and x_2 from equations (3.2) and (3.6), gives us the following four equations:

$$1 + C_1[(1/C_1 + C_2)[\exp(i(C_1 + C_2))] - (1/C_1 + C_2)] = \alpha_1 = -B\alpha_3 \tag{3.7}$$
$$C_1[(1/C_1 + C_2)[\exp(i(C_1 + C_2))] - (1/C_1 + C_2)] = \alpha_2 \tag{3.8}$$
$$1 + C_2[(1/C_1 + C_2)[\exp(i(C_1 + C_2))] - (1/C_1 + C_2)] = \alpha_4 = B\alpha_2 \tag{3.9}$$
$$C_2[(1/C_1 + C_2)[\exp(i(C_1 + C_2))] - (1/C_1 + C_2)] = \alpha_3 \tag{3.10}$$

Combining equations (3.7) and (3.10) gives

$$1 + (C_1/C_1 + C_2)[\exp(i(C_1 + C_2)) - 1] = -B(C_2/C_1 + C_2)[\exp(i(C_1 + C_2)) - 1] \quad (3.11)$$

and combining equations (3.8) and (3.9) gives

$$1 + (C_2/C_1 + C_2)[\exp(i(C_1 + C_2)) - 1] = B(C_1/C_1 + C_2)[\exp(i(C_1 + C_2)) - 1] \quad (3.12)$$

Solving for $\exp(i(C_1 + C_2))$ from equation (3.11) gives

$$1 - (C_1 + C_2/BC_2 + C_1) = \exp(i(C_1 + C_2)) \quad (3.13)$$

Using the result of equation (3.13) in equation (3.12) gives

$$C_1 = -(B - 1/B + 1)\, C_2 \quad (3.14)$$

Then using equation (3.14) to eliminate C_1 from equation (3.11) and solving for C_2, we have

$$C_2 = (B + 1/2i) \ln(B^2 - 1/B^2 + 1) \quad (3.15)$$

Combining this with equation (3.14) gives C_1:

$$C_1 = -(B - 1/2i) \ln(B^2 - 1/B^2 + 1) \quad (3.16)$$

Thus, the constants in equation (3.4) are determined in terms of known parameters.

Now what is S such that equation (3.4) is satisfied? This is easy to find if one remembers the commutation relations $[x_i, p_j] = i\hbar\delta_{ij}$. Consequently, if we try

$$S = (C_1/i\hbar)(p_1x_1 + p_1x_2) + (C_2/i\hbar)(p_2x_2 + p_2x_1) \quad (3.17)$$

then

$$\begin{aligned}[S, x_1] &= (-C_1/i\hbar)[\{[p_1, x_1]x_1\} + \{[p_1, x_1]x_2\}] \\ &= -(C_1/i\hbar)(-i\ \ )(x_1 + x_2) = C_1(x_1 + x_2) \\ [S, x_2] &= (-C_2/i\hbar)[\{[p_2, x_2]x_2\} + \{[p_2, x_2]x_1\}] \\ &= -(C_2/i\hbar)(-i\hbar)(x_2 + x_1) = C_2(x_1 + x_2)\end{aligned}$$

which is exactly equation (3.4). Therefore, an appropriate S is given by equation (3.17), and putting C_1 and C_2 in from equations (3.15) and (3.16) gives

$$\begin{aligned}S = [\ln(B^2 - 1/B^2 + 1)/2\hbar]\, &[-(B + 1)(p_2x_2 + p_2x_1) \\ &+ (B - 1)(p_1x_1 + p_1x_2)]\end{aligned} \quad (3.18)$$

where B is given in equation (2.12); and the unitary transformation operator $\mathcal{S}$ is $\exp(iS)$. This is the quantum mechanical transformation to diagonalized variables up to a phase factor.

However, since the commutation relations should be preserved under a unitary transformation (Messiah, 1966b), we also need to check them out. If they are not preserved, we are inconsistent. Therefore, under the transformation

$$\begin{aligned} q_1 &= \alpha_1 x_1 + \alpha_2 x_2 \\ q_2 &= \alpha_3 x_1 + \alpha_4 x_2 \\ p_1 &= (\alpha_1/m_1)p_1 + (\alpha_2/m_2)p_2 \\ p_2 &= (\alpha_3/m_1)p_1 + (\alpha_4/m_2)p_2 \end{aligned} \tag{3.19}$$

which is carried out by $\mathscr{S}$, do we have $[q_i, P_j] = i\hbar\delta_{ij}$ if we had $[x_i, p_j] = i\hbar\delta_{ij}$? We have under the transformation in equation (3.19),

$$\begin{aligned} [q_1, P_1] &= [x_1, p_1](\alpha_1^2/m_1) + [x_2, p_2](\alpha_2^2/m_2) \\ &= i\hbar(\alpha_1^2/m_1 + \alpha_2^2/m_2) \\ [q_2, P_2] &= [x_1, p_1](\alpha_3^2/m_1) + [x_2, p_2](\alpha_4^2/m_2) \\ &= i\hbar(\alpha_3^2/m_1) + i\hbar(\alpha_4^2/m_2) \\ [q_1, P_2] &= i\hbar(\alpha_1\alpha_3/m_1) + i\hbar(\alpha_2\alpha_4/m_2) \\ [q_2, P_1] &= i\hbar(\alpha_1\alpha_3/m_1) + i\hbar(\alpha_2\alpha_4/m_2) \end{aligned} \tag{3.20}$$

This means for our commutation relations to be preserved under the transformation which simultaneously diagonalizes the quadratic kinetic and potential energy forms, we must have

$$\begin{aligned} &(\alpha_1^2/m_1) + (\alpha_2^2/m_2) = 1 \\ &(\alpha_3^2/m_1) + (\alpha_4^2/m_2) = 1 \\ &(\alpha_3\alpha_1/m_1) + (\alpha_4\alpha_2/m_2) = 0 \end{aligned} \tag{3.21}$$

For our interaction Hamiltonian,

$$(\alpha_1^2/m_1) + (\alpha_2^2/m_2) = A^2(B^2 + 1) = (\alpha_3^2/m_1) + (\alpha_4^2/m_2)$$

and

$$(\alpha_3\alpha_1/m_1) + (\alpha_4\alpha_2/m_2) = -(A^2B) + A^2B = 0$$

Now from equation (2.12),

$$A^2 = 1/(1 + B^2) \tag{3.22}$$

Thus,

$$(\alpha_1^2/m_1) + (\alpha_2^2/m_2) = 1/(1 + B^2)(B^2 + 1) = 1$$

Consequently, equation (3.21) does indeed hold, and the commutation relations are preserved.

In passing, another way of determining C_1 and C_2 would be to use the conditions for preservation of commutation relations, equation (3.21), in conjunction with equations (3.7) through (3.10) and eliminate $\alpha_1, \alpha_2, \alpha_3$,

α_4. One can also use them to solve for C_1 and C_2 in terms of $\alpha_1, \alpha_2, \alpha_3$, and α_4. If this is done, after some tedious algebra, one finds

$$C_1 = [D/i(1+D)] \ln[\{(\alpha_1(1+D)-1)/D\}\{(\alpha_2(1+D)+D)/D\} \times \{\alpha_3(1+D)+1\}\{\alpha_4(1+D)-D\}]^{1/4} \quad (3.23)$$

and

$$C_2 = C_1/D \quad (3.24)$$

where

$$D = [(m_2/m_1)(m_1 m_2 + m_1^2 + m_2 - m_1)/(m_1 m_2 + m_2^2 - m_2 + m_1)]^{1/2} \quad (3.25)$$

These equations show the connections between the classical transformation constants, $\alpha_1, \alpha_2, \alpha_3, \alpha_4$, and the quantum mechanical transformation constants, C_1 and C_2.

Thus, we have used the nonunitary, classical transformation to diagonalized variables obtained from the simultaneous diagonalization of quadratic forms to arrive at the unitary, quantum mechanical transformation to diagonalized variables. We may summarize this procedure as follows:

(1) Follow through the steps of the simultaneous diagonalization of quadratic forms.
(2) Set the general form of the quantum mechanical transformation on coordinates and moments equal to the classical transformation from (1).
(3) Expand the quantum mechanical form of the transformation in the Baker-Hausdorff expansion.
(4) Impose the commutation relations on the coordinates and momenta and check that they are preserved under the transformation in (2).
(5) Select appropriate form of S in the quantum mechanical transformation operator $\mathscr{S} = \exp(iS)$ using the information in (3) and (4) and the form of the Hamiltonian.

4. *Conclusion*

The above is then a method of obtaining the explicit form of quantum mechanical transformations and, as shown of the example above, can be a useful method in many cases. Also, in other cases it may be a simpler alternative and could provide a very general method for going to normal coordinates quantum mechanically in many other models. As illustrated above, it works for the very frequently encountered model of coupled oscillators.

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