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# Generalised Fulton–Gouterman transformation for systems of Abelian symmetry

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**Abstract.** A two-level system which is coupled to a multitude of oscillators, such that the total system formally or geometrically is governed by a mirror symmetry, can be exactly diagonalised with respect to the two-level subsystem (FG transformation). This has been thoroughly exploited for the two-site exciton localisation problem as well as for two-site quantum transport. A generalisation to the  $N$ -level system is given, provided the  $N$  levels establish a regular representation of an Abelian group, and if the latter symmetry also governs the multi-oscillatory subsystem. Implications for the quantum transport problem are discussed.

## 1. Introduction

The coupling of a finite number  $N$  of one-particle levels (electron, proton, exciton) to a multi-oscillatory system has a long history both in solid state and molecular physics. In particular in the form of a particle or excitation transport problem this conformation of coupled subsystems has initiated a large amount of theoretical and experimental work. One of the earliest and most extensively studied of these problems is that of the polaron, where a number of different theoretical approaches have been developed. For a good review we recommend the book of Kuper and Whitfield (1963) and the article of Appel (1968). Of similar extent is the literature on the exciton problem, for which we again recommend the book of Kuper and Whitfield (1963) and also the book of Knox (1963). In recent years a great deal of interest has arisen in the quantum transport problem ('quantum diffusion', 'quantum tunnelling') of light particles (protons, muons), in crystals which also may be handled as a spatially arranged  $N$ -level system which is coupled to the phonon system. Another large group of publications has been devoted to the problem of tunnelling centres in crystals. A good introduction to this field is the article of Dick (1977). Here the  $N$  levels are representatives of the tunnelling wells around a central ion or vacancy, e.g. the system  $\text{KCl}:\text{OH}^-$  is of this kind. Finally we mention the quantum motion of hydrogen in organic molecules and hydrogen bonded ferroelectrics.

In the multitude of these systems mostly rather conventional methods have been employed for the theoretical description, involving rather crude approximations. It is only in the two-site problem that some effort has been made to get more accurate theoretical insight (Sander and Shore 1971, Wagner 1978, Junker and Wagner 1983) or even exact information. One of the most excessively cited two-site models is the 'small polaron' model of Holstein (1959).

One fascinating and non-conventional way of describing a two-state subsystem, which is coupled to oscillators, has been devised by Fulton and Gouterman (1961). In this method an ingenious unitary transformation is employed to diagonalise the full Hamiltonian with respect to the two-level subsystem. Later Shore and Sander (1973) used this method to discuss the two-site exciton problem. In particular they have studied the question of a sharp transition from high to low mobility in variation of the coupling constant ('localisation'). It is this question which has been discussed for a long time (namely Toyozawa 1968) among exciton researchers and which is of great importance in the field of quantum transport. To discuss this issue beyond the two-site arrangement it would be highly desirable to have a Fulton–Gouterman (FG) like transformation for the  $N > 2$  situation. It is the purpose of the present work to design such an extended transformation.

Fulton and Gouterman (1961) have shown that their transformation can be established for a specific class of systems which display a special kind of mirror symmetry (which may be formal). We exploit this symmetry argument by reformulating the FG transformation in a somewhat unusual manner in § 2. This gives us a good starting position for deriving an extended transformation in systems of Abelian symmetry (§ 3). In § 4 a special kind of Abelian symmetry, the cyclic symmetry, is discussed, which may prove to be of great interest in the quantum transport problem. Finally, in § 5 an outlook to physical problems is given.

In our presentation we freely make use of group-theoretical techniques, which we thus assume to be a standard tool. But if the reader wants to have a look at the details, we recommend the books of Hammermesh (1964) and of Heine (1960).

## 2. The transformation of Fulton and Gouterman

The Fulton–Gouterman transformation (FGT) has been devised to diagonalise a two-level system, which is coupled to a multi-oscillator system, with respect to the two-level subsystem, such that a set of two separate oscillatory systems is left. We describe the two-level system by Fermi creation and annihilation operators,  $a_r^+$ ,  $a_r$ ,  $r = 1, 2$ , and we require the occupation number conservation (particle number conservation)

$$a_1^+ a_1 + a_2^+ a_2 = 1. \quad (2.1)$$

The eigenvectors of the two levels will be denoted as  $|1\rangle$  and  $|2\rangle$ . It is now crucial that the system is governed by a kind of inversion symmetry, such that an inversion operator  $J$  can be defined with the properties

$$\begin{aligned} J|1\rangle &= |2\rangle, & J|2\rangle &= |1\rangle \\ Ja_1 &= a_2J, & Ja_2 &= a_1J, \end{aligned} \quad (2.2)$$

and which commutes with the Hamiltonian,

$$JH = HJ. \quad (2.3)$$

The effect of  $J$  onto the vibrational coordinates remains to be specified. It follows then that all eigenfunctions of  $H$  must be base functions of the two irreducible representations  $\Gamma_\gamma$ ,  $\gamma = 1$  (even parity) and  $\gamma = 2$  (odd parity) of the inversion group consisting of the two elements ( $E, J$ ). In this manner we arrive at two sets of functional

forms for the eigenfunctions of the coupled Hamiltonian,

$$\psi_{1m} = (1/\sqrt{2})[|1\rangle\Phi_m^{(1)}(Q) + |2\rangle J_Q \Phi_m^{(1)}(Q)], \quad \text{even} \quad (2.4a)$$

$$\psi_{2m} = (1/\sqrt{2})[|1\rangle\Phi_m^{(2)}(Q) - |2\rangle J_Q \Phi_m^{(2)}(Q)], \quad \text{odd} \quad (2.4b)$$

where  $\Phi_m^{(\gamma)}(Q)$  respectively are normalised functions in the vibrational subspace,  $Q$  representing the oscillatory coordinates. We may expect these forms to diagonalise the Hamiltonian if the  $\Phi_m^{(\gamma)}(Q)$  satisfy certain eigenvalue equations in the vibrational subspace. Now the most general Hamiltonian of oscillators coupled to a two-level system, which displays the inversion property, may be written in the form

$$\begin{aligned} H &= H_0(P, Q) + \{(E + J)[a_1^+ a_1 A(Q) + a_1^+ a_2 B(Q)]\} \\ &= H_0(P, Q) + (a_1^+ a_1 A(Q) + a_2^+ a_2 (J_Q A(Q)) + a_1^+ a_2 B(Q) + a_2^+ a_1 (J_Q B(Q))) \\ &= H_0(P, Q) + \frac{1}{2}(a_1^+ a_1 - a_2^+ a_2)[A(Q) - (J_Q A(Q))] + \frac{1}{2}[A(Q) + (J_Q A(Q))] \\ &\quad + \frac{1}{2}(a_1^+ a_2 + a_2^+ a_1)[B(Q) + (J_Q B(Q))] + \frac{1}{2}(a_1^+ a_2 - a_2^+ a_1)[B(Q) - (J_Q B(Q))] \end{aligned} \quad (2.5)$$

where  $E$  is the unity operation,  $J_Q$  the inversion operator in  $Q$  subspace, and where  $H_0(P, Q)$  denotes the pure vibrational subsystem,

$$H_0 = \frac{1}{2}\hbar \sum_i [P_i^2 + \Omega_i^2 Q_i^2], \quad J_Q H_0 = H_0 J_Q \quad (2.6)$$

Since  $H$  must be Hermitian, we must have

$$B(Q)^+ = (J_Q B(Q)). \quad (2.7)$$

Inserting (2.4a) in the Schrödinger equation  $H\psi - E\psi = 0$ , we get

$$\begin{aligned} (H - E_{1m})\psi_{1m} &\equiv (1/\sqrt{2})|1\rangle[(H_0 - E_{1m} + A(Q))\Phi_m^{(1)}(Q) + B(Q)J_Q \Phi_m^{(1)}(Q)] \\ &\quad + (1/\sqrt{2})|2\rangle[(H_0 - E_{1m} + (J_Q A(Q))J_Q \Phi_m^{(1)}(Q) + (J_Q B(Q))\Phi_m^{(1)}(Q)] = 0 \end{aligned} \quad (2.8)$$

which is seen to satisfy the equation, if  $\Phi_m^{(1)}$  simultaneously is a solution of the two projected equations

$$[H_0 - E_{1m} + A(Q)]\Phi_m^{(1)}(Q) + B(Q)J_Q \Phi_m^{(1)}(Q) = 0 \quad (2.9a)$$

and

$$[H_0 - E_{1m} + (J_Q A(Q))J_Q \Phi_m^{(1)}(Q) + (J_Q B(Q))\Phi_m^{(1)}(Q) = 0. \quad (2.9b)$$

However, it is immediately evident that these equations are not independent from each other, since the second one is generated from the first one by subjecting it to the inversion operation  $J_Q$  in  $Q$ -space. Hence the ansatz (2.4a) is shown to satisfy the Schrödinger equation, if  $\Phi_m^{(1)}$  is a solution of the Schrödinger equation (2.9a) in vibrational subspace. Similarly it is shown that the ansatz (2.4b) satisfies the Schrödinger equation, if  $\Phi_m^{(2)}$  is a solution of the vibrational Schrödinger equation

$$[H_0 - E_{1m} + A(Q)]\Phi_m^{(2)}(Q) - B(Q)J_Q \Phi_m^{(2)}(Q) = 0. \quad (2.10)$$

We now seek to simplify the formulation by devising a unitary transformation  $U$  which also has the property of disentangling the original problem into two vibrational subproblems. This is achieved if we require the transformed Hamiltonian  $\tilde{H} \equiv U^+ H U$  to have eigenfunctions of the form

$$\tilde{\psi}_{1m} \equiv U^+ \psi_{1m} = |1\rangle\Phi_m^{(1)}(Q) \quad (2.11a)$$

and

$$\tilde{\psi}_{2m} \equiv U^+ \psi_{2m} = |2\rangle \Phi_m^{(2)}(Q), \quad (2.11b)$$

which is tantamount to the requirement that the transformed Hamiltonian is diagonal with respect to the two-level subsystem. The inversion of (2.11) reads

$$U\tilde{\psi}_{1m} = \psi_{1m}, \quad U\tilde{\psi}_{2m} = \psi_{2m} \quad (2.12)$$

and if we identify these equations with equations (2.4) we have

$$U|1\rangle\Phi_m^{(1)}(Q) = (1/\sqrt{2})[|1\rangle\Phi_m^{(1)}(Q) + |2\rangle J_Q \Phi_m^{(1)}(Q)] \quad (2.13a)$$

$$U|2\rangle\Phi_m^{(2)}(Q) = (1/\sqrt{2})[|1\rangle\Phi_m^{(2)}(Q) - |2\rangle J_Q \Phi_m^{(2)}(Q)] \quad (2.13b)$$

from which we may directly read off the necessary form of  $U$ ,

$$U = (1/\sqrt{2})(a_1^+ a_1 - a_2^+ a_2 J_Q) + (1/\sqrt{2})(a_2^+ a_1 J_Q + a_1^+ a_2). \quad (2.14)$$

We may write (2.14) also in a more symmetric form,

$$U = (1/\sqrt{2})[\frac{1}{2} + \frac{1}{2}(a_1^+ a_2 - a_2^+ a_1)](1 - J_Q) \\ + (1/\sqrt{2})[\frac{1}{2}(a_1^+ a_1 - a_2^+ a_2) + \frac{1}{2}(a_1^+ a_2 + a_2^+ a_1)](1 + J_Q) \quad (2.15)$$

which is suitable for a pseudospin notation (see the appendix). Using the projective representation

$$a_i^+ a_j = |i\rangle\langle j| \quad (2.16)$$

we may rewrite  $U$  also in the form

$$U = (1/\sqrt{2})[|1\rangle\langle 1| - |2\rangle\langle 2| J_Q] + (1/\sqrt{2})[|2\rangle\langle 1| J_Q + |1\rangle\langle 2|]. \quad (2.17)$$

We also note the basic transformation properties of  $U$ :

$$U^+ f(Q) U = \frac{1}{2}(a_1^+ a_2 + a_2^+ a_1)(f(Q) - J_Q f(Q) J_Q) + \frac{1}{2}(f(Q) + J_Q f(Q) J_Q) \quad (2.18)$$

$$U^+(a_1^+ a_1 - a_2^+ a_2) U = a_1^+ a_2 + a_2^+ a_1$$

$$U^+ a_1^+ a_2 U = \frac{1}{2}(a_1^+ a_1 - a_2^+ a_2) J_Q - \frac{1}{2}(a_1^+ a_2 - a_2^+ a_1) J_Q$$

$$U^+ a_2^+ a_1 U = \frac{1}{2}(a_1^+ a_1 - a_2^+ a_2) J_Q + \frac{1}{2}(a_1^+ a_2 - a_2^+ a_1) J_Q$$

$$U^+ J_Q U = J_Q$$

and the transformed Hamiltonian reads

$$\tilde{H} \equiv U^+ H U = H_0(P, Q) + A(Q) + (a_1^+ a_1 - a_2^+ a_2) B(Q) J_Q \quad (2.19)$$

which is seen to be diagonal with respect to the two-level subsystem and indeed leads to equations of the form (2.9a) and (2.10) for the vibrational eigenfunctions. In passing, we note that the inversion operator  $J_Q$  in  $Q$ -space may be taken in the explicit unitary operator form

$$J_Q = \exp i\pi \sum_k \left( \frac{1}{\Omega_{uk}} (P_{uk}^2 + \Omega_{uk}^2 Q_{uk}^2) - \frac{1}{2} \right) \quad (2.20)$$

where  $Q_{uk}$  denote the 'odd' coordinates,  $(J_Q Q_{uk}) = -Q_{uk}$  (correspondingly the 'even' coordinates are denoted by  $Q_{gk}$ ).

We have presented the Fulton-Gouterman (1961) transformation in a way which easily lends itself to a generalisation to systems of higher symmetries than the pure

inversion symmetry. In the original paper (Fulton and Gouterman 1961) the semantics of the presentation has been somewhat different. A further quite useful display of the Fulton–Gouterman transformation can be made by means of spin- $\frac{1}{2}$  operators; this is given in the appendix.

### 3. Abelian symmetry

We now consider a set of orthogonal one-particle functions  $|r\rangle$ ,  $r = 1, 2, \dots, N$ , which are distributed in space in such a manner that they can be uniquely generated by the  $N$  symmetry operations  $R_r$  of a group  $G$ ,

$$|r\rangle = R_r|1\rangle, \quad r = 1, 2, \dots, N \tag{3.1}$$

$$\langle r|r'\rangle = \delta_{rr'}. \tag{3.2}$$

These functions then establish the *regular* representation of the group. We require that this group be Abelian

$$R_r R_{r'} = R_{r'} R_r. \tag{3.3}$$

Then it has precisely  $N$  irreducible representations  $\Gamma_\gamma$ ,  $\gamma = 1, 2, \dots, N$ , all of which are one-dimensional, and their characters also have the Abelian property

$$\chi_\gamma(R_r R_{r'}) = \chi_\gamma(R_r) \chi_\gamma(R_{r'}). \tag{3.4}$$

Further, we will need the orthogonality relation of characters,

$$\sum_{r=1}^N \chi_\gamma(R_r)^* \chi_{\gamma'}(R_r) = N \delta_{\gamma\gamma'}. \tag{3.5}$$

We also assume the vibrational subsystem to be governed by the symmetry group  $G$ . In particular the vibrational Hamiltonian

$$H_0 = \frac{1}{2}\hbar \sum_{\gamma,k} [P_{\gamma k} P_{\gamma k}^+ + \Omega_{\gamma k}^2 Q_{\gamma k} Q_{\gamma k}^+] \tag{3.6}$$

will then be invariant under the operations of the group,

$$R_r H_0 = H_0 R_r, \tag{3.7}$$

and each normal coordinate  $Q_{\gamma k}$  will be a base coordinate to one particular irreducible representation (index  $\gamma$ ):

$$R_r Q_{\gamma k} = \chi_\gamma(R_r) Q_{\gamma k} R_r \tag{3.8}$$

Any vector of the combined Hilbert space, which pertains to the irreducible representation  $\Gamma_\gamma$ , can then be created by the Wigner formula

$$\psi_\gamma = \sum_{r=1}^N \chi_\gamma(R_r) R_r \varphi, \tag{3.9}$$

where  $\varphi$  is some arbitrary function of the combined space. We now will show that the *most general base* vector of  $\Gamma_\gamma$  is already created by the choice  $\varphi = N^{-1/2}|1\rangle\Phi(Q)$ ,

$$\psi_\gamma = N^{-1/2} \sum_{r=1}^N \chi_\gamma(R_r) (R_r|1\rangle) R_r(Q)\Phi(Q). \tag{3.10}$$

To prove this we consider another choice  $\varphi = N^{-1/2}|a\rangle\Phi'(Q)$ ,

$$\psi'_\gamma = N^{-1/2} \sum_{r=1}^N \chi_\gamma(R_r)(R_r|a) R_r \Phi'(Q). \tag{3.11}$$

Now, by means of (3.1), (3.3) and (3.4)

$$\begin{aligned} |a\rangle &= R_a|1\rangle, & R_r \Phi'(Q) &= R_r R_a (R_a^{-1} \Phi'(Q)) \\ \chi_\gamma(R_r) &= \chi_\gamma(R_a^{-1}) \chi_\gamma(R_r R_a), \end{aligned} \tag{3.12}$$

whence

$$\psi'_\gamma = N^{-1/2} \sum_{r=1}^N \chi_\gamma(R_r R_a)(R_r R_a|1) R_r R_a [\chi_\gamma(R_a^{-1}) R_a^{-1} \Phi'(Q)]. \tag{3.13}$$

Since the combined operations  $R_r R_a = R_r$  for  $r = 1 \dots N$  also sweeps over all elements of the group, we may write

$$\psi'_\gamma = N^{-1/2} \sum_{r=1}^N \chi_\gamma(R_r) R_r |1\rangle R_r [\chi_\gamma(R_a^{-1}) R_a^{-1} \Phi'(Q)] \tag{3.14}$$

which evidently is the form (3.9) again, if we choose  $\Phi(Q) = \chi_\gamma(R_a^{-1}) R_a^{-1} \Phi'(Q)$ , whence we have proved our statement.

It is this statement which permits us to proceed in a similar manner to § 2. Since each eigenfunction of a Hamiltonian governed by the symmetry group  $G$  must be a base vector of one of the irreducible representations  $\Gamma_\gamma$ , we have exactly  $N$  different species of eigenvectors for our Abelian group, which is the same number as that of the electronic states. We thus may diagonalise the Hamiltonian with respect to the  $N$ -level subsystem in such a way that each of the  $N$  states  $|\gamma\rangle$  of the transformed picture respectively is attached to one of the irreducible representations  $\Gamma_\gamma$ . That is, we require the unitary transformation operator  $U$  to be chosen in such a way that the eigenvectors of the transformed Hamiltonian are of the form

$$\tilde{\psi}_{\gamma m} \equiv U^+ \psi_{\gamma m} = |\gamma\rangle \Phi_m^{(\gamma)}(Q), \tag{3.15}$$

or vice versa

$$\psi_{\gamma m} \equiv U \tilde{\psi}_{\gamma m} = U |\gamma\rangle \Phi_m^{(\gamma)}(Q) \tag{3.16}$$

where  $m$  is a quantum number pertaining to the vibrational subsystem. This procedure parallels that given in § 2 (namely (2.11) and (2.12)). Since  $\psi_{\gamma m}$  must be of the form (3.10), we have the equality

$$U |\gamma\rangle \Phi_m^{(\gamma)}(Q) = N^{-1/2} \sum_{r=1}^N \chi_\gamma(R_r) |r\rangle R_r(Q) \Phi_m^{(\gamma)}(Q) \tag{3.17}$$

from which we may easily deduce the form of the unitary operator  $U$ ,

$$\begin{aligned} U &= N^{-1/2} \sum_\gamma \sum_{r=1}^N \chi_\gamma(R_r) |r\rangle \langle \gamma| R_r(Q) \\ U^+ &= N^{-1/2} \sum_\gamma \sum_{r=1}^N \chi_\gamma^*(R_r) |\gamma\rangle \langle r| R_r^+(Q) \end{aligned} \tag{3.18}$$

where  $R_r(Q)$  is the symmetry operation in  $Q$ -space. We emphasise, however, that the

operators  $R_r(Q)$  must be chosen unitary themselves too to warrant the unitarity of  $U$  itself,

$$R_r^+(Q) = R_r^{-1}(Q). \tag{3.19}$$

However, this is no limitation of generality, since  $R_r(Q)$  is a representation of  $G$  and thus must be equivalent to a unitary representation, whence we may directly choose it as a unitary representation from the beginning.

Using (3.8), we derive the basic transformation property of the normal coordinates

$$\tilde{Q}_{\gamma k} \equiv U^+ Q_{\gamma k} U = N^{-1} Q_{\gamma k} \sum_{r=1}^N \chi_{\gamma}^*(R_r) \sum_{\gamma', \gamma''=1}^N \chi_{\gamma'}^*(R_r) \chi_{\gamma''}(R_r) |\gamma'\rangle \langle \gamma''| \tag{3.20}$$

which thus are seen to be no longer disentangled from the  $N$ -level subsystem, except for those of the unity representation. However,

$$U^+(Q_{\gamma k} Q_{\gamma k}^+) U = Q_{\gamma k} Q_{\gamma k}^+. \tag{3.21}$$

The corresponding formulae apply to the normal momenta  $P_{\gamma k}$ . For the  $N$ -level subsystem we may employ the basic projectors  $|r\rangle\langle s|$  with the property

$$\sum_{r=1}^N |r\rangle\langle r| = 1. \tag{3.22}$$

Their transformation is given by

$$U^+ |r\rangle\langle s| U = N^{-1} \sum_{\gamma, \gamma'=1}^N |\gamma\rangle\langle \gamma'| \chi_{\gamma}^*(R_r) \chi_{\gamma'}(R_s) R_r^+(Q) R_s(Q) \tag{3.23}$$

which thus also is seen to remain no longer disentangled from the second (that is the vibrational) subsystem.

Turning to the Hamiltonian, it is clear from (3.21) that the pure vibrational Hamiltonian  $H_0$  of (3.6) remains invariant,

$$U^+ H_0 U = H_0. \tag{3.24}$$

The interaction Hamiltonian  $W$  is written in the form

$$W = \sum_{r,s=1}^N |r\rangle\langle s| A_{rs}(Q) \tag{3.25}$$

and since

$$(R_r, W) = W, \quad \text{or } R_r W = W R_r, \tag{3.26}$$

where the bracket denotes the partial application of  $R_r$  onto  $W$ , sparing operators to the right of  $W$ , we may also write it in the form

$$W = N^{-1} \sum_{r=1}^N \sum_{u,v=1}^N [R_r |u\rangle\langle v| A_{uv}(Q)]. \tag{3.27}$$

If we apply the transformation operators (3.18) to this form, we first get

$$WU = N^{-3/2} \sum_{ruv=1}^N \sum_{\gamma=1}^N (R_r R_u |1\rangle) (R_r(Q) A_{uv}(Q)) \chi_{\gamma}(R_r R_v) \langle \gamma | R_r(Q) R_v(Q) \tag{3.28}$$



and subsequently

$$U^+ WU = N^{-2} \sum_{\substack{uv \\ r\gamma\gamma'}}^N |\gamma\rangle\langle\gamma'| \chi_\gamma^*(R_r R_u) \chi_\gamma(R_r R_v) [R_u^+(Q) A_{uv}(Q)] R_u^+(Q) R_v(Q) \tag{3.29}$$

and since  $\chi_\gamma^*(R_r R_u) \chi_\gamma(R_r R_v) = \chi_\gamma^*(R_r) \chi_\gamma(R_r) \chi_\gamma^*(R_u) \chi_\gamma(R_v)$  we may apply the orthogonality property (3.5) of the characters. Then we arrive at

$$U^+ WU = N^{-1} \sum_{\gamma=1}^N |\gamma\rangle\langle\gamma| \sum_{r,s=1}^N \chi_\gamma^*(R_r) \chi_\gamma(R_s) [R_r^+(Q) A_{rs}(Q)] R_r^+(Q) R_s(Q). \tag{3.30}$$

If, in place of the projectors  $|u\rangle\langle v|$ , we prefer a description in creation-annihilation operators  $a_r^+ a_s$ , the corresponding formulae read

$$U^+ Q_{\gamma k} U = N^{-1} Q_{\gamma k} \sum_{r=1}^N \chi_\gamma^*(R_r) \sum_{\gamma',\gamma''=1}^N a_{\gamma'}^+ a_{\gamma''} \chi_{\gamma'}^*(R_r) \chi_{\gamma''}(R_r) \tag{3.20a}$$

$$U^+ a_r^+ a_s U = N^{-1} \sum_{\gamma,\gamma'=1}^N a_\gamma^+ a_{\gamma'} \chi_\gamma^*(R_r) \chi_{\gamma'}(R_s) R_r^+(Q) R_s(Q) \tag{3.23a}$$

$$W = \sum_{r,s=1}^N a_r^+ a_s A_{rs}(Q) \tag{3.25a}$$

$$U^+ WU = N^{-1} \sum_{\gamma=1}^N a_\gamma^+ a_\gamma \sum_{r,s=1}^N \chi_\gamma^*(R_r) \chi_\gamma(R_s) [R_r^+(Q) A_{rs}(Q)] R_r^+(Q) R_s(Q). \tag{3.30a}$$

To illustrate these formulae, we may rederive the results of § 2. There we have considered the inversion group  $G(E, J)$  which only had the two elements  $E$  and  $J$  and the two irreducible representations  $\Gamma_1$  (even parity; characters  $\chi_1(E) = 1, \chi_1(J) = 1$ ) and  $\Gamma_2$  (odd parity; characters  $\chi_2(E) = 1, \chi_2(J) = -1$ ). We thus have two species of normal coordinates, and for simplicity we just take a single even coordinate  $Q_g ((JQ_g) = Q_g)$  and a single odd coordinate  $Q_u ((JQ_u) = -Q_u)$ , which by application of formula (3.20a) are transformed like

$$U^+ Q_g U = \frac{1}{2} Q_g \sum_{\gamma,\gamma''=1}^2 a_{\gamma'}^+ a_{\gamma''} [\chi_\gamma^*(E) \chi_{\gamma''}(E) + \chi_\gamma^*(J) \chi_{\gamma''}(J)] = Q_g \tag{3.31a}$$

$$U^+ Q_u U = \frac{1}{2} Q_u \sum_{\gamma,\gamma''=1}^2 a_{\gamma'}^+ a_{\gamma''} [\chi_\gamma^*(E) \chi_{\gamma''}(E) - \chi_\gamma^*(J) \chi_{\gamma''}(J)] = Q_u (a_1^+ a_2 + a_2^+ a_1). \tag{3.31b}$$

This coincides with formula (2.18a), if  $f(Q) = Q_g$  and  $f(Q) = Q_u$  is taken successively. In a corresponding manner the other formulae (2.18) can be derived. Defining the Hamiltonian

$$H = \frac{1}{2} \hbar (P_g^2 + P_u^2 + \Omega_g^2 Q_g^2 + \Omega_u^2 Q_u^2) + W \tag{3.32}$$

$$W = A_{11}(Q) a_1^+ a_1 + A_{22}(Q) a_2^+ a_2 + A_{12}(Q) a_1^+ a_2 + A_{21}(Q) a_2^+ a_1$$

we get from (3.30a)

$$U^+ WU = \frac{1}{2} a_1^+ a_1 [A_{11} + A_{12} J_Q + (J_Q A_{21}) J_Q + (J_Q A_{22}) J_Q^2] + \frac{1}{2} a_2^+ a_2 [A_{11} + A_{22} - A_{12} J_Q - (J_Q A_{21}) J_Q] \tag{3.33}$$

which merges into result (2.19), if we make the identifications  $A_{11} = A$ ,  $A_{22} = (J_Q A)$ ,  $A_{12} = B$ ,  $A_{21} = (J_Q B)$ .

4. Cyclic symmetry

The most simple Abelian group, and simultaneously the group of largest physical interest, is the cyclic group. It is generated by a single element

$$R_r = (R_1)^r, \quad (R_1)^N = E. \tag{4.1}$$

In this case the characters of  $\Gamma_\gamma$  are given in the simple form

$$\chi_\gamma(R_r) = \exp(2i\pi r\gamma/N), \quad \begin{matrix} \gamma = 1, 2, \dots, N \\ r = 1, 2, \dots, N \end{matrix} \tag{4.2}$$

where  $\gamma = N$  denotes the unity representation, and

$$\begin{aligned} \chi_\gamma(R_{N-r}) &= \chi_\gamma^*(R_r) \\ \chi_{N-\gamma}(R_r) &= \chi_\gamma^*(R_r). \end{aligned} \tag{4.3}$$

The set of basic formulae (3.20a), (3.23a) and (3.30a) then are simplified

$$U^+ Q_{\gamma k} U = Q_{\gamma k} \sum_{\gamma'} a_{\gamma'}^+ a_{\gamma'-\gamma} \tag{4.4}$$

$$U^+ a_r^+ a_s U = N^{-1} \sum_{\gamma, \gamma'=1}^N a_{\gamma'}^+ a_{\gamma'} \exp[2i\pi(\gamma's - \gamma r)/N] R_1(Q)^{s-r} \tag{4.5}$$

$$U^+ W U = N^{-1} \sum_{\gamma=1}^N a_{\gamma}^+ a_{\gamma} \sum_{r,s=1}^N \exp[2i\pi(s-r)\gamma/N] [(R_1^+(Q))^r A_{rs}(Q)] (R_1(Q))^{s-r} \tag{4.6}$$

and in particular

$$U^+ a_r^+ a_r U = N^{-1} \sum_{\gamma, \gamma'=1}^N a_{\gamma'}^+ a_{\gamma'} \exp[2i\pi(\gamma' - \gamma)r/N]. \tag{4.7}$$

In view of later applications in transport theory we may define here a kind of ‘occupation wave’

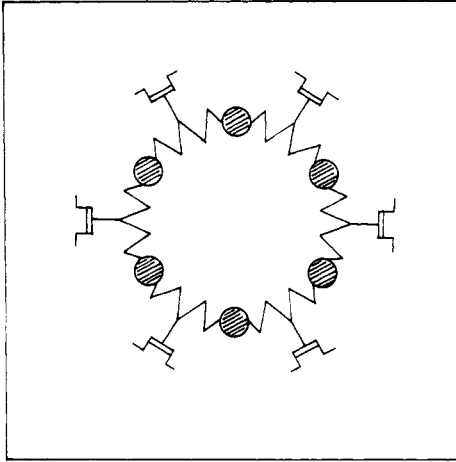
$$\Theta_\alpha = \sum_r \exp(-2i\pi\alpha r/N) a_r^+ a_r. \tag{4.8}$$

Then we find from (7)

$$U^+ \Theta_\alpha U = \sum_{\gamma=1}^N a_{\gamma}^+ a_{\gamma+\alpha}. \tag{4.9}$$

Let us illustrate the preceding formulae for a specific example. We consider a cyclic chain of  $N$  atoms of mass  $M$  and springs  $f$  between neighbouring atoms, as drawn in figure 1. We characterise the displacements of the mass points from their equilibrium position by Cartesian mass-reduced coordinates  $X_r$ , and introduce the symmetry operation  $R_r(Q)$ ,

$$(R_r(Q)X_1) = X_{r+1}, \quad X_{N+1} \equiv X_1. \tag{4.10}$$



**Figure 1.** A cyclic chain with harmonic nearest-neighbour interaction and with a one-particle level placed in the centres between each pair of mass points. The one-particle states are characterised by a potential well having a single level.

The pure vibrational Hamiltonian then reads

$$H_0 = \frac{1}{2}\hbar \sum_{r=1}^N \left[ P_r^2 + \frac{f}{M} (X_{r+1} - X_r)^2 \right], \tag{4.11}$$

which is diagonalised by the normal coordinates  $Q_\gamma$

$$X_r = N^{-1/2} \sum_{\gamma=1}^N \exp(-2\pi i r \gamma / N) Q_\gamma, \quad P_r = N^{-1/2} \sum_{\gamma=1}^N \exp(+2\pi i r \gamma / N) P_\gamma. \tag{4.12}$$

This yields

$$H_0 = \frac{1}{2}\hbar \sum_{\gamma=1}^N [P_\gamma P_\gamma^+ + \Omega_\gamma^2 Q_\gamma Q_\gamma^+] \tag{4.13}$$

where

$$\Omega_\gamma^2 = 4 \frac{f}{M} \sin^2 2\pi \gamma / N, \quad \gamma = 1, 2, \dots, N. \tag{4.14}$$

We now supplement this model by  $N$  one-particle states  $|r\rangle$  which are assumed to be located respectively between two adjacent mass points such that their energy depends linearly on the coordinates  $(X_{r+1} - X_r)$ , and further on that there is an equal static transition probability from state  $|r\rangle$  to the states  $|r \pm 1\rangle$ . This is incorporated in the interaction Hamiltonian

$$\begin{aligned} W &= \frac{\hbar}{2} \Delta \sum_{r=1}^N [a_r^+ a_{r+1} + a_{r+1}^+ a_r] + \hbar D \sum_{r=1}^N a_r^+ a_r (X_{r+1} - X_r) \\ &= \frac{\hbar}{2} \Delta \sum_{r=1}^N [a_r^+ a_{r+1} + a_{r+1}^+ a_r] \\ &\quad - 2i N^{-1/2} \hbar D \sum_{r=1}^N \sum_{\gamma=1}^N a_r^+ a_r \exp[-2i\pi(r + \frac{1}{2})\gamma / N] Q_\gamma \sin(\pi\gamma / N). \end{aligned} \tag{4.15}$$

Employing (4.4), (4.5) and (4.7), we get after some rearrangement

$$\begin{aligned}
 U^+ W U &= \frac{\hbar}{2} \Delta \sum_{\gamma=1}^N a_{\gamma}^+ a_{\gamma} [\exp(i2\pi\gamma/N) R_1(Q) + \exp(-i2\pi\gamma/N) R_1^{-1}(Q)] \\
 &\quad + \frac{\hbar D}{\sqrt{N}} \sum_{\gamma=1}^N [\exp(-i2\pi\gamma/N) - 1] Q_{\gamma} \\
 &= \frac{1}{2} \hbar \Delta \sum_{\gamma=1}^N a_{\gamma}^+ a_{\gamma} [\exp(i2\pi\gamma/N) R_1(Q) + \exp(-i2\pi\gamma/N) R_1^{-1}(Q)] \\
 &\quad + \hbar D (X_1 - X_N)
 \end{aligned} \tag{4.16}$$

which is seen to be diagonal with respect to the  $N$ -level subsystem. Each of the  $N$  levels in the transformed picture is thus respectively attached to a different irreducible representation  $\Gamma_{\gamma}$  of the cyclic group.

Concluding this section we develop a convenient explicit representation of the basic group operator  $R_1(Q)$ . From (4.1) and (4.10) we have

$$R_1 X_r \equiv (R_1 X_r R_1^{-1}) R_1 = X_{r+1} R_1. \tag{4.17}$$

Inserting this in the inversion of (12),

$$Q_{\gamma} = N^{-1/2} \sum_{r=1}^N \exp(2\pi i r \gamma / N) X_r, \quad P_{\gamma} = N^{-1/2} \sum_{r=1}^N \exp(-2\pi i r \gamma / N) P_r, \tag{4.18}$$

we have

$$R_1 Q_{\gamma} = \exp(-2\pi i \gamma / N) Q_{\gamma} R_1, \quad R_1 P_{\gamma} = \exp(2\pi i \gamma / N) P_{\gamma} R_1. \tag{4.19}$$

Now, from the theory of unitary transformations (see a forthcoming book, Wagner 1984) it is known that an operator effect of this nature may be established by an operator of the form

$$R_1^{(\gamma)} = \exp[-(\pi\gamma/N)(P_{\gamma} Q_{\gamma} + Q_{\gamma} P_{\gamma})] \equiv e^{-S_{\gamma}}, \quad \gamma \neq N, \frac{1}{2}N. \tag{4.20}$$

This may be directly verified by forming the commutator expansion

$$R_1^{(\gamma)} Q_{\gamma} R_1^{(\gamma)-1} = Q_{\gamma} + [Q_{\gamma}, S_{\gamma}] + \dots \tag{4.21}$$

By means of definition (4.18) we have

$$Q_{\gamma}^+ = Q_{N-\gamma} \quad \text{and} \quad P_{\gamma}^+ = P_{N-\gamma} \tag{4.22}$$

and hence  $R_1^{(\gamma)} R_1^{(N-\gamma)}$  will always form a unitary operator if we exclude  $\gamma = N$  and  $\gamma = \frac{1}{2}N$ . For  $\gamma = N$  we have

$$R_1 Q_N = Q_N R_1 \tag{4.23}$$

whence we may choose

$$R_1^{(N)} = 1. \tag{4.24}$$

If  $N$  is an even number,  $\gamma$  may also assume the value  $\frac{1}{2}N$ ; then

$$R_1 Q_{(N/2)} = -Q_{(N/2)} R_1 \quad (\text{for } N \text{ even}). \tag{4.25}$$

To have a unitary operator also in this case, we make recourse to the inversion operator

form (2.20) of § 2 and choose

$$R_1^{(N/2)} = \exp[(i\pi/\Omega)_{(N/2)}(P_{(N/2)}^2 + \Omega_{(N/2)}^2 Q_{(N/2)}^2) - i\pi/2] \quad \text{for } N = 2n \quad (\text{even}). \tag{4.26}$$

Thus the total form of  $R_1$  in  $Q$  space is given in the unitary form

$$R_1(Q) = \exp\left(-\frac{\pi}{N} \sum_{\gamma=1}^{N-1} \gamma(P_\gamma Q_\gamma + Q_\gamma P_\gamma)\right) \quad \text{for } N = 2n + 1 \quad (\text{odd}) \tag{4.27}$$

or

$$R_1(Q) = \exp\left[\left(\frac{i\pi}{\Omega}\right)_{(N/2)} (P_{(N/2)}^2 + \Omega_{(N/2)}^2 Q_{(N/2)}^2) - i\pi/2 - \frac{\pi}{N} \sum_{\gamma=1}^{N-1} \gamma(P_\gamma Q_\gamma + Q_\gamma P_\gamma)\right] \quad \text{for } N = 2n \quad (\text{even}).$$

### 5. Application in quantum transport

In the translationally invariant systems, like the cyclic system of § 4, quantum transport is characterised by an occupation transfer within the  $N$ -level system from site  $r$  to site  $r'$ . Specifically, if occupation  $\langle n_r \rangle_t = \langle a_r^+ a_r \rangle_t$ , at site  $r$  at time  $t=0$  deviates from the thermal occupation  $\langle n_r \rangle_T = \text{Tr}(n_r \exp(-\beta H)) / \text{Tr} \exp(-\beta H)$ , then by means of the Kubo response formalism the decay to thermal equilibrium can be written in the form ( $\beta = k_B T$ )

$$\langle n_r \rangle_t = \langle n_r \rangle_T + \frac{\langle n_r \rangle_{t=0}}{\langle n_r \rangle_T} \int_{-\infty}^{+\infty} d\omega \frac{(e^{\beta\omega} - 1)}{\omega - i\varepsilon} \langle n_r; n_r \rangle_\omega^H e^{-i\omega t} \tag{5.1}$$

where  $\langle A; A \rangle_\omega^H$  denotes the ‘spectral function’, which is the Fourier transform of the autocorrelation function  $\langle n_r(0)n_r(t) \rangle^H$  with respect to the original Hamiltonian  $H = H_0 + W$ ,

$$\langle n_r(0)n_r(t) \rangle^H = \text{Tr}(e^{-\beta H} n_r(0)n_r(t)) / \text{Tr} e^{-\beta H}, \quad \beta = k_B T. \tag{5.2}$$

The decay process (1) involves all phenomenologically defined transport quantities, which accordingly may be derived from it. It thus turns out that the auto-correlation function (5.2) is the decisive quantity to be calculated. By way of the cyclic invariance property of the trace operation all factors of the latter may be subjected to a unitary transformation  $U^+AU$ , whence

$$\langle n_r(0)n_r(t) \rangle^H = \langle (U^+ n_r U)_{t=0} (U^+ n_r U)_t \rangle^{U^+ H U}. \tag{5.3}$$

In this manner any correlation function with respect to some original Hamiltonian  $H$  may be transformed to a correlation function of altered elements, which pertains to a transformed Hamiltonian  $H = U^+ H U$ . Employing the unitary transformation of the preceding two sections, we have from equations (4.7) and (4.8)

$$\langle n_r(0)n_r(t) \rangle^H = N^{-2} \sum_{\gamma\gamma'}^N \sum_{\gamma''\gamma'''}^N \exp[2i\pi(\gamma - \gamma' + \gamma'' - \gamma''')r/N] \langle (a_{\gamma'}^+ a_{\gamma''})_{t=0} (a_{\gamma'''}^+ a_{\gamma''})_t \rangle^{\tilde{H}} \tag{5.4}$$

where

$$\begin{aligned} \tilde{H} = & \frac{1}{2}\hbar \sum_{\gamma=1}^N [P_{\gamma}P_{\gamma}^+ + \Omega_{\gamma}^2 Q_{\gamma}^+ Q_{\gamma}] \\ & + \frac{1}{2}\hbar \sum_{\gamma=1}^N a_{\gamma}^{\dagger} a_{\gamma} [\exp(i2\pi\gamma/N)R_1(Q) + \exp(-i2\pi\gamma/N)R_1^{\dagger}(Q)] \\ & + \hbar \frac{D}{\sqrt{N}} \sum_{\gamma=1}^N [\exp(-i2\pi\gamma/N) - 1] Q_{\gamma} \end{aligned} \tag{5.5}$$

Since this Hamiltonian is diagonal with respect to the  $N$ -level subsystem, only those correlation functions of (5.4) will survive for which either  $\gamma = \gamma' = \gamma'' = \gamma'''$  or  $\gamma = \gamma''$ ,  $\gamma' = \gamma'''$ ,

$$\langle n_r(a)n_r(t) \rangle^H = \frac{1}{N} + \frac{1}{N^2} \sum_{\substack{\gamma, \gamma' \\ (\gamma \neq \gamma')}}^N \langle (a_{\gamma}^{\dagger} a_{\gamma'})_{t=0} (a_{\gamma}^{\dagger} a_{\gamma'})_t \rangle^{\tilde{H}} \tag{5.6}$$

and the remaining correlation functions are fully governed by the *vibrational sub-dynamics* for the respective  $\gamma$ -states. The treatment becomes more elegant if the Kubo formalism is not applied to the single site occupation operators  $n_r = a_r^{\dagger} a_r$ , but to the ‘occupation wave’ superposition defined by (4.8). But we will not pursue this further at this place. We only pay notice to a conspicuous result implicit in (5.6), which is the fact that there are precisely  $\frac{1}{2}N(N - 1)$  transport pathways. This follows from (5.6) by counting all combinations.

In summing up, there seem to be two main virtues of the presented unitary transformation with respect to the quantum transport problem. On the one hand it allows for a clear distinction and characterisation of single transport paths. On the other hand it establishes for each level of the  $N$ -level subsystem in the transformed space a specific and well defined vibrational dynamics, which may be solved to some desired degree of accuracy. The vibrational eigenstates pertaining respectively to a pair of different states  $\gamma$  and  $\gamma'$  of the  $N$ -level subsystem then completely determine the considered transport path.

**Appendix. Spin- $\frac{1}{2}$  formulation of the FG transformation**

The most compact way of describing a two-level system is by spin- $\frac{1}{2}$  operators, which are introduced in the following manner,

$$\begin{aligned} \sigma_x = \frac{1}{2}(a_1^{\dagger} a_2 + a_2^{\dagger} a_1), & \quad \sigma_y = (1/2i)(a_1^{\dagger} a_2 - a_2^{\dagger} a_1) \\ \sigma_z = \frac{1}{2}(a_1^{\dagger} a_1 - a_2^{\dagger} a_2), & \quad \sigma_{+} = a_1^{\dagger} a_2, \quad \sigma_{-} = a_2^{\dagger} a_1 \end{aligned} \tag{A1}$$

and satisfy the commutation relations

$$\begin{aligned} [\sigma_x, \sigma_y]_{-} &= i\sigma_z, & \text{cycl.} \\ [\sigma_z, \sigma_{\pm}]_{-} &= \pm\sigma_{\pm} \\ [\sigma_{+}, \sigma_{-}]_{-} &= 2\sigma_z \end{aligned} \tag{A2}$$

as well as the anticommutation relations

$$\begin{aligned}
 [\sigma_x, \sigma_y]_+ &= 0, & \text{cycl.} \\
 [\sigma_+, \sigma_-]_+ &= 1 \\
 [\sigma_{\pm}, \sigma_z]_+ &= 0
 \end{aligned}
 \tag{A3}$$

and have the further properties

$$\begin{aligned}
 \sigma_x^2 = \sigma_y^2 = \sigma_z^2 &= \frac{1}{4}, & \sigma_-^2 = \sigma_+^2 &= 0 \\
 \sigma_x \sigma_y &= \frac{1}{2} i \sigma_z, & \text{cycl.} \\
 \sigma_{\pm} \sigma_z &= \frac{1}{2} \pm \sigma_z.
 \end{aligned}
 \tag{A4}$$

Hamiltonian (5) then reads

$$H = H_0(P, Q) + \sigma_z A_u(Q) + A_g(Q) + \sigma_x B_g(Q) + i \sigma_y B_u(Q)
 \tag{A5}$$

where the abbreviations  $A = \frac{1}{2}(A_g + A_u)$ ,  $B = \frac{1}{2}(B_g + B_u)$  and

$$\begin{aligned}
 A_g &= A + (J_Q A), & A_u &= A - (J_Q A) \\
 B_g &= B + (J_Q B), & B_u &= B - (J_Q B)
 \end{aligned}
 \tag{A6}$$

have been used, which indicate that *g* and *u* respectively denote the ‘even’ and ‘odd’ parity parts of *A* and *B*,  $(J_Q A_g) = A_g$ ,  $(J_Q A_u) = -A_u$ , etc. Further, by means of (7) we must have

$$B_u^+(Q) = -B_u(Q),
 \tag{A7}$$

whereas  $A_g$ ,  $A_u$  and  $B_g$  are Hermitian. The FG transformation operator (2.15) then reads

$$U = (1/\sqrt{2})[\frac{1}{2} + i\sigma_y](1 - J_Q) + (1/\sqrt{2})[\sigma_z + \sigma_x](1 + J_Q)
 \tag{A8}$$

and its basic transformation properties read

$$\begin{aligned}
 U^+ f_g(Q) U &= f_g(Q), & U^+ f_u(Q) U &= 2\sigma_z f_u(Q) \\
 U^+ \sigma_z U &= \sigma_x, & U^+ \sigma_x U &= \sigma_z J_Q, & U^+ \sigma_y U &= -i\sigma_y J_Q
 \end{aligned}
 \tag{A9}$$

where the indices *g* and *u* respectively hint at ‘even’ and ‘odd’ parity functions. The transformed Hamiltonian reads

$$\tilde{H} \equiv U^+ H U = H_0(P, Q) + A(Q) + 2\sigma_z B(Q) J_Q,
 \tag{A10}$$

We point out that the Hamiltonian form (A5) has been chosen to be slightly more general than in the original paper of Fulton and Gouterman (1961), who have chosen  $A_g = 0$  and  $B_u = 0$ .

It further should be noted that there is no restriction on the number of vibrational coordinates, but it is beneficial to separate them in even and odd parity ones,  $Q_{gk}$ ,  $Q_{uk}$ ,

$$J_Q Q_{gk} = Q_{gk} J_Q, \quad J_Q Q_{uk} = -Q_{uk} J_Q.
 \tag{A11}$$

Then an explicit form for the inversion operator may be introduced,

$$J_Q = \exp\left[ i\pi \sum_k b_{uk}^+ b_{uk} \right]
 \tag{A12}$$

where  $b_{pk}^+$  and  $b_{pk}$  are the vibrational creation and annihilation operators,

$$b_{pk} = (2\Omega_{pk})^{-1/2}(\Omega_{pk}Q_{pk} + iP_{pk}), \quad p = g, u. \quad (\text{A13})$$

The form (A12) has already been proposed by Fulton–Gouterman (1961) and others.

Finally, it may be enlightening to write down one of the most simple forms of a FG Hamiltonian,

$$H = \hbar(P_g^2 + \Omega_g^2 Q_g^2 + P_u^2 + \Omega_u^2 Q_u^2) + \hbar D\sigma_z Q_u + \hbar\sigma_x(\Delta_0 + \Delta_g Q_g + \Delta_{gg} Q_g^2 + \Delta_{uu} Q_u^2) \quad (\text{A14})$$

where  $D$ ,  $\Delta_0$ ,  $\Delta_g$ ,  $\Delta_{gg}$ ,  $\Delta_{uu}$  are constants.

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