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An exponential alternative to the Fulton–Gouterman transformation

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Abstract. The Fulton–Gouterman transformation (FGT) diagonalises special electron–phonon systems with respect to the electronic subsystem, but the transformation operator cannot be written in a simple exponential form. An alternative unitary transformation, displaying a simple exponential form, is presented.

1. Introduction

Although the Fulton–Gouterman transformation (FG 1961) is somewhat exotic in its nature, it holds a great fascination for the electron–phonon coupling problem, since it allows for an exact diagonalisation with respect to the electronic subsystem, provided the system displays some specific mirror symmetry (which may be real or abstract). Originally Fulton and Gouterman (1961) devised the transformation for an electronic two-level system, but recently this has been generalised to N levels, provided the latter establish a regular representation of an Abelian group (Wagner 1984a).

There is some indication that the FGT may acquire the status of an *argumentum crucis* for the quantum-transport problem. Quite generally the phonon-assisted quantum-transport problem may be characterised as the decay of a quasi-continuous sequence of oscillator states associated with one particular state $|1\rangle$ of the 'light particle' (electron, proton, muon, lithium, etc.) into a sequence associated with another state $|2\rangle$ of the quantum particle. The basic intricacy may thus be viewed as the decay of an 'initial' continuous set of states into a final continuous set. The energy levels in the two sets are pairwise degenerate, whence any arbitrarily small transitive coupling constant necessitates a degenerate type of perturbative approach. In particular, any straightforward golden-rule type of calculation is not adequate. However, a simple and well defined calculation can be achieved if the two sequences of states are separated by means of a unitary transformation. For the background of the quantum-transport problem we refer to papers of Dick (1968, 1977), Flynn and Stoneham (1970) Shore and Sander (1973), Kagan and Klinger (1974), Kuhn and Wagner (1981), Junker and Wagner (1983) and to a forthcoming paper of the author (Wagner 1984b).

The FGT is a unitary transformation, but it is of a form which assumes a rather non-simple structure if it is written as an exponential operator $U = \exp S$. The purpose of the present paper is to present another unitary transformation, which has the property of diagonalising the electron–phonon Hamiltonian considered by Fulton and Gouterman (1961) with respect to the two-level electronic subsystem, but which in addition displays a simple exponential form.

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2. Notation

For lucidity we consider the most simple representative of those Hamiltonian forms which may be handled by FG transformations

$$H = H_{\text{osc}}(P, Q) + D\sigma_z Q_u + \sigma_x(\Delta_0 + \Delta_g Q_g + \Delta_{uu} Q_u^2) \tag{1}$$

where H_{osc} is an oscillatory Hamiltonian

$$H_{\text{osc}} = \tfrac{1}{2}\Omega_g(P_g^2 + Q_g^2) + \tfrac{1}{2}\Omega_u(P_u^2 + Q_u^2) \tag{2}$$

with an 'odd' coordinate Q_u ('ungerade') and an 'even' coordinate Q_g ('gerade'). We further employ a spin-$\frac{1}{2}$ representation of the electronic two-level system given by

$$\begin{aligned} \sigma_x &= \tfrac{1}{2}[|1\rangle\langle 1| - |2\rangle\langle 2|] \\ \sigma_y &= \tfrac{1}{2}[|1\rangle\langle 2| + |2\rangle\langle 1|] \\ \sigma_z &= (1/2\mathrm{i})[|1\rangle\langle 2| - |2\rangle\langle 1|], \end{aligned} \tag{3}$$

and the spin operators satisfy commutation and anticommutation relations of the form

$$\begin{aligned} [\sigma_x, \sigma_y]_- &= \mathrm{i}\sigma_z, \qquad \text{cycl.} \\ [\sigma_x, \sigma_y]_+ &= 0, \qquad \text{cycl.} \end{aligned} \tag{4}$$

and have the further properties

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \tfrac{1}{4}. \tag{5}$$

We introduce a reflection operator J_Q ('inversion') in Q_u–P_u space with the properties

$$\begin{aligned} J_Q Q_u &= -Q_u J_Q, \qquad & J_Q P_u &= -P_u J_Q \\ J_Q Q_g &= Q_g J_Q, \qquad & J_Q P_g &= P_g J_Q \end{aligned} \tag{6}$$

and

$$J_Q^+ = J_Q^{-1} = J_Q, \qquad J_Q^2 = 1. \tag{7}$$

This operator may be written in the explicit form

$$J_Q = \exp[\mathrm{i}\pi(P_u^2 + Q_u^2 - \tfrac{1}{2})], \tag{8}$$

but we will only need its properties (6). The FG is defined by the unitary operator

$$U_{\text{FG}} = (1/\sqrt{2})[\tfrac{1}{2} + \mathrm{i}\sigma_y](1 - J_Q) + (1/\sqrt{2})[\sigma_z + \sigma_x](1 + J_Q) \tag{9}$$

and it transforms the Hamiltonian into the form

$$T_{\text{FG}}\colon \tilde{H} \equiv U_{\text{FG}}^+ H U_{\text{FG}} = H_{\text{osc}} + \tfrac{1}{2}DQ_u + \sigma_z(\Delta_0 + \Delta_g Q_g + \Delta_{uu} Q_u^2) J_Q(P_u, Q_u). \tag{10}$$

Considering $\Delta_0, \Delta_g, \Delta_{uu}$ as perturbation parameters the zero-order eigenfunctions of the transformed Hamiltonian read

$$\tilde{\psi}^{(0,\text{FG})}_{\pm\frac{1}{2},m_g,m_u} \equiv T_{\text{FG}} : \psi^{(0,\text{FG})}_{\pm\frac{1}{2},m_g,m_u} \equiv U^+_{\text{FG}} \psi^{(0,\text{FG})}_{\pm\frac{1}{2},m_g,m_u} = |\pm\tfrac{1}{2}\rangle \Phi^{(0)}_{m_g}(Q_g) \Phi^{(0)}_{m_u}(Q_u + D/2) \tag{11}$$

where $\Phi^{(0)}_m(Q)$ is the harmonic oscillator eigenfunction and $|\pm\frac{1}{2}\rangle$ are the two spin statevectors. Inverting equation (11) we have for the original zero-order eigenfunctions

$$\psi^{(0,\text{FG})}_{\pm\frac{1}{2},m_g,m_u} = (1/\sqrt{2}) \Phi^{(0)}_{m_g}(Q_g)[|+\tfrac{1}{2}\rangle \Phi^{(0)}_{m_u}(Q_u + D/2) \pm (-1)^{m_u} |-\tfrac{1}{2}\rangle \Phi^{(0)}_{m_u}(Q_u - D/2)] \tag{12}$$

where the property

$$J_Q \Phi^{(0)}_{m_u}(Q_u + D/2) = (-1)^{m_u} \Phi^{(0)}_{m_u}(Q_u - D/2) \tag{13}$$

has been employed. From equation (12) we observe that the 'natural' zero-order wavefunctions of the FG-transformed Hamiltonian (10) turn out to be the properly symmetrised (which is parity ordered) zero-order wavefunctions of the original Hamiltonian and thus may be used as a base for non-degenerate perturbation theory.

3. Alternative transformation

We now discuss a transformation of the form

$$U = e^S, \qquad S = \mathrm{i}(\pi/2)\sigma_y J_Q, \qquad S^2 = -(\pi/4)^2, \tag{14}$$

which may also be written in the non-exponential form

$$U = (1/\sqrt{2})(1 + 2\mathrm{i}\sigma_y J_Q) \tag{14a}$$

where J_Q is the reflection operator as defined by equations (6). We evaluate the transformation properties of U by summing up the commutator expansion

$$T\colon A \equiv U^+ A U = A + [A, S] + (1/2!)[[A, S], S] + \ldots \tag{15}$$

The basic commutators read

$$\left.\begin{aligned} &[\sigma_z, S] = (\pi/2)\sigma_x J_Q \\ &[\sigma_x, S] = -(\pi/2)\sigma_z J_Q \\ &[Q_u, S] = \mathrm{i}\pi\sigma_y Q_u J_Q \\ &[Q_u J_Q, S] = \mathrm{i}\pi\sigma_y Q \end{aligned}\right. \tag{16}$$

from which the respective commutator series are easily found to be

$$\left.\begin{aligned} &T\colon \sigma_z \equiv \sigma_x J_Q \\ &T\colon \sigma_x = -\sigma_z J_Q \\ &T\colon Q_u = 2\mathrm{i}\sigma_y Q_u J_Q \\ &T\colon (Q_u\sigma_z) = Q_u\sigma_z \\ &T\colon P_u = 2\mathrm{i}\sigma_y P_u J_Q \end{aligned}\right. \tag{17}$$

whence the transformed Hamiltonian (1) assumes the form

$$T\colon H = H_{\mathrm{osc}} + D\sigma_z Q_u - \sigma_z(\Delta_0 + \Delta_g Q_g + \Delta_{uu} Q_u^2) J_Q(P_u, Q_u) \tag{18}$$

which again is seen to be diagonal with respect to the two-level subsystem (pseudo-spin system), but the diagonality is of a different make from the one established by the FGT. Specifically, the oscillatory displacement term $D\sigma_z Q_u$ may now have positive and negative prefactors $\pm D/2$ for $\sigma_z = \pm\frac{1}{2}$. Thus for $\Delta_0 = \Delta_g = \Delta_{uu} = 0$ the eigenvectors of the transformed Hamiltonian (18) read

$$\tilde{\psi}^{(0)}_{\pm\frac{1}{2}, m_g, m_u} \equiv U^+ \psi^{(0)}_{\pm\frac{1}{2}, m_g, m_u} = |\pm\tfrac{1}{2}\rangle \Phi^{(0)}_{m_g}(Q_g) \Phi^{(0)}_{m_u}(Q_u \pm D/2)] \tag{19}$$

whence the correct original eigenfunctions must be taken as

$$\psi^{(0)}_{\pm\frac{1}{2},m_g,m_u} \equiv U\tilde{\psi}^{(0)}_{\pm\frac{1}{2},m_g,m_u} = (1/\sqrt{2})\Phi^{(0)}_{m_g}(Q_g)[|\pm\tfrac{1}{2}\rangle\Phi^{(0)}_{m_u}(Q_u\pm\tfrac{1}{2})\mp|\mp\tfrac{1}{2}\rangle(-1)^{m_u}\Phi^{(0)}_{m_u}(Q_u\mp\tfrac{1}{2})] \tag{20}$$

which again is the basis (12), as expected, but it is now the $\sigma_z=+\frac{1}{2}$ states of $T:H$ which denote the 'odd' parity states and the $\sigma_z=-\frac{1}{2}$ states pertain to 'even' parity, whereas in the FG case (see (12)) the association is the other way around.

4. Generalisation

As in the Fulton–Gouterman case the presented transformation is easily generalised to the multimode case

$$U=e^S, \qquad S=\mathrm{i}(\pi/2)\sigma_y J_Q, \qquad J_Q=\exp\left(\mathrm{i}\pi\sum_k(P_{uk}^2+Q_{uk}^2-\tfrac{1}{2})\right) \tag{21}$$

and the most general Hamiltonian which may be brought to diagonal form with respect to the spin operators reads ($p=u, g$)

$$\begin{aligned}H=\sum_{p,k}\tfrac{1}{2}\Omega_{pk}[P_{pk}^2+Q_{pk}^2]&+\tfrac{1}{2}[A(Q,P)+(J_QA(Q,P)J_Q)]\\&+\sigma_z[A(Q,P)-(J_QA(Q,P)J_Q)]\\&+\sigma_x[B(Q,P)+(J_QB(Q,P)J_Q)]\\&+\mathrm{i}\sigma_y[B(Q,P)-(J_QB(Q,P)J_Q)]\end{aligned} \tag{22}$$

where $A(Q,P)$ and $B(Q,P)$ are arbitrary functions of Q_{pk}, P_{pk}, but such that

$$A^+=A, \qquad J_QB(Q,P)=B(Q,P)^+J_Q. \tag{23}$$

This is just the same as in the FG case and for details we refer to the earlier paper of the author (Wagner 1984a). The generalised transformation properties read

$$T:\sigma_z\equiv\sigma_xJ_Q, \qquad T:\sigma_x=-\sigma_zJ_Q, \qquad T:\sigma_y=\sigma_y, \qquad T:F_g(P,Q)=F_g(P,Q), \qquad T:F_u(P,Q)=2\mathrm{i}\sigma_yF_u(P,Q)J_Q, \tag{24}$$

where F_g and F_u respectively is an 'even' or an 'odd' function of Q_{pk}, P_{pk},

$$J_qF_g=F_gJ_Q, \qquad J_QF_u=-F_uJ_Q. \tag{25}$$

5. Conclusion

We have learned that in the Fulton–Gouterman approach the $\sigma_z=\frac{1}{2}$ zero-order wavefunctions (see equation (12)) are associated with the even parity functions in the original frame, whereas in our transformation $\sigma_z=\frac{1}{2}$ associates with the odd parity original zero-order functions (see equation (20)). Since there are only two spin-levels as well as two irreducible representations of the inversion group, one may conclude that the FG transformation and ours constitute the only two transformations which diagonalise the Hamiltonian with respect to the spin subsystem.

If one has an N-level subsystem which is coupled to an oscillatory system, and if the N levels establish a regular representation of an Abelian group, it has been shown earlier (Wagner 1984a) that a generalisation of the FGT can be found which again diagonalises the Hamiltonian with respect to the N-level subsystem. In this case also alternative transformations may be devised in the spirit of the above development. Accordingly any zero-order sequence of oscillatory states associated with a definite level $|u\rangle$ of the N-level subsystem in the transformed frame may be associated with any of the N-irreducible representations of the original frame, and one may thus expect $N!$ unitary transformations which accomplish a diagonalisation with respect to the N-level subsystem. But it is not yet known whether any of these may be written in a simple exponential form.

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