

Fulton-Gouterman ground states for soft tunneling systems

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The two-site and periodic N -site model of a tunneling particle in a "soft" surrounding (phonons, electronic excitations) is considered. The emphasis is on the Fulton-Gouterman (FG) transcription of these models, which lays open a peculiar topological property. The latter always supplements any symmetry-broken bath wave function by mirror images of finite weight in other spatial regions. In this manner an antilocalizing tendency emerges. We analyze this tendency and show that localization, if defined in the very strict sense, is overcome by the FG topology. From this result we deduce a temporal limitation for the stability of a strictly localized state, which, however, does not seem to be in conflict with the particular kind of symmetry breaking discussed in recent literature.

I. INTRODUCTION

Much discussion has grown up recently about the transport behavior of a tunneling particle coupled to a heat bath of harmonic oscillators. In a real physical system the background oscillators may represent the phonon system (phonon-assisted quantum diffusion) or may be reviewed as representations of other elementary excitations, e.g., excitonic, electronic, spin excitations, etc. For a good review of modern work we refer to the articles of Leggett *et al.*^{1,2} Specifically these approaches have pondered a particular coupling setup known as Ohmic dissipation, and it has been shown that this coupling law leads to a particular kind of symmetry-broken ground state, if the coupling strength exceeds a critical value.²⁻⁴

Further insight into the problem may be gained from an approach which up to the present has not been exploited very much. As shown by Fulton and Gouterman⁵ a two-level system (=two-site system), which is coupled to an oscillatory system in such a manner that the total Hamiltonian displays a reflection symmetry, may be subjected to a unitary transformation (FG transformation),⁶ which diagonalizes the system with respect to the two-level subsystem. This method can be generalized to the N -site situation,⁷ if the symmetry of the system is governed by an Abelian group.

It was Shore and Sander⁸ who first employed the FG transformation as a tool to investigate the localization problem in a mode-assisted transfer process (excitonic self-trapping). They have found that the vibrational part of the ground-state wave function pertaining to the left or right site is given, respectively, as a displaced oscillator function with a small supplement of its mirror image. The latter establishes mode mixing in the oscillatory bath and makes the self-trapping process a smooth one, which is in contrast to a sharp transition as surmised earlier.

In the present work we apply the FG transformation to the two most prominent tunneling models considered so far—the two-site and the spatially periodic N -site model with local bath coupling, respectively. We first give a brief review of the generalized Fulton-Gouterman transcription of a Hamiltonian displaying an Abelian symme-

try. We then apply this transcription to a two-site tunneling center and evaluate the ground-state energy-expectation value by use of a displaced oscillator trial wave function which subsequently is supplemented by a mirror-image contribution. Thereafter we turn to the FG equations of the periodic site model and again employ a displaced oscillator trial form. We finally make some remarks about the spin-bath models which correspond to the oscillatory bath models considered before.

The main emphasis of this work is onto the *peculiar topological properties* displayed by the Fulton-Gouterman Hamiltonians, which have an impact onto the spatial extension of the solutions.

II. GENERALIZED FULTON-GOUTERMAN TRANSFORMATION

For later reference we briefly review the background of the FG concept.⁷ We consider N -particle states $|m\rangle$ with tunneling between nearest sites m and $m + \mu$ and a linear coupling to a bath of oscillators. We require that the system displays the symmetry of an Abelian group (elements R_m) such that

$$|m\rangle = R_m |0\rangle, \quad R_m = (R_1)^m. \quad (1)$$

The Hamiltonian then reads

$$H = -\frac{\Delta}{g} \sum_{\mu, m} (|m\rangle \langle m + \mu| + \text{H. c.}) + \frac{1}{2} \sum_{\Gamma, \lambda} \Omega_{\Gamma\lambda} (P_{\Gamma\lambda} P_{\Gamma\lambda}^* + Q_{\Gamma\lambda} Q_{\Gamma\lambda}^*) + \frac{1}{2} \sum_m |m\rangle \langle m| R_m \left[\sum_{\Gamma, \lambda} \Omega_{\Gamma\lambda} D_{\Gamma\lambda} Q_{\Gamma\lambda}^* \right], \quad (2)$$

where a linear coupling to a bath has been assumed, which for convenience is written as a superposition of normal coordinate couplings. $\{Q_{\Gamma\lambda}, P_{\Gamma\lambda}\}$ are the symmetry-adapted normal coordinates, (branch λ , irreducible representation Γ), such that

$$R_m Q_{\Gamma\lambda} = \chi_{\Gamma}^*(R_m) Q_{\Gamma\lambda}. \quad (3)$$

$\chi_\Gamma(R_m)$ is the character of element R_m in the irreducible representation Γ . g is the number of nearest neighbors μ . We note the symmetry requirement

$$[H, R_m] = 0. \quad (4)$$

The particles states $|m\rangle$ constitute an N -dimensional (regular) representation in which each of the irreducible representations appears once. Since each eigenfunction of the Hamiltonian must be an irreducible representation of the group, we may write it in the Wigner form

$$\psi^{(\Gamma)} = \frac{1}{\sqrt{N}} \sum_m \chi_\Gamma(R_m) R_m (|0\rangle \Phi^{(\Gamma)}(Q)), \quad (5)$$

which we insert in the Schrödinger equation. Employing the orthonormality of states $|m\rangle$ and the orthogonality theorem of group theory we find the Fulton-Gouterman equations⁷

$$\begin{aligned} H_{\text{FG}}^{(\Gamma)} \Phi^{(\Gamma)}(Q) &= \left[H_{\text{bath}} + \frac{1}{2} \sum_{\Gamma', \lambda} \Omega_{\Gamma' \lambda} D_{\Gamma' \lambda} Q_{\Gamma' \lambda}^* \right. \\ &\quad \left. - \frac{\Delta}{g} \sum_{\mu} \chi_\Gamma(R_\mu) R_\mu \right] \Phi^{(\Gamma)}(Q) \\ &= E^{(\Gamma)} \Phi^{(\Gamma)}(Q), \end{aligned} \quad (6)$$

$$H_{\text{bath}} = \frac{1}{2} \sum_{\Gamma', \lambda} \Omega_{\Gamma' \lambda} (P_{\Gamma' \lambda} P_{\Gamma' \lambda}^* + Q_{\Gamma' \lambda} Q_{\Gamma' \lambda}^*), \quad (7)$$

which is a *rigorous substitute* of the original Schrödinger equation. In this manner the original eigenvalue problem is replaced by N -eigenvalue equations, each referring to a single irreducible representation, respectively, but each pertaining to the vibrational subspace only. It is this reduction which represents the main virtue of the Fulton-Gouterman transcription and offers both computational advantages as well as physical insights. In particular it is the last term of $H_{\text{FG}}^{(\Gamma)}$ which establishes a *specific topological quality*, since it has the effect of supplementing each wave function by reflected contributions, which are centered in different spatial regions. These are generated by the symmetry operators R_μ , which in our discussion below will be either reflectional or translational operators. Specifically for the ground state $\Phi_0(Q)$ we find [$\Gamma = E$, $\chi_E(R_\mu) = 1$],

$$\begin{aligned} H_{\text{FG}}^{(\Gamma=E)} \Phi_0^{(\Gamma=E)}(Q) &= \left[H_{\text{bath}} + \frac{1}{2} \sum_{\Gamma', \lambda} \Omega_{\Gamma' \lambda} D_{\Gamma' \lambda} Q_{\Gamma' \lambda}^* \right. \\ &\quad \left. - \frac{\Delta}{g} \sum_{\mu} R_\mu \right] \Phi_0^{(\Gamma=E)}(Q) \\ &= E_0^{(\Gamma=E)} \Phi_0^{(\Gamma=E)}(Q). \end{aligned} \quad (8)$$

For completeness we note that the FG equations can also be established by means of a unitary transformation U_{FG} . For this we refer to the original papers.^{5,7}

III. TWO-SITE TUNNELING CENTER COUPLED TO A BATH OF OSCILLATORS

We idealize the particle system to one of two states only, $|r\rangle$ and $|l\rangle$, which now constitute the regular base

of the system $\{|m\rangle\}$.⁹ We also assume the system to be governed by reflection symmetry (a simple case of Abelian symmetry) generated by a single element G , which is a reflection operator, $\{R_m\} = \{G, G^2 = E\}$. The group has two irreducible representations $\Gamma = g, \mu$, which designate the two parities $p = \pm 1$, and the characters are $\chi_p(G) = p$, $\chi_p(E) = 1$. The Hamiltonian then reads

$$\begin{aligned} H &= -\Delta \frac{1}{2} (|l\rangle \langle r| + |r\rangle \langle l|) \sigma_x + \frac{1}{2} \sum_{\Gamma, \lambda} \Omega_{\Gamma \lambda} (P_{\Gamma \lambda}^2 + Q_{\Gamma \lambda}^2) \\ &\quad + \frac{1}{2} (|l\rangle \langle l| - |r\rangle \langle r|) \sigma_z \sum_{\lambda} \Omega_{u \lambda} D_{u \lambda} Q_{u \lambda}, \end{aligned} \quad (9)$$

where $\{Q_{u \lambda}, P_{u \lambda}\}$ are odd-parity modes and where we have used the pseudospin notation

$$\begin{aligned} \sigma_x &= \frac{1}{2} (|l\rangle \langle r| + |r\rangle \langle l|), \\ \sigma_z &= \frac{1}{2} (|l\rangle \langle l| - |r\rangle \langle r|), \\ \sigma_y &= \frac{1}{2i} (|l\rangle \langle r| - |r\rangle \langle l|). \end{aligned} \quad (10)$$

We remark that the even modes $Q_{g \lambda}$ have the prefactor $|1\rangle \langle 1| + |r\rangle \langle r| = 1$, hence there is no coupling to them. Therefore we henceforth may disregard them and drop the index u attached to the bath coordinates. We define

$$H_{\text{bath}} = \frac{1}{2} \sum_{\lambda} \Omega_{\lambda} (P_{\lambda}^2 + Q_{\lambda}^2). \quad (11)$$

The Wigner formula (5) amounts to a parity ordering of the wave functions

$$\psi^{(\Gamma)} = \frac{1}{\sqrt{2}} [|l\rangle \Phi^{(\Gamma)}(Q) + p |r\rangle G \Phi^{(\Gamma)}(Q)]. \quad (12)$$

Therefore we get only two FG equations

$$\begin{aligned} H_{\text{FG}}^{(\Gamma)} \Phi^{(\Gamma)}(Q) &= \left[H_{\text{bath}} + \frac{1}{2} \sum_{\lambda} \Omega_{\lambda} D_{\lambda} Q_{\lambda} - p \frac{\Delta}{2} G \right] \Phi^{(\Gamma)}(Q) \\ &= E^{(\Gamma)} \Phi^{(\Gamma)}(Q). \end{aligned} \quad (13)$$

In passing we note that these equations could have been found also via a unitary transformation defined by the operator

$$\begin{aligned} U_{\text{FG}} &= \frac{1}{\sqrt{2}} (|l\rangle \langle l| G_Q + |r\rangle \langle r| - |r\rangle \langle l| \\ &\quad + |l\rangle \langle r| G_Q), \end{aligned} \quad (14)$$

which is the form used by Shore and Sander.⁸ G_Q is the reflection operator in the vibrational subspace. For the trial even-ground-state wave function ($\Gamma = g, p = 1$) we choose a product of displaced oscillator wave functions

$$\Phi_0^{(g)}(Q) = \prod_{\lambda} \pi^{-1/4} \exp \left[-\frac{1}{2} \left[Q_{\lambda} + \frac{\delta_{\lambda}}{2} \right]^2 \right], \quad (15)$$

where δ_{λ} are variational parameters. Inserting (15) into (13) we are confronted with the overlap integral

$$\mathcal{L} = \langle \Phi_0^{(g)}(\mathcal{Q}) | G \Phi_0^{(g)}(\mathcal{Q}) \rangle = \exp \left[-\frac{1}{4} \sum_{\lambda} \delta_{\lambda}^2 \right], \quad (16)$$

which characterizes the ‘‘Debye-Waller’’ screening. The ground-state energy is then given by

$$E_0^{(g)} = \frac{1}{2} \sum_{\lambda} \Omega_{\lambda} - \frac{1}{8} \sum_{\lambda} \Omega_{\lambda} (2D_{\lambda} - \delta_{\lambda}) \delta_{\lambda} - \frac{\Delta}{2} \mathcal{L}. \quad (17)$$

A vanishing overlap integral would mean localization in the two-site system, since in this case the lowest state of odd parity would be degenerate with the even-parity ground state. Hence a symmetry-broken state, for example $|r\rangle \Phi_0(\mathcal{Q})$, would become a good eigenfunction of Hamiltonian (9). We now specify our calculation to a coupling setup of power-law form

$$\Omega_{\lambda}^2 D^2(\Omega_{\lambda}) \rho(\Omega_{\lambda}) = 4\alpha \Omega_D x_{\lambda}^m, \quad x_{\lambda} = \frac{\Omega_{\lambda}}{\Omega_D}, \quad (18)$$

where $\rho(\Omega_{\lambda})$ is the frequency density in the oscillatory system and Ω_D is the Debye frequency. Two power laws have been considered as physically significant. $m=1$ characterizes the ‘‘Ohmic dissipation’’ case, which mainly plays a role in one-dimensional systems or in systems where electronic excitations across the Fermi surface play the role of the bath.¹⁰ Case $m=3$ is often taken for three-dimensional tunneling in nonmetallic systems.

(1) In a naive approximation we first choose $\delta_{\lambda} = D_{\lambda}$ and therefore we find from (16)

$$\begin{aligned} \mathcal{L}^{(0)} &= \exp \left[-\frac{1}{4} \sum_{\lambda} D_{\lambda}^2 \right] \\ &= \exp \left[-\frac{1}{4} \int_0^{\Omega_D} d\Omega \rho(\Omega) D^2(\Omega) \right] \\ &= \exp \left[-\alpha \int_0^1 dx x^{m-2} \right] = \exp \left[-\frac{\alpha}{m-1} \right]. \end{aligned} \quad (19)$$

The divergence for $m=1$ (Ohmic dissipation), also called infrared divergence, leads to a vanishing overlap and hence to localization of the particle.

(2) Minimizing the energy with respect to the displacements leads to a self-consistency equation

$$\delta_{\lambda} = \frac{\Omega_{\lambda} D_{\lambda}}{\Omega_{\lambda} + \Delta \mathcal{L}(\delta_{\lambda})}, \quad (20)$$

where \mathcal{L} is given by Eq. (16). By means of the ansatz

$$\Lambda = \frac{\Delta}{\Omega_D} \mathcal{L}, \quad (21)$$

Eq. (20) is transmuted into a self-consistency equation for Λ ,

$$\Lambda = \frac{\Delta}{\Omega_D} \exp \left[-\alpha \int_0^1 dx \frac{x^m}{(x+\Lambda)^2} \right]. \quad (22)$$

Specifically for the Ohmic dissipation case ($m=1$) this reads

$$\Lambda = \frac{\Delta}{\Omega_D} \left[\frac{\Lambda}{1+\Lambda} \exp \left[\frac{1}{1+\Lambda} \right] \right]^{\alpha}. \quad (23)$$

This equation is seen to yield nonlocalized solutions $\Lambda \neq 0$ only for coupling constants $\alpha < \alpha_{cr} = 1$, provided we choose $\Delta e / \Omega_D < 1$. (We do not consider the less interesting case $\Delta e / \Omega_D \geq 1$). If α exceeds the critical value, the solution jumps to localization. This behavior is shown in Fig. 1.

(3) We now take account of the remarkable topological property of the FG Hamiltonian which is established by the reflective term of Eq. (13). Operating the FG Hamiltonian onto the wave function always yields a small quantity ($\sim \Delta$) of the mirror image of this wave function. Using this observation, first made by Shore and Sander⁷ in the context of exciton self-trapping, we supplement the displaced oscillator wave function $\Phi_0^{(g)}(\mathcal{Q})$ by an admixture of its mirror image ($\sim \gamma$) and employ the trial wave function

$$\begin{aligned} \Phi_0^{(\text{ref})}(\mathcal{Q}) &= (1 + 2\gamma \mathcal{L} + \gamma^2)^{-1/2} \\ &\times [\Phi_0^{(g)}(\mathcal{Q}) + \gamma G \Phi_0^{(g)}(\mathcal{Q})], \end{aligned} \quad (24)$$

where γ is a new variational parameter. This reflective ansatz (24) cannot be written in product form and thus establishes mode mixing in the bath. To get a perception of the geometrical meaning of this ansatz, we return to the original form of the wave function for $p=1$, which is given by expression (12)

$$\begin{aligned} \psi_0^{(g)} &= \frac{1}{\sqrt{2}} (1 + 2\gamma \mathcal{L} + \gamma^2)^{-1/2} \\ &\times \{ [\Phi_0^{(g)}(\mathcal{Q}) + \gamma G \Phi_0^{(g)}(\mathcal{Q})] |l\rangle \\ &+ [G \Phi_0^{(g)}(\mathcal{Q}) + \gamma \Phi_0^{(g)}(\mathcal{Q})] |r\rangle \}. \end{aligned} \quad (25)$$

Without the reflective part ($\gamma=0$), $\psi_0^{(g)}$ is a symmetrized linear combination of localized states (states of broken symmetry) shown in Fig. 2 by solid lines. Roughly speaking, in this wave function the left state $|1\rangle$ of the particle is attached to an oscillatory function which is displaced

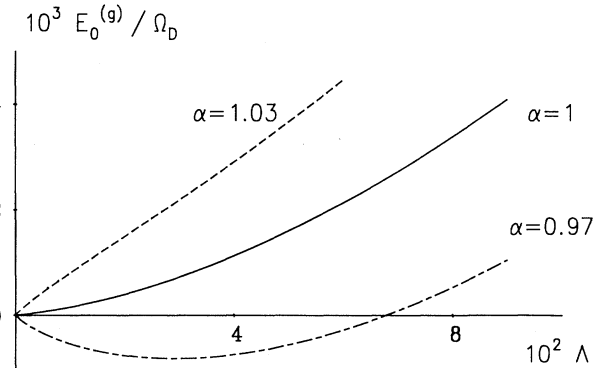


FIG. 1. Ground-state energy $E_0^{(g)}$ with a simple displaced oscillatory ansatz as a function of the localization parameter Λ ($\Lambda=0$, localization). Coupling law: Ohmic dissipation ($m=1$). $\alpha=0.97, 1.03$ and $\alpha=\alpha_{cr}=1$, $\Delta/\Omega_D=0.36$.

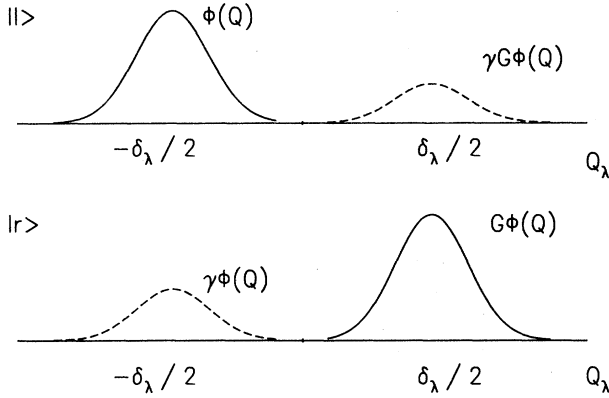


FIG. 2. Geometrical illustration of the wave function. Solid lines: Simple displaced oscillatory part ($\gamma=0$). Dashed lines: Supplements of the reflective ansatz ($\gamma \neq 0$) establish a mode mixing.

to the left, and similarly the right state $|r\rangle$ is attached to an oscillatory wave function displaced to the right. The supplements which are introduced by the reflective ansatz (24) and (25) are illustrated by dashed lines. This most clearly exemplifies the effect of the specific topological property inherent in the FG Hamiltonian (13). There is, as one might say, a reflection of the oscillatory wave function across the barrier. Minimizing the energy with respect to the admixture parameter γ , and introducing the simplified ansatz

$$\delta_\lambda = \frac{\Omega_\lambda D_\lambda}{\Omega_\lambda + \Omega_D \Lambda}, \quad (26)$$

we find for the ground-state energy

$$E_0^{(g)} = \frac{1}{2} \sum_\lambda \Omega_\lambda - \frac{1}{2} \Omega_D \frac{\alpha}{1 + \Lambda} - \frac{1}{2} \Delta e^\alpha \Lambda^\alpha + \frac{\Delta}{8\alpha} \frac{\Delta}{\Omega_D} (\Lambda \ln \Lambda - 1) \text{ for } \Lambda \ll 1 \quad (27)$$

in leading order for small values of Λ , where Λ is the remaining global variational parameter. In this manner a logarithmic barrier against localization is established if localization is defined in the strict sense. This is shown in Fig. 3, where even for $\alpha > \alpha_{cr}$ there is a logarithmic descent of $E_0^{(g)}$ immediately above $\Lambda=0$ which establishes a minimum at $\Lambda > 0$. The dashed line in Fig. 3 illustrates the energy $E_0^{(g)}$ which we get by varying only the displacements, taking $\gamma=0$. For $(\Delta/\Omega_D) \ll 1$, $\alpha > 1$ minimization of Eq. (27) yields

$$\Lambda = \exp[-(2\alpha\Omega_D/\Delta)^2] \quad (28)$$

from which we find the ground-state energy

$$E_0^{(g)} = E_{loc} - \frac{1}{2} \Delta e^\alpha \exp\left[-4\alpha^3 \left(\frac{\Omega_D}{\Delta}\right)^2\right], \quad (29)$$

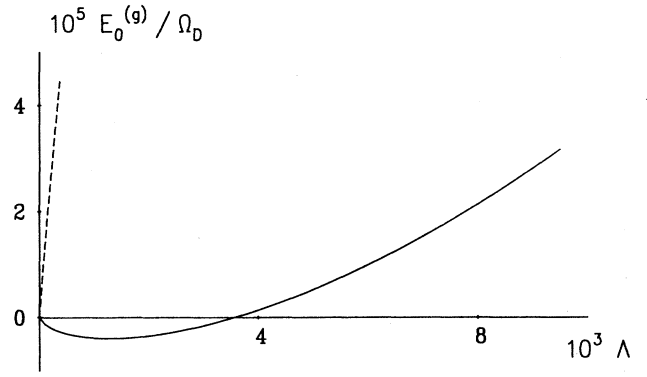


FIG. 3. Ground-state dependence $E_0^{(g)}$ on the localization parameter Λ ($\Lambda=0$, localization) in the case of the reflective ansatz ($\gamma \neq 0$, solid line) and in the case of the ansatz without reflective supplement ($\gamma=0$, dashed line). Coupling law: Ohmic dissipation ($m=1$); $\alpha=1.03 > \alpha_{cr}$, $\Delta/\Omega_D=0.36$.

where E_{loc} denotes the energy of the localized state ($\Lambda=0$),

$$E_{loc} = \frac{1}{2} \sum_\lambda \Omega_\lambda - \frac{1}{2} \alpha \Omega_D - \frac{\Delta^2}{8\alpha \Omega_D}. \quad (30)$$

IV. MULTISITE PERIODIC ARRAY OF ONE-PARTICLE STATES COUPLED TO A BATH OF OSCILLATORS

Another simple Abelian group, and simultaneously the group of greatest physical interest, is the translational group. For lucidity we confine ourselves to the one-dimensional translational group, which, by imposing periodic boundary conditions, is the cyclic group generated by one single element,

$$R_r = (R_1)^r, \quad (R_1)^N = E. \quad (31)$$

The irreducible representations of the cyclic group are given by $\Gamma = k = 0, \pm 1, \pm 2, \dots, \pm N/2$ with characters

$$\chi_k(R_r) = \exp\left[i \frac{2\pi}{N} kr\right], \quad (32)$$

where $k=0$ denotes the unity representation. We thus specify our calculation to a one-dimensional cyclic chain of particle sites with nearest-neighbor tunneling interaction ($\mu=1, -1$). The Hamiltonian reads

$$H = \frac{1}{2} \sum_q \Omega_q (P_q P_{-q} + Q_q Q_{-q}) - \frac{\Delta}{2} \sum_m (|m\rangle \langle m+1| + |m+1\rangle \langle m|) + \frac{1}{2} \sum_m |m\rangle \langle m| R_m \left[\sum_q \Omega_q D_q Q_{-q} \right], \quad (33)$$

where we have confined ourselves to a simple branch of

normal modes $\Gamma = q = 0, \pm 1, \pm 2, \dots, \pm N/2$, and we henceforth drop the index λ . For our practical computation we will again employ a power-law strength function

$$\Omega_q^2 D^2(\Omega_q) \rho(\Omega_q) = 4\alpha \Omega_D \left[\frac{\Omega_q}{\Omega_D} \right]^m \quad (34)$$

in accordance with Eq. (18). The Wigner prescription (5)

for the general group-theoretical form of eigenfunctions now leads to the Bloch functions

$$\psi^{(k)} = \frac{1}{\sqrt{N}} \sum_m \exp \left[i \frac{2\pi}{N} km \right] |m\rangle R_m \Phi^{(k)}(Q). \quad (35)$$

Following the general argumentation of Sec. II we find for the N FG equations

$$\begin{aligned} H_{\text{FG}}^{(k)} \Phi^{(k)}(Q) &= \left[\frac{1}{2} \sum_q \Omega_q (P_q P_{-q} + Q_q Q_{-q}) + \frac{1}{2} \sum_q \Omega_q D_q Q_{-q} - \frac{\Delta}{2} (e^{i(2\pi/N)k} R_1 + e^{-i(2\pi/N)k} R_{-1}) \right] \Phi^{(k)}(Q) \\ &= E^{(k)} \Phi^{(k)}(Q). \end{aligned} \quad (36)$$

We again choose a product of displaced oscillator wave functions as trial functions,

$$\Phi_0^{(k)}(Q) = \prod_q \pi^{-1/4} \exp \left[-\frac{1}{2} \left[Q_q + \frac{\delta_q}{2} \right] \left[Q_{-q} + \frac{\delta_{-q}}{2} \right] \right]. \quad (37)$$

From Eq. (3) we know the effect of the translational operator R_1 onto the normal coordinates Q_q ,

$$R_{\pm 1} Q_q = \exp \left[\mp i \frac{2\pi}{N} q \right] Q_q$$

from which we find

$$R_{\pm 1} \Phi_0^{(k)}(Q) = \prod_q \pi^{-1/4} \exp \left[-\frac{1}{2} \left[e^{\mp i(2\pi/N)q} Q_q + \frac{\delta_q}{2} \right] \left[e^{\pm i(2\pi/N)q} Q_{-q} + \frac{\delta_{-q}}{2} \right] \right] \quad (38)$$

or

$$\Phi_0^{(k)*}(Q) R_{\pm 1} \Phi_0^{(k)}(Q) = \mathcal{L} \prod_q \pi^{-1/2} \exp \left\{ \left[Q_q + \frac{\delta_q}{2} e^{\pm i(\pi/N)q} \cos \left[\frac{\pi}{N} q \right] \right] \left[Q_{-q} + \frac{\delta_{-q}}{2} e^{\mp i(\pi/N)q} \cos \left[\frac{\pi}{N} q \right] \right] \right\}, \quad (39)$$

where

$$\mathcal{L} = \exp \left\{ -\frac{1}{8} \sum_q \delta_q \delta_{-q} \left[1 - \cos \left[\frac{2\pi}{N} q \right] \right] \right\}. \quad (40)$$

The effective overlap matrix element then reads

$$\begin{aligned} \langle \Phi_0^{(k)}(Q) | e^{i(2\pi/N)k} R_1 + e^{-i(2\pi/N)k} R_{-1} | \Phi_0^{(k)}(Q) \rangle \\ = 2\mathcal{L} \cos \left[\frac{2\pi}{N} k \right]. \end{aligned} \quad (41)$$

The lowest (i.e., zero phonon) Bloch band for the tunneling particle is thus given by

$$\begin{aligned} E_0^{(k)} &= \frac{1}{2} \sum_q \Omega_q - \frac{1}{8} \sum_q \Omega_q (2D_q \delta_{-q} - \delta_q \delta_{-q}) \\ &\quad - \Delta \mathcal{L} \cos \left[\frac{2\pi}{N} k \right], \end{aligned} \quad (42)$$

where each of these states $E_0^{(k)}$ is to be understood as the lowest state of the particular FG equation (36) pertaining to the respective irreducible representation k . Thus, in

each single- k case we have to minimize the respective expression for $E_0^{(k)}$ with respect to the variational parameters δ_q .

The most important outcome of this calculation is the modification of the Debye-Waller exponent in the effective overlap integral \mathcal{L} [see Eq. (40)], which is the q -dependent factor

$$B_q = 1 - \cos \left[\frac{2\pi}{N} q \right]. \quad (43)$$

Since $B_q \sim q^2$ for small q , this factor has the ability to compensate infrared divergencies in the exponent of Eq. (40) if the displacements δ_q diverge for $q \rightarrow 0$. We take cognizance of the fact that the appearance of B_q is a consequence of the particular topological characteristics of the FG Hamiltonian.

To exemplify the impact of the quantity B_q onto infrared divergency in a more explicit manner, we have to specify the dispersion law of the bath modes. We first assume a bath of acoustic phonons:

$$\Omega_q = 2\Omega_D \left| \frac{q}{N} \right| \quad (44)$$

which yields for small $|q|$ values

$$B_q = \frac{1}{2} \left[\pi \frac{\Omega_q}{\Omega_D} \right]^2. \quad (45)$$

Taking the rough choice $\delta_q = D_q$ we find localization (i.e., $\mathcal{L} = 0$) for $m \leq -1$. A more accurate choice is found by minimization of Eq. (42) and yields

$$\delta_q = \frac{\Omega_q D_q}{\Omega_q + \Delta \mathcal{L} B_q}, \quad (46)$$

$$E_0^{(k=0)} \cong E_L - \Delta \mathcal{L}^{(0)} \left[1 + \frac{\pi^4}{24} \alpha \frac{\Delta}{\Omega_D} \mathcal{L}^{(0)} \right] \quad (47)$$

in the strong-coupling limit, where we have defined

$$\mathcal{L}^{(0)} = \exp \left[-\frac{1}{8} \sum_q D_q D_{-q} B_q \right] = \exp \left[-\frac{\pi^2}{8} \alpha \right] \quad (48)$$

and the localization energy we get for $\Delta \mathcal{L} = 0$,

$$E_L = \frac{1}{2} \sum_q \Omega_q - \frac{1}{2} \alpha \Omega_D. \quad (49)$$

Figure 4 illustrates the effective bandwidth $E_0^{(k=0)} - E_L$, which is just the lowering of the energy with respect to the localization energy E_L .

The second choice is an excitonic bath,

$$\Omega_q = \Omega_D \left[\frac{2q}{N} \right]^2. \quad (50)$$

Then (for small $|q|$ values)

$$B_q = \frac{\pi^2}{2} \frac{\Omega_q}{\Omega_D}, \quad (51)$$

and for the rough choice $\delta_q = D_q$, we find localization for

$m \leq 0$. A better choice of δ_q [minimization of Eq. (42)] yields again Eq. (46). Employing (51) we are left with

$$E_0^{(k=0)} \cong E_L - \Delta \mathcal{L}^{(0)} \left[1 + \frac{\pi^4}{8} \alpha \frac{\Delta}{\Omega_D} \mathcal{L}^{(0)} \right] \quad (52)$$

in the strong-coupling limit, where in this case

$$\mathcal{L}^{(0)} = \exp \left[-\frac{1}{8} \sum_q D_q D_{-q} B_q \right] = \exp \left[-\frac{\pi^2}{4} \alpha \right]. \quad (53)$$

Thus, in physically relevant systems ($m = 1, 2, 3$) we always find suppression of localization, if the latter is defined in the strict sense. This suppression is quantitatively (but not qualitatively) enforced, if the trial functions are supplemented by contributions in other spatial regions, such as terms of the form $R_{\pm 1} \Phi_0^{(k)}(Q)$. This would be the corresponding extension to the reflective ansatz of Sec. III.

V. SPIN BATHS, TWO-SITE AND MULTISITE MODELS

It turns out that the preceding two models with oscillatory baths may be easily related to the corresponding models with spin baths. Spin baths may be viewed as oscillatory baths, in which double (triple, etc.) excitations of the single oscillator are disregarded, since then the oscillators would act as two-level systems (i.e., spin systems). Taking into account now the statistical weight of double (triple, etc.) excitations of a single oscillator, which is $\sim N$, as contrasted to the statistical weight for single excitations of two (three, etc.) oscillators, which is $\sim N^2$ ($\sim N^3$, etc.) we deduce that we may neglect double (and higher) excitations of single oscillators for large N ($\approx 10^8$). Thus, the results of the preceding sections also refer to spin-bath models. An exact treatment of the two-site model in a spin bath very recently has been given by Chvosta.¹¹ His results coincide with those given in Sec. II.

VI. SUMMARY

This work emphasizes a peculiar topological property of mode-assisted tunneling systems, which is laid open by means of the Fulton-Gouterman transformation. This transformation is initiated by group theory and is applicable if the particle sites constitute a regular representation of an Abelian symmetry group. It transmutes one of the three basic Hamiltonian constituents into the form of a reflection operator (two-site model) or translational operators (N -site model). In this manner it establishes the effect that whenever the bath wave functions have a localization around some displaced equilibrium configuration, they necessarily must have a counterpart which is localized around the mirror-image equilibrium configuration. This counterpart must remain finite as long as the tunneling parameter Δ itself is finite. In this manner a kind of a bridge is established between different

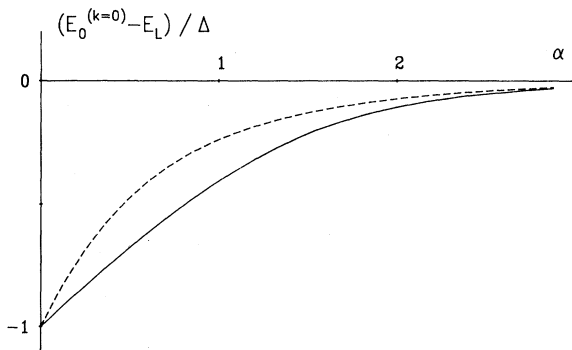


FIG. 4. Lowering of the ground-state energy $E_0^{(k=0)}$ below the localization energy E_L in the multisite model with acoustic phonon bath as a function of the coupling strength α . Dashed line: naive approximation $\delta_a = D_q$. Solid line: variation of displacements δ_q . $\Delta/\Omega_q = 0.25$.

displaced equilibrium configurations, and this bridge has an antilocalizing tendency.

We have investigated this tendency by means of displaced oscillatory trial wave functions and mirror images thereof. We have considered power-law coupling strength functions ($\sim \Omega^m$) and have given special attention to the Ohmic dissipation case ($m=1$). For the two-site model we have found a logarithmic barrier against strict localization in the Ohmic dissipation case, localization becoming possible only for $m < 1$. In the multisite model we have found that infrared divergency is overcome by a phase factor. Again there is no strict localization for $m=1$, if displaced oscillatory wave functions are used for the bath. The appearance of this phase factor is a peculiar new feature in the multisite situation. It has the effect that the critical power m for the onset of localization now depends on the dispersion law of the bath modes. For $\Omega(q) \sim q^2$ (excitonic or optical-phonon bath) localization arises for $m \leq 0$, whereas for $\Omega(q) \sim |q|$ (acoustic phonon bath) localization would arise for $m \leq -1$. Both $m=0$ and $m=-1$ do not seem to be of

relevance in physical systems.

It should be stressed that our results do not seem to be in conflict with the particular kind of symmetry breaking discussed in recent literature,¹⁻⁴ since this broken symmetry is not tantamount to a complete localization in one well. Rather, the outcome of our calculation may be exploited to give some new insight with regard to the temporal evolution of a strictly localized state for $\alpha > \alpha_c$. Since the Fulton-Gouterman ground state falls below the strictly localized state by an amount $E_{\text{trial}} - E_{\text{loc}}$, as given by Eqs. (29) and (30), we may define a time domain τ given by

$$\tau \equiv (E_{\text{loc}} - E_{\text{trial}})^{-1} = 2\Delta^{-1} e^{-\alpha} \exp[4\alpha^3 (\Omega_D / \Delta)^2],$$

which for $\alpha > 1$, $(\Delta / \Omega_D) \rightarrow 0$ tends stronger to infinity than any finite power of (Ω_D / Δ) . Thus the physical interpretation would be that the strictly localized solution is stable as long as $t < \tau$, which in most practical cases is far beyond the access of measurement.

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