Transport of a quantum particle in a dimer under the influence of two correlated dichotomic colored noises

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The transport of a quantum particle in a dimer is investigated for the case in which the influence of phonons from different branches is modeled by a dichotomic stochastic process with exponentially decaying correlations. For physical reasons, these processes might be correlated. An exact equation for the correlations between matrix elements of the density operator and both stochastic processes is constructed, and eigenvalues of the corresponding matrix are found numerically. Correlations between the noises reduce the range of incoherent transport. Various criteria for distinguishing between coherent and incoherent motion are also discussed.

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I. INTRODUCTION

Transport of quantum particles, such as electrons and excitons, in a surrounding medium, has been the subject of many experimental and theoretical investigations. At very low temperatures the particle motion is assumed to be coherent, and it can be described by a solution of the Schrödinger equation [1]. With increasing temperature, the phase of the wave function is disturbed by the influence of phonons. At high enough temperatures, the decay of the phase is so rapid that the motion of the particle may be described as a hopping process, and can be successfully described by the Pauli master equation or by the diffusion equation [2]. Both limiting cases as well as the whole range in between are represented in the Haken-Strobl-Reineker treatment [3] in which the influence of phonons is described by a δ-correlated Gaussian Markov process giving rise to fluctuations of the site energies and the transfer matrix element. This model has been successfully used for the description of a series of experimental results; details may be found in [4].

The δ-correlated Gaussian white noise of the Haken-Strobl-Reineker model implies that the phonon-generated fluctuations also have a white spectrum. This may be questioned in the case of low temperatures when only low-energy phonon modes are excited. Also, Gaussian white noise is unphysical, and therefore replacement of a δ-correlated Gaussian white noise with a dichotomic colored noise represents a straightforward generalization, especially as the Gaussian white noise may in certain limits be modeled by a dichotomic colored noise [5]. This type of noise is very well known from textbooks [6], and becomes more and more popular in the literature; we refer the reader to an excellent review [7], and some more recent references may be found in [8].

Recently, Chvosta [9] and Kraus and Reineker [10] have considered the motion of a quantum particle under the influence of a dichotomic colored noise in a dimer, and obtained a number of interesting results. In particular, Kraus and Reineker [10] have shown that the motion is much more complicated than the Haken-Strobl-Reineker model would suggest, and that the criterion for the transition from coherent to incoherent motion becomes rather complex. Kraus and Reineker have assumed that both sites and the interaction coupling are subject to influence of independent noises. However, as all these noises have the same physical origin, namely, the influence of the phonons, they may not be independent, and it has been shown that effects of correlations between seemingly different noises can be very strong [11]. In the present paper we extend the results of Kraus and Reineker to the case when all noises present in the system's Hamiltonian are correlated, and find their origin in two independent noises representing the internal fluctuations resulting from the influence of phonons from the acoustic and optical branches. In addition, these two noises may be asymmetric, i.e., they may influence either site with a different strength. Also, the sites themselves may be asymmetric, i.e., they may have different energies. However, in order not to complicate the whole picture too much, we assume while solving numerically the equations of motion that the interaction term does not exhibit fluctuations.

This paper is organized as follows. In Sec. II we present the model Hamiltonian, derive the equation of motion, and introduce the necessary parametrization. In Sec. III we discuss various criteria for distinguishing between coherent and incoherent motion. Numerical results are also presented and discussed. Concluding remarks are given in Sec. IV, and a detailed form of the equations of motion is given in the Appendix.

II. MODEL HAMILTONIAN AND EQUATIONS OF MOTION

A. Model Hamiltonian

The complete time-dependent Hamiltonian of the model, describing the dynamics of quantum particles in

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a dimer, consists of two parts,

$$H(t) = H_0 + H_1(t)\,. \tag{2.1}$$

The first part, describing the coherent motion of the quantum particle, is given by

$$H_0 = \varepsilon_1 a_1^\dagger a_1 + \varepsilon_2 a_2^\dagger a_2 + J(a_1^\dagger a_2 + a_2^\dagger a_1)\,, \tag{2.2}$$

where $a_i^\dagger$, a_i are creation and annihilation operators for the quantum particle at site i, and ε_1 and ε_2 are the energies of the dimer. J describes the coherent transport of the particles between the two sites. The coherent transport is disturbed by the influence of phonons. Instead of treating them quantum mechanically, we average the fast variables [12], and add a stochastic part

$$H_1(t) = \varepsilon_1(t) a_1^\dagger a_1 + \varepsilon_2(t) a_2^\dagger a_2 + J(t)(a_1^\dagger a_2 + a_2^\dagger a_1) \tag{2.3}$$

to the Hamiltonian, which results in fluctuations of the energies ε_i and of the interaction J. $\varepsilon_i(t)$ and $J(t)$ are stochastic processes. Unlike in the original paper of Kraus and Reineker [10], we assume that the energy fluctuations at different sites and the fluctuations of the interaction are not independent. Instead, we assume that

$$\varepsilon_i(t) = \sum_{n=1}^{N} \mu_{in}\xi_n(t)\,, \tag{2.4}$$

where $i = 1, 2, 3$, and $\varepsilon_3(t) \equiv J(t)$. The noises $\xi_n(t)$ express the influence of different phonon branches, and we assume that they are independent Markovian symmetric dichotomic colored noises: $\langle \xi_n(t)\rangle = 0$, $\xi_n^2(t) = \Delta_n^2$, and

$$\langle \xi_n(t)\xi_m(t')\rangle = \delta_{nm}\Delta_n^2 \exp(-\lambda_n|t-t'|)\,. \tag{2.5}$$

In the following, we will always assume that there are only two phonon branches, i.e., $N = 2$.

B. Equation of motion for the density matrix

We describe the transport of a quantum particle by a density operator ρ which obeys the Liouville equation

$$\dot\rho = -i[H(t), \rho]\,. \tag{2.6}$$

On account of the fluctuating part $H_1(t)$ of the Hamiltonian, ρ contains fluctuations as well. However, as the full Hamiltonian is Hermitian, the density operator ρ is always Hermitian and normalized to unity:

$$\rho_{11} + \rho_{22} = 1\,, \quad \text{and} \quad \rho_{12} = (\rho_{21})^*\,. \tag{2.7}$$

We now introduce three variables X_i,

$$X_1 = \tfrac{1}{2}(\rho_{11} - \rho_{22})\,, \tag{2.8}$$

$$X_2 = \tfrac{1}{2}(\rho_{12} + \rho_{21})\,, \tag{2.9}$$

$$X_3 = \tfrac{i}{2}(\rho_{21} - \rho_{12})\,, \tag{2.10}$$

and the Liouville equation (2.6) with $H(t)$ given by (2.1), is now equivalent to three equations for the variables X_i:

$$\begin{aligned}\dot X_1 &= -2[J + J(t)]X_3\,,\\ \dot X_2 &= [\varepsilon_1 - \varepsilon_2 + \varepsilon_1(t) - \varepsilon_2(t)]X_3\,,\\ \dot X_3 &= 2[J + J(t)]X_1 - [\varepsilon_1 - \varepsilon_2 + \varepsilon_1(t) - \varepsilon_2(t)]X_3\,.\end{aligned} \tag{2.11}$$

If we now express $\varepsilon_i(t)$ by $\xi_n(t)$ $(n = 1, 2)$ using (2.4), we obtain

$$\begin{aligned}\dot X_1 &= -2[J + \mu_{31}\xi_1(t) + \mu_{32}\xi_2(t)]X_3\,,\\ \dot X_2 &= [\delta_0 + \delta_1\xi_1(t) + \delta_2\xi_2(t)]X_3\,,\\ \dot X_3 &= 2[J + \mu_{31}\xi_1(t) + \mu_{32}\xi_2(t)]X_1\\ &\quad - [\delta_0 + \delta_1\xi_1(t) + \delta_2\xi_2(t)]X_2\,,\end{aligned} \tag{2.12}$$

where $\delta_0 = \varepsilon_1 - \varepsilon_2$, and $\delta_n = \mu_{1n} - \mu_{2n}$ $(n = 1, 2)$.

Equations ((2.12) are still exact. We now have to average the fluctuations. Taking the stochastic average of Eqs. (2.12), we obtain on the right-hand sides of the averaged equations terms proportional to $\langle \xi_n X_i\rangle$. To calculate their derivatives, we use a theorem of Shapiro and Loginov [13] and arrive at

$$\tfrac{d}{dt}\langle \xi_n X_i\rangle = \langle \xi_n \dot X_i\rangle - \lambda_n \langle \xi_n X_i\rangle\;. \tag{2.13}$$

Inserting the equation of motion (2.12) into (2.13), expressions of the form $\langle \xi_n\xi_m X_i\rangle$ and $\langle \xi_n\xi_n X_i\rangle$ occur. The latter expression immediately results in $\Delta_n^2\langle X_i\rangle$ when the property $\xi_n^2(t) = \Delta_n^2$ is used. To find the equation of motion for the other correlation function, $\langle \xi_n\xi_m X_i\rangle$, we apply the above-mentioned theorem again and obtain $(n, m = 1, 2,\ n \neq m)$

$$\begin{aligned}\tfrac{d}{dt}\langle \xi_n\xi_m X_i\rangle &= \langle \xi_n\xi_m \dot X_i\rangle\\ &\quad - (\lambda_n + \lambda_m)\langle \xi_n\xi_m X_i\rangle\;.\end{aligned} \tag{2.14}$$

Upon inserting the equation of motion (2.12) into (2.14), we get terms proportional to $\langle \xi_1\xi_2\xi_1 X_j\rangle$ and $\langle \xi_2\xi_1\xi_2 X_j\rangle$. These result in $\Delta_1^2\langle \xi_2 X_j\rangle$ and $\Delta_2^2\langle \xi_1 X_j\rangle$, respectively. In this way we finally obtain a closed set of 12 differential equations for $\langle X_i\rangle$, $\langle \xi_1 X_i\rangle$, $\langle \xi_2 X_i\rangle$, and $\langle \xi_1\xi_2 X_i\rangle$ $(i = 1, 2, 3)$.

If either Δ_1 or Δ_2 vanishes, we in fact have a system with only one phonon branch, and there is a full correlation between fluctuations at both sites and the interaction. We assume that neither of $\Delta_{1,2}$ vanishes, and we introduce variables

$$y_1 = \langle X_1 \rangle\,,\; y_2 = \langle X_2 \rangle\,, y_3 = \langle X_3 \rangle\,,$$
$$y_4 = \frac{1}{\Delta_1}\langle \xi_1 X_1 \rangle\,,\; y_5 = \frac{1}{\Delta_1}\langle \xi_1 X_2 \rangle\,,$$
$$y_6 = \frac{1}{\Delta_1}\langle \xi_1 X_3 \rangle\,, y_7 = \frac{1}{\Delta_2}\langle \xi_2 X_1 \rangle\,, \tag{2.15}$$
$$y_8 = \frac{1}{\Delta_2}\langle \xi_2 X_2 \rangle\,,\quad y_9 = \frac{1}{\Delta_2}\langle \xi_2 X_3 \rangle\,,$$
$$y_{10} = \frac{1}{\Delta_1\Delta_2}\langle \xi_1\xi_2 X_1 \rangle\,,\; y_{11} = \frac{1}{\Delta_1\Delta_2}\langle \xi_1\xi_2 X_2 \rangle\,,$$
$$y_{12} = \frac{1}{\Delta_1\Delta_2}\langle \xi_1\xi_2 X_3 \rangle\,.$$

If we now denote by $\boldsymbol{y}$ the vector $(y_1,\ldots,y_{12})$, we can write our 12 equations of motion for the averages as

$$\dot{\boldsymbol{y}} = L\boldsymbol{y}\,. \tag{2.16}$$

The detailed form of L is given in the Appendix.

Note at this point that we have only 12 equations for real variables, instead of 16 equations for complex variables of Ref. [10]. This is so because we have explicitly used the properties of the density operator ρ, namely, its normalization and Hermiticity. Also our matrix L is more symmetric than that of Kraus and Reineker, and this is a consequence of introducing variables in the form $\langle \xi_n X_i \rangle/\Delta_n$, not just $\langle \xi_n X_i \rangle$. Such a choice of variables reveals symmetries of the problem more clearly, and also makes the numerical procedures work more efficiently.

C. Parametrization of the equation of motion

In principle, we should deal with 13 parameters: three static parameters (ε_1, ε_2, J), six coupling parameters (μ_{jn}, $j=1,2,3$, $n=1,2$), and four parameters describing the stochastic processes ξ_n ($\Delta_{1,2}$, $\lambda_{1,2}$). To simplify our work, we assume that there are no fluctuations in the interaction term ($\mu_{3n}=0$, $n=1,2$). As it turns out, admitting fluctuations in this term introduces some additional complications, but does not change the main results significantly (details will be published elsewhere). However, we are still left with 11 free parameters.

On the other hand, the coupling and noise parameters enter the equations of motion only in certain combinations (cf. the Appendix), namely,

$$\delta_1\Delta_1 = \mu_{11}\Delta_1 - \mu_{21}\Delta_1\,,$$
$$\delta_2\Delta_2 = \mu_{12}\Delta_2 - \mu_{22}\Delta_2\,. \tag{2.17}$$

The correlations between the fluctuations at both sites read

$$\langle \varepsilon_1(t)\varepsilon_1(t') \rangle = \mu_{11}\Delta_1\mu_{11}\Delta_1 \exp(-\lambda_1|t-t'|) + \mu_{12}\Delta_2\mu_{12}\Delta_2 \exp(-\lambda_2|t-t'|)\,, \tag{2.18}$$

$$\langle \varepsilon_2(t)\varepsilon_2(t') \rangle = \mu_{21}\Delta_1\mu_{21}\Delta_1 \exp(-\lambda_1|t-t'|) + \mu_{22}\Delta_2\mu_{22}\Delta_2 \exp(-\lambda_2|t-t'|)\,, \tag{2.19}$$

$$\langle \varepsilon_1(t)\varepsilon_2(t') \rangle = \mu_{11}\Delta_1\mu_{21}\Delta_1 \exp(-\lambda_1|t-t'|) + \mu_{12}\Delta_2\mu_{22}\Delta_2 \exp(-\lambda_2|t-t'|)\,. \tag{2.20}$$

Now we introduce three parameters Δ, r, and q, such that

$$\mu_{11}\Delta_1 = \Delta r\,,\quad \mu_{21}\Delta_1 = \Delta(1-r)\,,$$
$$\mu_{22}\Delta_2 = \Delta q\,,\quad \mu_{12}\Delta_2 = \Delta(1-q)\,. \tag{2.21}$$

With these parameters, the correlation functions (2.18)–(2.20) read

$$\langle \varepsilon_1(t)\varepsilon_1(t') \rangle = \Delta^2 r^2 \exp(-\lambda_1|t-t'|) + \Delta^2(1-q)^2 \exp(-\lambda_2|t-t'|)\,, \tag{2.22}$$
$$\langle \varepsilon_2(t)\varepsilon_2(t') \rangle = \Delta^2(1-r)^2 \exp(-\lambda_1|t-t'|) + \Delta^2 q^2 \exp(-\lambda_2|t-t'|)\,, \tag{2.23}$$
$$\langle \varepsilon_1(t)\varepsilon_2(t') \rangle = \Delta^2 r(1-r) \exp(-\lambda_1|t-t'|) + \Delta^2 q(1-q) \exp(-\lambda_2|t-t'|)\,. \tag{2.24}$$

Δ is the "absolute" strength of the effective noises, while r and q measure both the relative strength of the two noises $\xi_{1,2}$ at the two sites, and the correlations between the fluctuations at these sites. In particular, setting $r=q=1$ and $\lambda_1=\lambda_2$ gives the uncorrelated noises case, while $r=q=\frac{1}{2}$ and $\lambda_1=\lambda_2$ maximizes the correlations between the fluctuations at the two sites. The parametrization (2.21) is of course arbitrary, but it is sufficient for our purposes.

The parameters r and q can take any values for which the correlation functions (2.22)–(2.24) are well defined. For instance, if $\lambda_1=\lambda_2$, they must satisfy

$$r(1-r) + q(1-q) \geq 0\,. \tag{2.25}$$

This allows for one of these parameters to take a small negative value, provided the other one is sufficiently large. However, in the following we will mostly assume that r and q are confined to the 0–1 interval.

We are thus left with seven parameters: two static (δ_0 and J), three describing the strength and correlations of the noises (Δ, r, and q), and two decay constants (λ_1 and λ_2).

III. SOLUTION OF THE TRANSPORT PROBLEM

Equation (2.16), describing the dynamics of the system (2.1), has a formal solution given by

$$\boldsymbol{y}(t) = \exp(Lt)\boldsymbol{y}(0)\,, \tag{3.1}$$

and it is clear that if one is interested only in the frequencies and not in the actual form of $y_k(t)$, it is sufficient to find the eigenvalues of the matrix L. Thus we arrive at a non-Hermitian eigenvalue problem [14]

$$Ly = \Gamma y, \tag{3.2}$$

where the eigenvalues Γ are in general complex:

$$\Gamma_k = \gamma_k + i\omega_k. \tag{3.3}$$

The imaginary parts, ω_k, describe possible oscillations, the real parts, which are always ≤ 0, the damping of the system. Because the matrix L is real, all eigenvalues appear in complex conjugate pairs. Note that, unlike in Ref. [10], there is no eigenvalue identically equal to zero. This eigenvalue in the paper of Kraus and Reineker corresponds to the conserved normalization of the density matrix, and we have already used the fact that this quantity is conserved by reducing the number of equations of motion.

In the following, we numerically find eigenvalues Γ_k by the Householder elimination for various values of parameters.

A. Criteria for distinguishing between coherent and incoherent motion

In the case of white noise, four eigenvalues exist. Two of them are purely real (zero and a finite negative value), the other two may be real and negative or complex. The former case corresponds to a purely exponential exchange of occupation probabilities, which is characteristic for incoherent motion, the latter one to damped oscillations, describing the coherent motion [3].

The question arises, whether there is a simple criterion to separate the ranges of coherent and incoherent motion if the noises are not white but colored. It is clear that the oscillating modes, their number or persistence, should determine the character of the motion. Kraus and Reineker [10] numerically solved the equations of motion for the uncorrelated noises case and found the number of oscillating modes for different values of parameters. They regarded as coherent the motion with maximal number (= 8) of oscillating modes, and with less-than-eight oscillating modes, as incoherent. Kraus and Reineker presented their results in the J/Δ^2-$1/\lambda$ plane, and thus they divided the whole plane into the regions corresponding to coherent and incoherent motion. In the present research, we also numerically found eigenvalues of L and determined the number of oscillating modes. For the $r = q = 1$ and $\lambda_1 = \lambda_2$ case (uncorrelated noises) and using the above-said criterion, we obtained a picture identical to that of Kraus and Reineker (Fig. 1; cf. also Fig. 9 of Ref. [10]). In Fig. 1 region I corresponds to coherent, and region II to incoherent motion, respectively. Note at this point that we have, by reducing the number of equations of motion from 16 to 12, eliminated four nonoscillating modes. Indeed, with our choice of variables (2.8)–(2.10), we should have another variable, $X_4 = \frac{1}{2}(\rho_{11} + \rho_{22})$, to regain the lacking four equations. It is now straightforward to show using Eq. (2.6) and the Shapiro-Loginov theorem [13] that $\langle X_4 \rangle$ is constant, while $\langle \xi_1 X_4 \rangle$, $\langle \xi_2 X_4 \rangle$, and $\langle \xi_1 \xi_2 X_4 \rangle$ decay exponentially. Thus the oscillating modes for our $r = q = 1$ and $\lambda_1 = \lambda_2$ case are identical to the oscillating modes described by Kraus and Reineker.

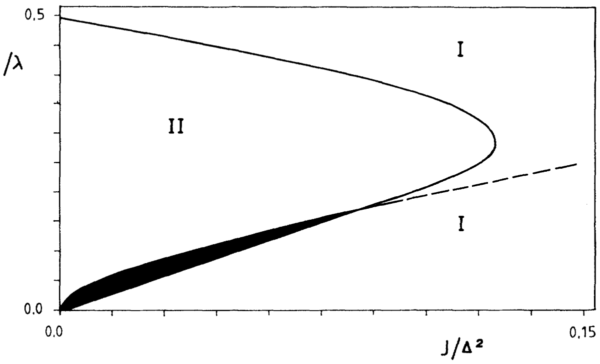

FIG. 1. Number of complex eigenvalues of the matrix L. $q = r = 1$, $\lambda_1 = \lambda_2 = \lambda$ (uncorrelated noises), $\delta_0 = 0$. Region I: eight complex eigenvalues — coherent motion; region II: less than eight complex eigenvalues — incoherent motion; shaded area: less than six complex eigenvalues. Below the dashed borderline the longest-living mode displays damped oscillations, above this line it is purely exponential.

Another criterion is possible: the motion is regarded as coherent or incoherent according to what type of motion prevails for long times. Thus the eigenvalue with smallest absolute value of its real part (the longest-living mode) determines the character of the whole motion. The dashed line in Fig. 1 corresponds to the borderline between different types of motion: above the borderline the longest-living mode is purely exponential, while below that line it displays damped oscillations. For small values of J/Δ^2 this line is tangent to the border between regions I and II, and for $r = q = 1$ and $\lambda_1 = \lambda_2$ its slope equals 2.

B. Numerical results

We start with results for a case with "symmetric" noises: $\lambda_1 = \lambda_2$, $\delta_0 = 0$, and $r = q$ (Fig. 2). The noises influence the two sites in the same way, the relative strength of the effective noises at both sites is identical, and the only thing that matters is the correlation between the noises. One can see that the larger the correlation, the smaller the region in which incoherent transport occurs. In particular, for $r = q = \frac{1}{2}$ (maximal correlation), region II vanishes altogether, and all motion is coherent (this result may also be found analytically; cf. the Appendix). Also the borderline between regions characterized by various types of behavior of the longest-living mode moves upward in the J/Δ^2-$1/\lambda$ plane, i.e., the range of parameters, for which this mode displays oscillatory behavior, grows as $r = q$ change from 0 to $\frac{1}{2}$. However, the borderline between regions I and II, as well as the borderline between the regions of oscillatory and nonoscillatory behavior of the longest-living mode, change smoothly with changes of the parameters $r = q$.

If the effective noise at one site is stronger than that on

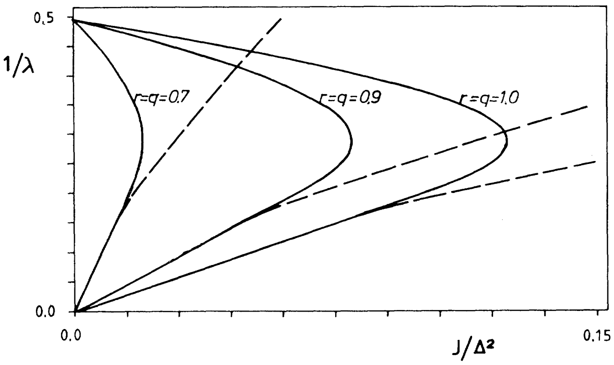

FIG. 2. Number of complex eigenvalues of the matrix L for "symmetric" noises: $\lambda_1 = \lambda_2 = \lambda$, $\delta_0 = 0$, and $r = q = 1$, $r = q = 0.9$, and $r = q = 0.7$, respectively. To the left of each line the motion is incoherent, to the right, coherent, for corresponding values of parameters. Dashed lines indicate the borderlines between regions in which the longest-living mode displays and does not display damped oscillations.

the other one, the situation changes dramatically. Figure 3 shows the region of incoherent motion for $\lambda_1 = \lambda_2$, $\delta_0 = 0$, $r = 1$, and $q = 0.9$; for comparison, the region for $r = q = 1$ is also shown. One can see that the region of incoherent motion is very small, and closer inspection reveals that with these values of parameters, we can have either eight complex eigenvalues, or four, but not six. In fact, we have observed this abrupt reduction of the region of incoherent motion for as small differences between r and q as the accuracy of numerical calculations would allow. Apparently, any difference between r and q destroys an additional symmetry of the matrix L. To substantiate this point, in Fig. 4 we show frequencies corresponding to the L-L line of Fig. 3: for the symmetric case $r = q = 1$ in Fig. 4(a), and for the asymmetric case $r = 1$, $q = 0.9$ in Fig. 4(b). Note that the mode marked by an arrow is

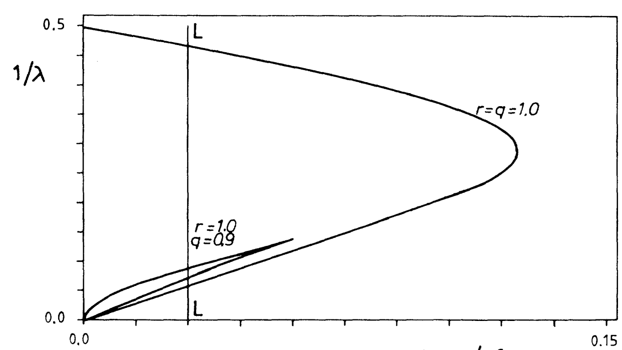

FIG. 3. Number of complex eigenvalues of the matrix L for asymmetric noises: $\lambda_1 = \lambda_2 = \lambda$, $\delta_0 = 0$, $r = 1$, and $q = 0.9$ (inner curve). For comparison, the borderline between regions I and II for a symmetric case ($r = q = 1$) is also shown (outer curve; cf. also Fig. 2). The L-L line corresponds to a "cut," along which the following figure is drawn.

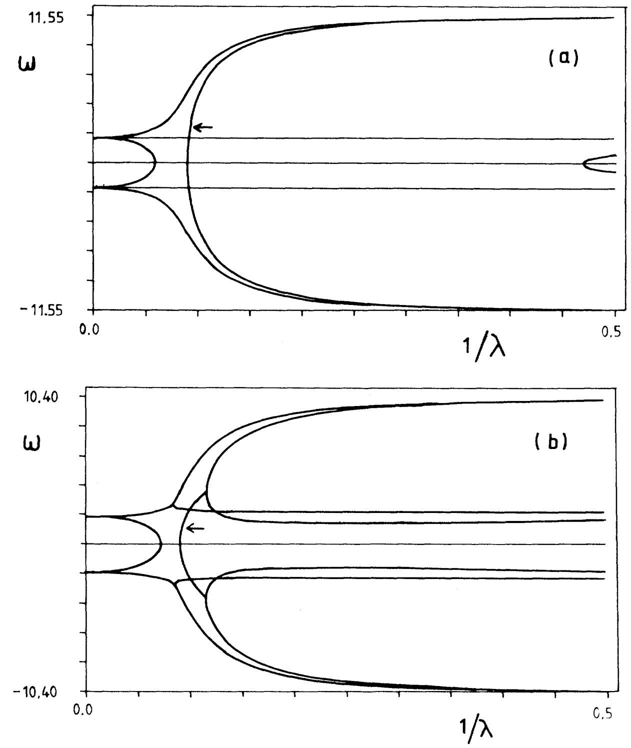

FIG. 4. Frequencies (imaginary parts of the eigenvalues) for parameters corresponding to the L-L "cut" of Fig. 3: $\lambda_1 = \lambda_2 = \lambda$, $\delta_0 = 0$, $J/\Delta^2 = 0.03$, and $r = q = 1$ (a), and $r = 1$ and $q = 0.9$ (b). See description in text.

not degenerated for the symmetric case, and is doubly degenerated for the asymmetric case. The zero frequency mode is sixfold degenerated for the symmetric case in between the arrow-marked mode and the bifurcation occurring for larger values of $1/\lambda$, and this area corresponds to the six-frequency region. For the asymmetric case, the zero frequency mode is only four times degenerated to the right of the arrow-marked mode, and the six frequency region is missing.

If $\lambda_1 = \lambda_2$ and one of the parameters r, q, takes a small negative value [cf. inequality (2.25) above], the region of incoherent motion is also very small and reduced to the four-frequency area. What might be more interesting, though, is that the borderline between regions of oscillatory and nonoscillatory behavior of the longest-living mode has a slope smaller than 2 in the vicinity of the origin of the coordination frame. In such a case one of the criteria for distinguishing between coherent and incoherent motion appears to give coherence enhancement (reduction of the area with less than eight oscillating modes), while the other, coherence reduction (enhancement of the area with nonoscillatory behavior of the longest-living mode). However, for larger values of J/Δ^2, this borderline grows faster than the borderline for the $r = q = 1$ case.

A similar abrupt reduction of the region of incoherent motion can be seen for a case with $\lambda_1 \neq \lambda_2$, even for

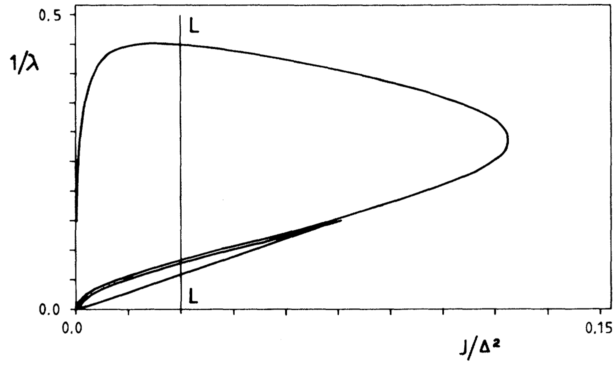

FIG. 5. Number of complex eigenvalues for symmetric uncorrelated noises and an asymmetric unperturbed Hamiltonian: $\lambda_1 = \lambda_2 = \lambda$, $r = q = 1$, $\delta_0 = 0.1$, $J/\Delta^2 = 0.03$. Note the "gap" of coherent motion in the area, where incoherent motion appears for the $\delta_0 = 0$ case (cf. Fig. 2). The L-L line corresponds to a "cut," along which the following figure is drawn.

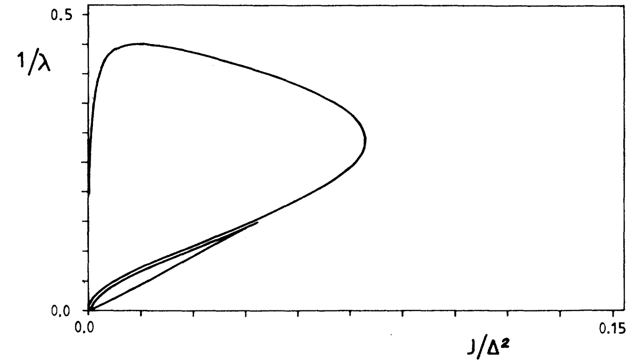

FIG. 7. Number of complex eigenvalues for symmetric correlated noises and an asymmetric unperturbed Hamiltonian: $\lambda_1 = \lambda_2 = \lambda$, $r = q = 0.9$, $\delta_0 = 0.1$.

$r = q = 1$. Again, the six-frequency region is missing.

If the unperturbed Hamiltonian H_0 is asymmetric ($\delta_0 \neq 0$) and $\lambda_1 = \lambda_2$, a new phenomenon occurs. The region of incoherent transport is reduced for large values of $1/\lambda_1$ and small values of J/Δ^2, but what is most peculiar, a gap of coherent motion appears in the area where for $\delta_0 = 0$ only four oscillating modes exist (Fig. 5). This gap corresponds to a double-degenerated "bubble" in the frequency spectrum (Fig. 6). Apparently, setting $\delta_0 \neq 0$ destroys another additional symmetry of the matrix L. Figure 5 shows results for the uncorrelated noises case; if the noises are correlated, or even asymmetric, both effects — reduction of the incoherent motion region for large $1/\lambda$ and small J/Δ^2, and the gap in the four-frequency area— persist, and the region of incoherent motion always lies within that for the same values of parameters but with $\delta_0 = 0$. Figure 7 shows results for a symmetric correlated noises case. However, the borderline between the regions of the two types of the longest-living mode behavior is not much affected by setting $\delta_0 \neq 0$, as compared to that with the same values of parameters but with $\delta_0 = 0$. It might also be noted that the larger absolute value of δ_0, the slower the convergence of the iteration procedure used to calculate the eigenvalues of L.

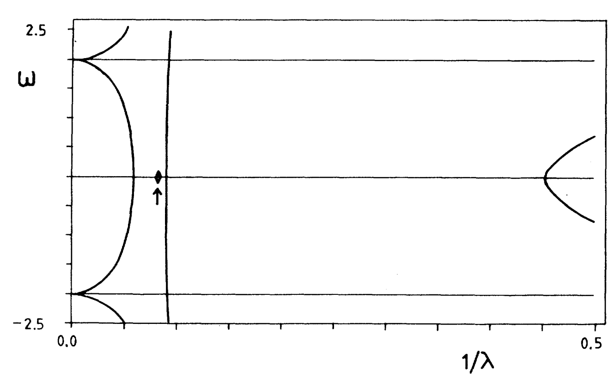

FIG. 6. Frequencies for parameters corresponding to the L-L "cut" of Fig. 5: $\lambda_1 = \lambda_2 = \lambda$, $r = q = 1$, $\delta_0 = 0.1$. Note the doubly degenerated "bubble" marked by an arrow [cf. Fig. 4(a)].

Finally, in Fig. 8 we present borderlines of regions characterized by different behavior of the longest-living mode, for all cases described above. Only the borderlines for $\delta_0 = 0.1$ are not shown, since within the presented range of parameters, they coincide with corresponding lines for the $\delta_0 = 0$ cases. No abrupt changes between these lines can be seen, and shapes of the lines change smoothly with the parameters.

IV. CONCLUDING REMARKS

In this paper we have investigated the influence of a heat bath with two correlated dichotomic colored noises on the transport properties of a quantum particle. In

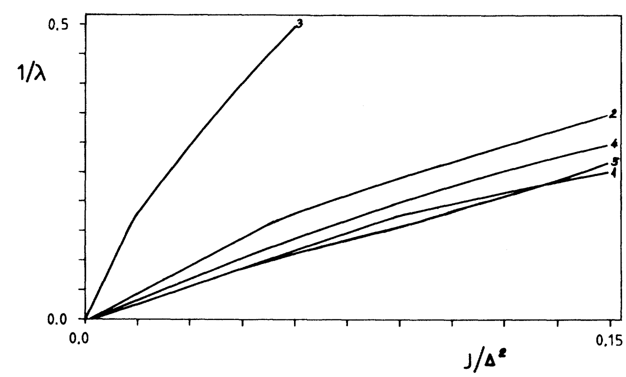

FIG. 8. Borderlines between regions of oscillatory and nonoscillatory behavior of longest-living mode for various values of parameters. $\lambda_1 = \lambda_2 = \lambda$, $\delta_0 = 0$, and $r = q = 1$ (1), $r = q = 0.9$ (2), $r = q = 0.7$ (3), $r = 1$, $q = 0.9$ (4), and $r = 0.9$, $q = -0.08$ (5). Lines for $\delta_0 = 0.1$ coincide with corresponding lines for $\delta_0 = 0$ within the presented range of parameters J/Δ^2 and $1/\lambda$.

the derivation of the equation of motion for the density operator we have allowed fluctuations of the excitation energies at the two sites, as well as of the transfer matrix elements. As we have explicitly used trace (normalization) and Hermitian properties of the density operators and chosen variables suitably, we have reduced the number of necessary equations from 16 to 12, and brought them to a more convenient form. In the numerical treatment, only excitation energy fluctuations have been considered.

We have used two criteria in order to distinguish between coherent and incoherent motion. First, according to Kraus and Reineker [10], motion of the system under consideration is regarded as coherent if at least eight of its modes oscillate, and we have argued that one should not use a similar criterion but with six modes. Second, the character of motion has been determined according to what type of behavior prevailed for long times (longest-living mode): oscillatory (coherent) or nonoscillatory (incoherent). By numerically calculating eigenvalues of the matrix L, we have found that if the two noises are correlated, the region of incoherent motion shrinks (for maximal correlations between the noises incoherent motion is removed altogether), and that the criterion determining the character of motion by number of its oscillatory modes, is unstable to small changes of parameters. These two points require some more attention.

First, the correlation-induced enhancement of coherent motion is fairly simple to understood. Correlations between the two noises mean that fluctuations at one site are not totally independent from that at the other site. As a consequence, the system behaves in a more orderly way and the noises are less prone to destroy phase properties of the system. In particular, when the correlations between the effective noises maximize, we have in fact only one noise acting simultaneously at both sites in the same way, which results in a coherent motion of the whole system.

Second, our observations of instability of the six-frequency region of incoherent motion under small changes of parameters, and stability of the four-frequency one, suggests introducing two types of incoherent motion: weak incoherence (six oscillating modes), which can be destroyed if some additional symmetry of the matrix L is removed, and strong incoherence (four oscillating modes), which is stable. Note that the "gap" introduced by a detuning δ_0 is not a hallmark of instability: infinitesimally small detunings introduce infinitesimally narrow gaps. On the other hand, the characterization of motion by its longest-living mode behavior is stable, so perhaps the latter criterion should be used. Another possibility exists: the motion is coherent or incoherent according to how the physically measurable quantities, $\langle X_1\rangle$, $\langle X_2\rangle$, and $\langle X_3\rangle$, behave. This, however, suggests a possible dependence on initial conditions. This problem is at present under investigation.

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APPENDIX: DETAILED FORM OF THE EQUATIONS OF MOTION

The equation of motion for the vector $\boldsymbol{y} = (y_1, \ldots, y_{12})$ reads

$$\dot{\boldsymbol{y}} = L\boldsymbol{y}\,, \tag{A1}$$

where L is a 12×12 real matrix given by ($\lambda_+ = \lambda_1 + \lambda_2$)

$$L=\begin{bmatrix}
0 & 0 & -2J & 0 & 0 & 0 & 0 & -2\mu_{31}\Delta_1 & -2\mu_{32}\Delta_2 & 0 & 0 & 0\\
0 & 0 & \delta_0 & 0 & 0 & 0 & 0 & \delta_1\Delta_1 & \delta_2\Delta_2 & 0 & 0 & 0\\
2J & -\delta_0 & 0 & 2\mu_{31}\Delta_1 & 2\mu_{32}\Delta_2 & -\delta_1\Delta_1 & -\delta_2\Delta_2 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & -2\mu_{31}\Delta_1 & -\lambda_1 & 0 & 0 & 0 & -2J & 0 & 0 & 0 & -2\mu_{32}\Delta_2\\
0 & 0 & -2\mu_{32}\Delta_2 & 0 & -\lambda_2 & 0 & 0 & 0 & -2J & 0 & 0 & -2\mu_{31}\Delta_1\\
0 & 0 & \delta_1\Delta_1 & 0 & 0 & -\lambda_1 & 0 & \delta_0 & 0 & 0 & 0 & \delta_2\Delta_2\\
0 & 0 & \delta_2\Delta_2 & 0 & 0 & 0 & -\lambda_2 & 0 & \delta_0 & 0 & 0 & \delta_1\Delta_1\\
2\mu_{31}\Delta_1 & -\delta_1\Delta_1 & 0 & 2J & 0 & -\delta_0 & 0 & -\lambda_1 & 0 & 2\mu_{32}\Delta_2 & -\delta_2\Delta_2 & 0\\
2\mu_{32}\Delta_2 & -\delta_2\Delta_2 & 0 & 0 & 2J & 0 & -\delta_0 & 0 & -\lambda_2 & 2\mu_{31}\Delta_1 & -\delta_1\Delta_1 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -2\mu_{32}\Delta_2 & -2\mu_{31}\Delta_1 & -\lambda_+ & 0 & -2J\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta_2\Delta_2 & \delta_1\Delta_1 & 0 & -\lambda_+ & \delta_0\\
0 & 0 & 0 & 2\mu_{32}\Delta_2 & 2\mu_{31}\Delta_1 & -\delta_2\Delta_2 & -\delta_1\Delta_1 & 0 & 0 & 2J & -\delta_0 & -\lambda_+
\end{bmatrix}. \tag{A2}$$

If we set $\mu_{31} = \mu_{32} = 0$ and introduce the parameters (2.22), (A2) simplifies to $[x = (2r-1)\Delta,\ y = (2q-1)\Delta]$

$$L = \begin{bmatrix} 0 & 0 & -2J & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \delta_0 & 0 & 0 & 0 & 0 & x & -y & 0 & 0 & 0 \\ 2J & -\delta_0 & 0 & 0 & 0 & -x & y & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\lambda_1 & 0 & 0 & 0 & -2J & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\lambda_2 & 0 & 0 & 0 & -2J & 0 & 0 & 0 \\ 0 & 0 & x & 0 & 0 & -\lambda_1 & 0 & \delta_0 & 0 & 0 & 0 & -y \\ 0 & 0 & -y & 0 & 0 & 0 & -\lambda_2 & 0 & \delta_0 & 0 & 0 & x \\ 0 & -x & 0 & 2J & 0 & -\delta_0 & 0 & -\lambda_1 & 0 & 0 & y & 0 \\ 0 & y & 0 & 0 & 2J & 0 & -\delta_0 & 0 & -\lambda_2 & 0 & -x & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda_+ & 0 & -2J \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -y & x & 0 & -\lambda_+ & \delta_0 \\ 0 & 0 & 0 & 0 & 0 & y & -x & 0 & 0 & 2J & -\delta_0 & -\lambda_+ \end{bmatrix} . \quad \text{(A3)}$$

The Kraus and Reineker case of uncorrelated noises [10] may be recovered by setting $r = q = 1$ and $\lambda_1 = \lambda_2$. If $r = q = \frac{1}{2}$ ($x = y = 0$) and $\delta_0 = 0$, eigenvalues of L are calculated from

$$\Gamma(\Gamma+\lambda_1)(\Gamma+\lambda_2)(\Gamma+\lambda_1+\lambda_2)[\Gamma^2+4J^2][(\Gamma+\lambda_1)^2+4J^2][(\Gamma+\lambda_2)^2+4J^2][(\Gamma+\lambda_1+\lambda_2)^2+4J^2]=0\,, \quad \text{(A4)}$$

and we have four real nonpositive eigenvalues [$\Gamma = 0$, $-\lambda_1$, $-\lambda_2$, and $-(\lambda_1+\lambda_2)$, respectively], and four pairs of complex conjugate eigenvalues [$\Gamma = \pm 2iJ$, $-\lambda_1 \pm 2iJ$, $-\lambda_2 \pm 2iJ$, and $-(\lambda_1+\lambda_2) \pm 2iJ$, respectively]. We can see that in this case there are eight oscillating modes regardless of the values of J and $\lambda_{1,2}$, and the incoherent motion is removed altogether.

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