Nonlinear dynamics of spin-boson systems: 
Quantum mechanical and quasi-classical treatment

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Abstract

We investigate a quasi-particle coupled to polarization vibrations in a dimer model. This model (harmonic oscillator coupled to a two-level system) is interesting for various physical situations, e.g. the transport of excitons in dimers or the spin-\( \frac{1}{2} \) case of the Jaynes-Cummings model. We found that a complementary approach to the usual quasi-classical treatment of the spin-boson model may be more suitable for the spin-\( \frac{1}{2} \) case. © 1998 Elsevier Science B.V. All rights reserved.

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1. Model and basic equations

We consider the dynamics of a quasi-particle (electron or exciton) in a molecular dimer. The quasi-particle is moving between the two sites of the dimer and its motion is coupled to local vibrational modes at the two sites. For simplicity we assume that there is exactly one quasi-particle excited on the dimer. Furthermore, we restrict ourselves to the symmetric dimer. The full Hamiltonian [1–3] can be simplified by some transformations and its non-trivial part is

\[
H = T \sigma_z + \omega (b^\dagger b + \frac{1}{2}) - \eta \sigma_z (b^\dagger + b). 
\]

In the dimer model the three terms describe the transfer of the quasi-particle between the two sites with transfer matrix element \( T \), the vibrational modes with frequency \( \omega \) and the coupling between quasiparticle and oscillator where \( \eta \) is the coupling constant. The subsystem of the quasiparticle can be considered as a spin system (with the spin-operators \( \sigma_j \)). This Hamiltonian can be applied to various other physical situations, e.g. the spin-\( \frac{1}{2} \) case of the Jaynes-Cummings model without rotating wave approximation.

2. Quasi-classical description and spectral statistics

In order to get quasi-classical equations of motion we use the time-dependent variational principle (TDVP) which is based on the fact that the solutions of the Schrödinger equation are just those functions for which the action

\[
S[\psi] = \int dt \langle \psi(t) | ( - i \partial_t + H) | \psi(t) \rangle = \int dt \mathcal{L} 
\]

(\( \langle \psi | \psi \rangle = 1 \)) is stationary [4,5].
Assuming that the combined quantum system behaves nearly classical, i.e. the correlations between boson and spin (quasi-particle) degrees of freedom are negligible, we are led to the factorized ansatz

$$|\psi(t)\rangle = e^{i\omega t |t|} |q(t), p(t)\rangle \otimes |s(t)\rangle,$$

where $|q(t), p(t)\rangle$ is a coherent state of the oscillator and $|s(t)\rangle$ is a state of the spin subsystem alone.

Inserting the ansatz, Eq. (3), in the Lagrangian $\mathcal{L}$ and performing the variation with respect to $q(t), p(t)$ and $s(t)$, we get equations of motion for the classical variables $q(t), p(t)$ and the spin state $|s(t)\rangle$. Additionally, we derive the equations of motion for the spin expectation values $\hat{s}_i(t) = i\langle s(t)|[H_s, \sigma_i]_+ |s(t)\rangle$, where $H_s$ is the spin part of the Hamiltonian. In this way, we arrive at

$$\begin{align*}
\dot{s}_x &= 2\sqrt{2}\omega \eta q s_x, \\
\dot{s}_y &= -2\sqrt{2}\omega \eta q s_x - 2Ts_z, \\
\dot{s}_z &= 2Ts_z, \\
\dot{q} &= p, \quad \dot{p} = -\omega^2 q - \sqrt{2}\omega \tau.
\end{align*}$$

These equations of motion can also be obtained by replacing the operators by corresponding c-numbers in the Heisenberg equations. For strong coupling $\eta$ and high energies this system shows chaotic behavior. A more detailed investigation of the system, Eq. (4), can be found in Refs. [1,2,6].

In order to investigate whether or not the system shows chaotic behavior in the quantum mechanical treatment we investigate the eigenvalue spectrum of the Hamiltonian of Eq. (1). We find avoided level crossings in the spectra (considering odd or even parity) which might be a sign of chaotic behavior (see Fig. 1a, solid lines). But the two-peak structure of the level spacing distribution (Fig. 1b, solid lines) derived from the spectra fits neither a Wigner distribution nor a Poissonian distribution which are typical for systems with chaotic and regular behavior, respectively, in their classical counterparts.

A more detailed investigation of the level spacings shows that the deviations from the dominating linear part ($\omega b^+ b$) seem to oscillate quite regularly. In order to understand this seemingly regular behavior we consider the strong coupling limit analytically. For strong coupling $\eta$, the dynamics of the system is essentially governed by the combined vibronic/two-level normal mode oscillations originating from the diagonalization of the last two terms $H_{\text{vib, int}}$ of Hamiltonian of Eq. (1). Using the unitary transformation

$$U = \exp\left(\frac{\eta \sigma_z}{\omega} (b^\dagger b - \bar{b})\right),$$

the part $H_{\text{vib, int}}$ can be put into diagonal form. Applying this transformation to the full
Hamiltonian of Eq. (1) we get the transformed one
\[ \hat{H} = \mathbb{H}^{-1} H \mathbb{H} \]
with
\[ \mathbb{H} = \hat{b} + \frac{\epsilon}{2} - \frac{\eta^2}{2} + T'[\mathscr{A}(\gamma)\sigma^+ + \mathscr{A}(\gamma)\sigma^-]. \]

(6)

Here \( \sigma^\pm \) represent the spin-flip operators and \( \gamma(t) = e^{t\gamma t^{-}\gamma} \) is the displacement operator \([7]\).

For simplicity of notation, we introduced \( \gamma = 2\eta/\omega \).

In the analytical calculation we neglect the contribution of the non-diagonal boson matrix elements and obtain approximate eigenvalues, where \( L_n \) are the Laguerre polynomials:
\[ E^+_n = \omega n + \frac{\epsilon^2}{2} - \frac{\eta^2}{2} \mp (1)^n T e^{-\omega^2/2} L_n(x^2). \]

(7)

The comparison with the numerical diagonalization of the Hamiltonian shows very good agreement in the strong coupling range with the spectra (Fig. 1a, \( \gamma \geq 3 \)) and with the level spacings (even for \( \gamma \approx 1 \), Fig. 1b).

In contrast to the classical equations, Eq. (4), the equations
\[ \dot{s}_x = -2T e^{-i\gamma t/p} \sin(\gamma p) \hat{s}_z, \]
\[ \dot{s}_y = -2T e^{-i\gamma t/p} \cos(\gamma p) \hat{s}_z, \]
\[ \dot{s}_z = 2T e^{-i\gamma t/p} \{ \sin(\gamma p) \hat{s}_x + \cos(\gamma p) \hat{s}_y \}, \]
\[ \dot{q} = \hat{p} - i \gamma T e^{-i\gamma t/p} \{ \sin(\gamma p) \hat{s}_x + \cos(\gamma p) \hat{s}_y \}, \]
\[ \dot{p} = -\omega^2 \hat{q}. \]

(8)

\( t' = \gamma \sqrt{2/\omega} \) derived from the transformed Hamiltonian \( \hat{H} \) using the TDVP, show a regular behavior especially in the strong coupling limit because the exponential factor \( e^{-i\gamma t/p} \) leads to nearly decoupled equations for spin and oscillator. Effectively, the transfer matrix element is reduced to \( T e^{-\omega^2/2} \) as compared to the corresponding Heisenberg equations, which is caused by the fluctuations \( \langle P^n \rangle - \langle P \rangle^n \neq 0 \) in the boson mode \( Q = (1/\sqrt{2})(b^+ + b), \quad P = i \sqrt{\omega^2/2}(b^+ - b) \). In contrast to the linear coupling \( \propto \sigma Q \) in Eq. (1) we have coupling terms of infinite order in \( P \) (sine and cosine functions, if we express the boson operators in Eq. (6) as oscillator coordinate and momentum operators).

3. Quantum mechanical dynamics

In this section we investigate the time evolution of the state vector \( |\psi(t)\rangle \) for various initial conditions, especially for strong coupling (more detailed discussions can be found in Ref. [2]). The time propagation can be calculated in the basis of the simultaneous eigenvectors of \( h^\dagger h \) and \( \sigma_z \):
\[ |\psi(t)\rangle = \sum_{n=0}^{\infty} C_n(t)|n\rangle + \sum_{n=0}^{\infty} C_n(t)|n\rangle. \]

(9)

In this representation the Schrödinger equation for the Hamiltonian of Eq. (1) is equivalent to the set of first-order differential equations for the coefficients \( C_n(t) \) and \( C_n(t) \).

The time dependence of a state vector \( |\psi(t)\rangle \) governed by the original Hamiltonian \( H \), Eq. (1), may equivalently be described by a state vector \( |\bar{\psi}(t)\rangle \) governed by the transformed Hamiltonian \( \bar{H} \), Eq. (6). The relation between corresponding states and operators is given via the unitary transformation of Eq. (5). For an initially coherent state \( |\psi_0\rangle = |q_0,p_0\rangle \otimes |\uparrow\rangle \), \( s_0 = (\phi_0,\theta_0) \) we get
\[ |\bar{\psi}(t)\rangle = e^{-i\omega t/\sqrt{2}} (|q_0 - \gamma/2, p_0 \rangle \otimes |\uparrow\rangle + \sin(\omega t/\sqrt{2}) |q_0 + \gamma/2, p_0 \rangle \otimes |\downarrow\rangle). \]

(10)

Considering the dynamics of the transformed system described by the Hamiltonian in Eq. (6), it was found from the classical equations, Eq. (8), that in the strong coupling limit the spin-part shows only a minor time dependence, whereas the boson mode performs a simple rotation in its phase space, the \((q,p)\)-plane.

Starting with a Bose/spin coherent state polarized in positive \( \sigma_z \) direction \( |\psi_0\rangle = |q_0,p_0\rangle \otimes |\uparrow\rangle \), we can consider the time dependence of the state in the transformed system \( |\bar{\psi}(t)\rangle = |q_0, p_0 \rangle \otimes |\uparrow\rangle \), which is obviously a Bose/spin coherent state with \( \bar{q}_0 = q_0 - \gamma/2, \bar{p}_0 = p_0 \). The time dependence of \( |\bar{\psi}(t)\rangle \) can now be approximated by the expression
\[ |\bar{\psi}(t)\rangle = e^{i\omega t} |q_0, p_0 \rangle \otimes |\uparrow\rangle, \]

where the additional phase \( \phi(t) \) accounts for the time dependence of the quantum phase. (see Ref. [2]). In the original system (applying the
transformation $\pi$ to the corresponding operators)
$q(t)$ and $p(t)$ are explicitly given by

\[ q(t) = \gamma/2 + (q_0 - \gamma/2) \cos(\omega t) + (p_0/\omega) \sin(\omega t), \]

\[ p(t) = p_0 \cos(\omega t) - \omega(q_0 - \gamma/2) \sin(\omega t). \]

Hence, $|\psi(t)\rangle$ will perform an elliptic motion around the center $q = \gamma/2$, $p = 0$.

In particular, for the initial state $q_0 = \gamma/2$ and $p_0 = 0$, the state vector will show no motion and thus will appear to be trapped at this point. Obviously, similar arguments will hold for a state polarized in negative $\sigma_z$ direction. These predictions, based on the results of the quasi-classical treatment in the transformed system, fit perfectly to the results of the quantum treatment, i.e. the numerical integration of the Schrödinger equation using the expansion in Eq. (9) for the state vector. The infinite sums were truncated at an appropriate number of states $N$, determined by the dynamical behavior of the system.

For states starting in the vicinity of a trapped state we also get good agreement between quantum and classical description. The Q-function performs a rotation around the trapped state. There is no significant difference between quantum mean-value and quasi-classical calculation concerning the oscillator variables, whereas the quantum mean-value of the spin-operator varies smoothly as compared to its quasi-classical counterpart.

4. Conclusions

We have investigated the properties of a system described by a harmonic oscillator coupled to a two-level system. We used an approach complementary to the usual quasi-classical treatment. Identifying an integrable Hamiltonian in the strong coupling case, we found that, especially in the strong coupling limit, the system is nearly integrable in contrast to the pronounced chaotic behavior of the usual quasi-classical description. Although both Hamiltonians considered are equivalent (related by an unitary transformation $\pi$), the resulting quasi-classical equations lead to a qualitatively different (chaotic/regular) behavior.

Thus the transition from the quantum description to the quasi-classical approximation depends on the selection of a suitable reference Hamiltonian. Considering the quasi-classical treatment using the transformed Hamiltonian we can identify quantum initial states where a quasi-classical approximation is reasonable. Furthermore, we can find trapped states even in the quantum mechanical treatment.

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References