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Finite temperature variational analysis of the tunneling and localization in spin–phonon model

Zoran Ivić [a,*], Dragan Kostić [a], Darko Kapor [b]

[a] *The "Vinča" Institute of Nuclear Sciences, Theoretical Physics Department, 020, 11001 Belgrade, P.O. Box 522, Serbia and Montenegro*
[b] *Department of Physics, Faculty of Sciences, University of Novi Sad, Trg D. Obradovića 4, Novi Sad, Serbia and Montenegro*

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Abstract

Temperature dependence of the effective tunneling frequency of the spin–phonon model for a few particular types of coupling has been studied within the framework of the simple variational method.

Our analysis shows that for the Ohmic type of coupling, temperature drives the system towards delocalization. The same type of behavior has been noticed for super-Ohmic case, but in the so-called "adiabatic regime", while in the nonadiabatic case we predict localization transition, analogous to that observed for Ohmic coupling, when temperature dependent coupling constant $S(T)$ approaches critical value $S(T) \sim 1/2$. In contrast to these results, for super-Ohmic ($r = 3$) case, there was no substantial difference with respect to zero-temperature case. Brief discussion of the validity of the method has been given.

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A simple model representing a particle tunneling between the two equivalent minima coupled to a collection of the harmonic oscillators, which simulate the influence of the dissipative environment (phonons for example), provides a good basis for the study of the underlying microscopic mechanisms describing the various phenomena in chemical and physical [1–9] and even in the biological systems [10–12]. Particular interest in this model has originated recently due to the development of the new theoretical techniques and their application in the examination of the modern fundamental concepts such as macroscopic quantum coherence and tunneling [1,3].

* Corresponding author.
E-mail address: zivic@rt270.vin.bg.ac.yu (Z. Ivić).

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Essential features of the system may be described on the basis of the well-known spin–phonon (or equivalently spin–boson) Hamiltonian:

$$H = -J\sigma_z - \sigma_x \sum_q \left(\lambda_q^* b_q + \lambda_q b_q^\dagger\right) + \sum_q \hbar\omega_q b_q^\dagger b_q, \tag{1}$$

where $2J$ defines so-called tunneling matrix element, $b_q^\dagger$ and b_q are Bose operators creating and annihilating the phonon quanta of frequency ω_q, σ_i $(i = x, y, z)$ are Pauli matrices, while λ_q denotes the coupling parameter. Each particular application is specified through the choice of the explicit q-dependence of the λ_q and ω_q or by the particular choice of the spectral density of states whose connection to phonon dispersion law and spin–phonon coupling parameter is defined as: $\mathcal{J}(\omega) = \sum_q |\lambda_q|^2 \delta(\omega - \omega_q)$. Its particular choice in the form $\mathcal{J}(\omega) \sim \omega^r e^{-\omega/\omega_B}$ (ω_B—cut off frequency), describes a variety of realistic situations in a various contexts.

The problem of major concern is the examination of the system dynamics in dependence of (i) the mutual ratio of the values of the basic physical parameters determining the energy spectrum of the system: ω_B—width of the phonon band, tunneling splitting—$2J$ and $E_B = \sum_q |\lambda_q|^2/(\hbar\omega_q)$—the ground state energy of the system in the absence of tunneling ($J = 0$), and (ii) the type of coupling and the nature of phonons which are specified by the explicit q dependence of the ω_q and λ_q or by the particular choice of the exponent r in the expression for the spectral density of states.

This problem has been extensively studied by means of various theoretical tools and it was found that the system can display regimes with substantially different physical behavior in dependence of the values of coupling constant ($S = \frac{E_B}{\hbar\omega_B}$) and adiabatic parameter ($B = \frac{2J}{\hbar\omega_B}$). Thus in the weak coupling limit, the mean position of the particle exhibits damped oscillations between localized states with transition to an exponential decay when the friction constant exceeds the bare tunneling frequency [6].

On the other hand, in the strong coupling regime, particle substantially influences the phonon subsystem which in turn affects system dynamics considerably and, in the final instance, the suppression of the tunneling (localization) may arise [1,3,9,13–16]. In that sense, depending on the value of the adiabatic parameter, two physically very distinct situations emerge.

In particular, we found [15] that, irrespectively of the type of coupling, the whole parameter space of the system, comprised by the adiabatic parameter and coupling constant ((S, B)-plane in other words), is divided in two distinct regions corresponding to the two different mechanisms of the lattice response (reaction field), which dominate tunneling dynamics and which, in final instance, may lead to a localization. In the first one, so-called symmetry preserving region, system dynamics is determined by the quantum nature of the phonon field and localization is achieved through the reduction of the effective tunneling frequency. In the second region (symmetry breaking [15]), particle can highly affect the medium which in turn substantially modifies its dynamics and may cause localization. Transition between these two regions is determined by so-called symmetry breaking boundary. This is the line in (S, B)-plane, whose explicit form is different for each type of coupling. In the strong coupling limit all these curves converge towards the $S \simeq B/4$. In this region the tunneling frequency is slightly reduced and tends to its bare value in the strong coupling limit while the system dynamics may be described by a discrete nonlinear Schrödinger equation [17–19]. Analogous, slightly modified, results were found by Kireev and Mann [20] who used improved interpolation variational method taking into account also phonon squeezing.

In the present paper we shall examine the system properties in the symmetry preserving region. In particular, we shall restrict ourselves to the examination of the behavior of the effective tunneling frequency in dependence of system parameters, type of coupling and temperature. For that purpose we shall use a temperature dependent variational method of Silbey and coworkers [7] utilized in the analysis of the dynamics of the spin–phonon model. In respect to that treatment of the problem which deals with the strict antiadiabatic limit ($B \ll 1$), here we shall extend such an approach towards the adiabatic limit. In particular, we shall focus our attention to the examination how the temperature modifies previously [14] observed characteristic dependence of the effective tunneling frequency on the coupling constant and adiabatic parameter. Thus, following [7], we first perform the modified Lang–Firsov unitary transformation [21] of the system Hamiltonian