Tunneling of a quantum breather in a one-dimensional chain

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We investigate a chain of particles (bonds) with harmonic interbond and anharmonic intrabond interactions. In the classical limit we consider a breather solution that is strongly localized (essentially a single-site excitation). For the quantum case we study tunneling of this excitation to a neighboring site. In that case we neglect the anharmonicity except for the two sites between which the tunneling occurs. Within this model the breather tunneling reduces to the tunneling in a dimer coupled to two adjacent harmonic chains. Application of Feynman's path instanton technique yields the tunneling splitting ΔE. For the isolated dimer we reproduce the exponential factor for the splitting $\Delta E^{(0)}$, obtained earlier by a perturbative approach. Assuming the frequency ω of the breather to be much larger than the inverse instanton width we use an adiabatic approximation to derive ΔE for the dimer coupled to the harmonic chains. We find that ΔE can be obtained from $\Delta E^{(0)}$ just by scaling the Planck constant. We argue that independent of the density of states of the harmonic chains tunneling can never be suppressed, if ω is large enough. [S1063-651X(98)11407-1]

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I. INTRODUCTION

Initiated by early papers of Ovchinnikov [1], Kosevich *et al.* [2], and Takeno *et al.* [3,4] there exists now a clear understanding of the generic existence of discrete breathers. These classical solutions to the Hamiltonian equations of motion are time periodic and spatially localized. They are structurally stable provided the plane wave spectrum of small amplitude excitations has finite bounds. This can be achieved by considering a spatial lattice, with degrees of freedom associated to each lattice site. Existence proofs demonstrate that the existence of these solutions is not restricted to low lattice dimensions [5]. (For reviews on this subject, see [6,7].)

A logical step is then to consider the fate of these classical solutions in the presence of quantum fluctuations. We may think about a quantum object corresponding to a breather solution. Contrary to a classical breather, localized in the vicinity of a certain lattice site, such a quantum object will be able to tunnel from site to site, forming a quantum breather band. Taking into account the coupling of the breather to its environmental degrees of freedom may strongly influence the tunneling probability amplitude. Therefore the central issue is to calculate the probability amplitude of the breather intersite tunneling, which will determine the width of the band. An interesting question may be whether such an effect, known for particle tunneling (see, e.g., [8,9]) as tunneling suppression in the Ohmic case, can be observed for the quantum breathers as well. It is worthwhile mentioning in this context that quantization of solitons (other nonlinear objects that are close but certainly different from breathers) was discussed in the literature; see, e.g., [10]. Tunneling of fluxons in Josephson junction chains (soliton solutions of the sine-Gordon equation) interacting with plasmons was recently considered in [11].

Since classical breathers can be localized essentially on one site (bond), one can start by considering a system of just two sites (bonds), for example, the dimer discussed in [12,13]. Classical trajectories in this system may be not invariant under permutation of the sites (bonds), whereas the Hamiltonian is invariant. Quantization yields pairs of eigenstates, corresponding to these classical symmetry breaking trajectories, with exponentially small splittings of the eigenenergies.

This dimer model is particularly interesting, because its classical version is an integrable system, due to the existence of two integrals of motion that are the total dimer energy E and a measure J for the intensity of the classical excitation. The pairs of eigenstates of the quantum dimer correspond to tunneling between tori in the classical phase space. This type of problem has already been studied earlier by several authors (see, e.g., [14,15]). Two cases were considered that are, respectively, dynamical and potential tunneling. The latter is what one usually understands as tunneling, i.e., a quantum transition of a particle through a potential barrier in a configuration space that is energetically forbidden in classical mechanics, whereas the former corresponds to tunneling in the phase space where no such energy barrier exists. Despite the absence of the energy barrier no classical solution of Newton's equation of motion exist that connects the two tori.

In the case of the two tori that appear in [12,13], as will be shown in the next section, an effective potential barrier can be defined and the problem of dynamical tunneling can be mapped onto a potential tunneling. This becomes possible since the dimer has two conservation laws. If we were left with just the energy conservation, we would be faced with a

proper dynamical tunneling again (see [16]).

The tunneling splitting for all the levels of the dimer was calculated in Ref. [13]. However, to study a possible delocalization of the classical breather due to quantum behavior one has to investigate an extended system. A step in this direction was made in the paper [16] where a dimer coupled to a single harmonic oscillator was studied. A consideration of an extended system with a macroscopic number of bonds is the principal aim of this paper, which will be organized as follows. The next section introduces an extended model with N bonds and then shows that subdiving this chain into a dimer coupled to adjacent harmonic chains may be a good approximation. Section III reinvestigates the isolated dimer, classically and quantum mechanically, and uses Feynman's path integral method in order to derive the exponential factor that mainly determines the tunneling splitting. The extended model will be studied in Sec. IV, where the main result of our paper will be derived. The final section contains a discussion and some conclusions.

II. MODEL

We are going to consider the quantum tunneling of a breather in a one-dimensional chain described by the Hamiltonian

$$H=\frac{\omega_0}{2}\sum_i (p_i^2+x_i^2)+\frac{\gamma}{8}\sum_i (p_i^2+x_i^2)^2 + C\sum_i (x_i x_{i+1}+p_i p_{i+1}). \tag{2.1}$$

Here the label i numbers the bonds. It will be assumed in what follows that the breather is strongly localized and corresponds actually to an excitation of only one bond in this chain. Then tunneling will correspond to transferring this excitation to a neighboring bond. Since all the other bonds remain lowly excited during this process we may neglect the corresponding anharmonic terms in Eq. (2.1). However, the anharmonicity in the two bonds participating in the tunneling transfer will be fully taken into account. Then the problem reduces to a consideration of tunneling in a dimer coupled to a bath represented by two harmonic chains. The system is described by the Hamiltonian

$$H=H_d+H_{ph}+H_1, \tag{2.2}$$

where

$$H_d=\sum_{\alpha=1,2}\left[\frac{\omega_0}{2}(p_\alpha^2+x_\alpha^2)+\frac{\gamma}{8}(p_\alpha^2+x_\alpha^2)^2\right]+C(x_1x_2+p_1p_2) \tag{2.3}$$

represents the dimer of two bonds (chosen to be 1 and 2), which may be strongly excited. The bath is represented by the remaining part of the chain

$$H_{ph}=\frac{\omega_0}{2}\sum_{n\neq 1,2}(p_n^2+x_n^2)+C\sum_{n\neq 0,1,2}(x_n x_{n+1}+p_n p_{n+1}) \tag{2.4}$$

in which the anharmonic terms are omitted. The interaction between the dimer and the harmonic bath is given by

$$H_1=C(x_0x_1+p_0p_1+x_2x_3+p_2p_3). \tag{2.5}$$

The harmonic part (2.4) consists of two open ended harmonic chains, each of which can be diagonalized by means of the transformation

$$x_n=\sum_\mu \begin{cases} x_\mu^L \mathcal{N}_\mu^L \sin q_\mu^L(n-1), & -(N_L-1)\leqslant n\leqslant 0 \\ x_\mu^R \mathcal{N}_\mu^R \sin q_\mu^R(n-2), & 3\leqslant n\leqslant N_R+2 \end{cases}$$

and

$$p_n=\sum_\mu \begin{cases} p_\mu^L \mathcal{N}_\mu^L \sin q_\mu^L(n-1), & N_L-1\leqslant n\leqslant 0 \\ p_\mu^R \mathcal{N}_\mu^R \sin q_\mu^R(n-2), & 3\leqslant n\leqslant N_R+2. \end{cases}$$

The superscripts L and R denote the left and right hand chains with N_L and N_R bonds, respectively. The wave numbers $q_\mu^L=\pi\mu/(N_L-1), \mu=1,\ldots,N_L$, $q_\mu^R=\pi\mu/(N_R+1), \mu=1,\ldots,N_R$, and $\mathcal{N}_\mu^{L/R}$ are normalization coefficients.

Equation (2.4) now reads

$$H_{ph}=\frac{1}{2}\sum_\mu \lambda_\mu^L[(p_\mu^L)^2+(x_\mu^L)^2]+\frac{1}{2}\sum_\mu \lambda_\mu^R[(p_\mu^R)^2+(x_\mu^R)^2], \tag{2.6}$$

where the eigenfrequencies are $\lambda_\mu^{L/R}=\omega_0+2C\cos q_\mu^{L/R}$. The interaction in the normal coordinates becomes

$$H_1=\sum_\mu C_\mu^L(x_1x_\mu^L+p_1p_\mu^L)+C_\mu^R(x_2x_\mu^R+p_2p_\mu^R), \tag{2.7}$$

where $C_\mu^L=-C\mathcal{N}_\mu^L \sin q_\mu^L$ and $C_\mu^R=C\mathcal{N}_\mu^R \sin q_\mu^R$.

The problem of breather tunneling reduces now to investigating the tunneling transfer of an excitation from one bond of the dimer to the other under the influence of the harmonic bath. On one hand this problem differs from the standard problem of a particle tunneling between two minima in a double-well potential in the configuration space, since here we deal with dynamical tunneling from one torus to another in the phase space. On the other hand there are many similarities in these two problems, which will be discussed in what follows.

III. TUNNELING IN THE DIMER

Tunneling in the dimer described by the Hamiltonian H_d (2.3) was studied in detail in [12,13]. Here we try to approach the problem by means of the path integral technique and obtain some results that will be necessary for our more general problem.

A. Classical properties

The canonical transformation

$$y=\tfrac{1}{4}[x_2^2+p_2^2-x_1^2-p_1^2],$$

$$\varphi=\arctan\frac{p_2}{x_2}-\arctan\frac{p_1}{x_1},$$

$$J=\frac{1}{2}[x_2^2+p_2^2+x_1^2+p_1^2],$$

$$\chi=\frac{1}{2}\left(\arctan\frac{p_2}{x_2}+\arctan\frac{p_1}{x_1}\right) \tag{3.1}$$

allows one to represent the dimer Hamiltonian (2.3) in the form

$$H_d=\omega_0 J+\gamma\left(\frac{J}{2}\right)^2+\gamma y^2+2C\sqrt{\left(\frac{J}{2}\right)^2-y^2}\cos\,\varphi. \tag{3.2}$$

Here y and J play the roles of the coordinates while φ and χ are the corresponding momenta. The Hamiltonian H_d does not depend on the momentum χ, which means that its conjugate coordinate J is one of the two integrals of motion. The following restrictions should be also applied: $|y|<J/2$ and $|\varphi|<\pi/2$.

The second integral of motion is the total energy E. Since the Poisson bracket of J and H_d vanishes, the dimer model is integrable. The momentum φ is excluded from the Hamiltonian equations of motion by means of the energy conservation and the equation

$$\ddot{y}=-\frac{dV(y)}{dy} \tag{3.3}$$

is obtained, which describes motion along the coordinate y at a given energy E in the potential

$$V(y)=\frac{\gamma^2}{2}y^4-\gamma\left[E-\omega_0 J-\gamma\left(\frac{J}{2}\right)^2-2\frac{C^2}{\gamma}\right]y^2. \tag{3.4}$$

Note that the motion described by Eq. (3.3) is not exactly the same as the motion of a particle in a usual double-well potential. The difference is due to the fact that the two integrals of motion, the conserved total energy E of the dimer and the amplitude J, play now the role of parameters. Thus the shape of the potential $V(y)$ depends explicitly on E and J, which is a consequence of dealing with the dynamics in the four-dimensional phase space of the dimer. [This is a general property of an integrable system with two degrees of freedom and a separatrix that separates symmetry noninvariant from symmetry invariant trajectories. The Hamiltonian is assumed to be invariant under the discrete symmetry operation P with $P^2=1$. The two actions J_1 and J_2 in one of the symmetry broken phase space regions parametrize the isolated periodic orbits (J_1) and its quasiperiodic perturbations J_2, where $\omega_2=\partial H/\partial J_2$ vanishes on the separatrix. Performing now a canonical variable transformation $\{J_1,J_2,\phi_1,\phi_2\}\rightarrow\{J_1,z,\phi_1,p_z\}$ will lead to a Hamiltonian $H(J_1,z,p_z)$. Fixing J_1 (which is the boson number in our case) leads to an effective one-particle problem. This case can be finally always described by an effective potential, which will depend on both the total energy H and the chosen value for the action J_1.]

Multiplying Eq. (3.3) by $\dot{y}$ it follows that the quantity

$$E_t=\tfrac{1}{2}\dot{y}^2+V(y)=-\tfrac{1}{2}(E-E_1)(E-E_2)$$

with

$$E_1=\omega_0 J+\gamma J^2/4+CJ,\quad E_2=\omega_0 J+\gamma J^2/4-CJ \tag{3.5}$$

does not vary in time. E_t plays the role of the effective energy for the motion described by Eq. (3.3). Note that E_t does not coincide with the real energy E of the dimer. They are even measured in different units.

The potential (3.4) becomes a double-well potential if the coefficient of the y^2 term is negative. In order to have a permutation symmetry breaking trajectory the condition

$$0>E_t\geqslant-\frac{1}{2}\left[E-\omega_0 J-\gamma\left(\frac{J}{2}\right)^2-2\frac{C^2}{\gamma}\right]^2$$

has to be satisfied.

It follows from Eq. (3.2) that for $\gamma J\leqslant 2C$ the choice of the possible energies is restricted by the conditions

$$E_1\geqslant E\geqslant E_2, \tag{3.6}$$

which implies that E_t is positive in this case. Then only symmetry conserving periodic trajectories are possible. At $\gamma J=2C$ a bifurcation occurs, and for $\gamma J>2C$ the energy range $E_1<E<E_3=\omega_0 J+\gamma J^2/2+C^2/\gamma$ becomes accessible to permutation symmetry broken trajectories. These are the conditions for an appearance of permutation symmetry broken isolated periodic orbits as described in Ref. [13].

A permutation symmetry broken trajectory means that the system dwells in one of the two wells of the potential (3.4). Now we are able to consider tunneling from one minimum of the potential $V(y)$ to the other one applying the standard formulation of the instanton technique in the path integral approach. This will be done first for the isolated dimer and then for the dimer interacting with the bath.

B. Quantum properties

The amplitude of the tunneling transition in the potential $V(y)$ can be found by calculating the phase space path integral [17]

$$Z=\int \mathcal{D}[y]\int \mathcal{D}[\varphi]\int \mathcal{D}[J]\int \mathcal{D}[\chi]\exp\left\{\frac{i}{\hbar}\int_{-T/2}^{T/2}\left[-J(t)\dot{\chi}(t)-y(t)\dot{\varphi}(t)+S[y(t),\varphi(t),J(t),\chi(t)]\right]\right\}, \tag{3.7}$$

where

$$S_d[y(t),\varphi(t),J(t),\chi(t)]=S_-(T/2)-S_-(-T/2)+S_+(T/2)-S_+(-T/2)+\overline{S_d},$$

$$\overline{S_d}=-\int_{-T/2}^{T/2}H_d(y(t),\varphi(t),J(t))dt \tag{3.8}$$

and

$$S_\pm(t)=\tfrac{1}{4}[J(t)\pm 2y(t)]\sin[2\chi(t)\pm\varphi(t)].$$

Note that in contrast to the usual phase space path integral representation, we have performed a partial integration in the exponent. Choosing the dimer energy $E=E_3$ we may consider the tunneling motion between the two minima of the potential $V(y)$ located at $y_\pm=\pm\sqrt{J^2/4-C^2/\gamma^2}$. This means that the integral in the action (3.8) should be calculated using the conditions that $y(T/2)=y(-T/2)=y_+$ or y_- and $J(T/2)=J(-T/2)=J_0$. For $\gamma J_0>2C$ the value of J_0 (integral of motion for the classical paths) characterizes the particular tunneling process. This procedure corresponds to calculating the splitting due to the phase space tunneling between the two isolated periodic orbits

$$y_\pm=\pm\sqrt{J_0^2/4-C^2/\gamma^2},\quad \varphi=0,\quad J=J_0,\quad \chi=-(\omega_0+\gamma J_0)t. \tag{3.9}$$

Since H_d does not depend explicitly on χ, the path integration over χ and then over J can be carried out straightforwardly. One can see from this integration that only the paths along which $J(t)\equiv J_0$ contribute to the integral (3.7). Then keeping only the terms relevant to tunneling one obtains

$$Z\sim\int \mathcal{D}[y]\int \mathcal{D}[\varphi]\exp\left\{\frac{i}{\hbar}\left[-\int_{-T/2}^{T/2}y(t)\dot{\varphi}(t)-H_d[y(t),\varphi(t),J_0]\right]\right\}. \tag{3.10}$$

Switching to the imaginary time, $t=-i\tau$, one finds for $T\to\infty$ the well-known instanton for the potential (3.4) with $E=E_3$:

$$y(\tau)=\sqrt{\frac{J_0^2}{4}-\frac{C^2}{\gamma^2}}\tanh\left\{\gamma\tau\sqrt{\frac{J_0^2}{4}-\frac{C^2}{\gamma^2}}\right\}, \tag{3.11}$$

corresponding to the imaginary time solution of Eq. (3.3). Then the tunneling splitting becomes

$$\Delta E\sim e^{-(1/\hbar)S_E}, \tag{3.12}$$

where the Euclidean action is calculated with the help of the instanton (3.11),

$$S_E=-\sqrt{J_0^2-4C^2/\gamma^2}+J_0\ln\left(\frac{2C\gamma}{\gamma J_0-\sqrt{\gamma^2J_0^2-4C^2}}\right).$$

Comparing this result with the results obtained in [12,13] by the perturbation theory approach by taking into account that J_0 has to be replaced by its quantized value $J_0=n\hbar$, $n=0,1,2,\ldots$, we find that they coincide up to the preexponential factor. The latter can be found by properly accounting for the quantum fluctuations in the above path integral. Unfortunately, the action (3.8) contains a kinetic term proportional to $\cos\varphi$, rather than a quadratic form, which complicates the calculation of the quantum fluctuations. Nevertheless, while considering tunneling of a breather interacting with the harmonic bath we will be able to arrive at a certain conclusion concerning this preexponential factor as well.

IV. BREATHER IN THE 1D CHAIN

A. Classical properties

In order to consider tunneling in the 1D chain described by the Hamiltonian (2.2) we study some of its classical properties first. To be more specific we need to find isolated periodic orbits between which the quantum phase space tunneling occurs. This can be achieved by applying the same trick as in Refs. [13,16]. The system has two integrals of motion one of which is the total energy, i.e., the Hamiltonian itself, and the second one is the quantity

$$B=\frac{1}{2}\sum_{i=-N_L}^{N_R}(p_i^2+x_i^2).$$

Hence, we can find isolated periodic orbits by using the condition $\nabla H=\omega\nabla B$ in the phase space. This condition directly leads to the equations

$$x_\mu^{L/R}=\frac{C_\mu^{L/R}}{\omega-\lambda_\mu^{L/R}}x_{1/2},$$

$$p_\mu^{L/R}=\frac{C_\mu^{L/R}}{\omega-\lambda_\mu^{L/R}}p_{1/2},$$

which allow one to eliminate the bath coordinates. Then applying also the canonical transformation (3.1) and assuming that the left hand chain is identical to the right hand chain, one finds isolated periodic orbits in the form

$$y_\pm=\pm\sqrt{J_0^2/4-C^2/\gamma^2},\quad \varphi=0,\quad J=J_0,\quad \chi=-\omega t \tag{4.1}$$

with ω defined by the equation

$$\omega_0+\gamma J_0+\sum_\mu \frac{2C_\mu^2}{\omega-\lambda_\mu}=\omega. \tag{4.2}$$

Comparing this solution with Eq. (3.9) we find that it has the same structure as for the isolated dimer and only the coefficient in the linear time dependence of the momentum χ is now renormalized due to the interaction with the bath. We also obtain the energy

$$E=E_3+2J_0\sum_\mu (2\omega-\lambda_\mu)\frac{C_\mu^2}{(\omega-\lambda_\mu)^2}$$

of the system corresponding to such an isolated orbit. It contains two terms corresponding to the dimer and all the other, bath, degrees of freedom separately. It is interesting to note that the energy E_3 of the dimer is also a conserved quantity, meaning that when moving along this orbit there is no exchange of energy between the dimer and the remaining part of the chain.

B. Quantum properties

Now we will consider how the interaction with the harmonic bath influences the tunneling in the dimer between the two isolated orbits (4.1) found in the previous subsection. Let us calculate the path integral

$$Z=\prod_\mu \int_{-\infty}^{\infty}dx_{0\mu}^L\int_{-\infty}^{\infty}dx_{0\mu}^R\int \mathcal{D}[x_\mu^L(t)]\int \mathcal{D}[p_\mu^L(t)]\int \mathcal{D}[x_\mu^R(t)]\int \mathcal{D}[p_\mu^L(t)]\int \mathcal{D}[y(t)]\int \mathcal{D}[\varphi(t)]\int \mathcal{D}[J(t)]\int \mathcal{D}[\chi(t)]$$

$$\times\exp\left\{\frac{i}{\hbar}\int_{-T/2}^{T/2}dt\left[-\sum_\mu (\dot{x}_\mu^L p_\mu^L+\dot{x}_\mu^R p_\mu^R)-J\dot{\chi}-y\dot{\varphi}+S[y,\varphi,J,\chi,\{x_\mu^L\},\{p_\mu^L\},\{x_\mu^R\},\{p_\mu^R\}]\right]\right\}, \tag{4.3}$$

where

$$S[y,\varphi,J,\chi,\{x_\mu^L\},\{p_\mu^L\},\{x_\mu^R\},\{p_\mu^R\}]=S_-(T/2)-S_-(-T/2)+S_+(T/2)-S_+(-T/2)+\overline{S},$$

$$\overline{S}=-\int_{-T/2}^{T/2}H(y(t),\varphi(t),J(t),\{x_\mu^L(t)\},\{p_\mu^L(t)\},\{x_\mu^R(t)\},\{p_\mu^R(t)\})dt \tag{4.4}$$

with the Hamiltonian H defined by Eq. (2.2). The action (4.4) is calculated using the conditions that $x_\mu^L(-T/2)=x_\mu^L(T/2)=x_{0\mu}^L$ and $x_\mu^R(-T/2)=x_\mu^R(T/2)=x_{0\mu}^L$, all other conditions being the same as in the case of the isolated dimer. Note that in Eq. (4.3) we have taken the trace with respect to $x_{0\mu}^L$ and $x_{0\mu}^R$.

Integration over the harmonic coordinates is straightforward and the propagator (4.3) becomes (see, e.g., [18])

$$Z=\tilde{Z}\int \mathcal{D}[y(t)]\int \mathcal{D}[\varphi(t)]\int \mathcal{D}[J(t)]\int \mathcal{D}[\chi(t)]$$

$$\times\exp\left\{\frac{i}{\hbar}\int_{-T/2}^{T/2}dt[-J\dot{\chi}-y\dot{\varphi}]+\overline{S_d}[y,\varphi,J]+S_L[y,\varphi,J,\chi]+S_R[y,\varphi,J,\chi]\right\}, \tag{4.5}$$

where $\overline{S_d}$ is given by Eq. (3.8) and

$$S_{L,R}[y,\varphi,J,\chi]=\int_{-T/2}^{T/2}dt\int_{-T/2}^{T/2}dt'\sqrt{A_{L,R}(t)A_{L,R}(t')}[K_{L,R}(t-t')\cos\psi_{L,R}(t,t')+L_{L,R}(t-t')\sin\psi_{L,R}(t,t')] \tag{4.6}$$

with

$$K_{L,R}(t)=\frac{1}{2}\sum_{\mu}\ (C_{\mu}^{L,R})^2\frac{\cos\ \lambda_{\mu}^{L,R}(T/2-|t|)}{\sin\ \lambda_{\mu}^{L,R}T/2}$$

and

$$L_{L,R}(t)=\frac{1}{2}\mathrm{sgn}(t)\sum_{\mu}\ (C_{\mu}^{L,R})^2\frac{\sin\ \lambda_{\mu}^{L,R}(T/2-|t|)}{\sin\ \lambda_{\mu}^{L,R}T/2}.$$

Here

$$\psi_{L,R}(t,t')=\chi(t)-\chi(t')\mp\tfrac{1}{2}[\varphi(t)-\varphi(t')],$$

$$A_{L,R}(t)=J(t)/2\pm y(t);$$

$\tilde{Z}$ is the factor due to all the integrations carried out in Eq. (4.5). It also includes terms containing $S_{\pm}(\pm T/2)$. A detailed knowledge of $\tilde{Z}$ is not important for calculation of the tunneling splitting.

The action in the propagator (4.5) is rather complicated and is far from being a quadratic form. It contains also nonlocal terms $S_{L,R}[y,\varphi,J,\chi]$ due to the interaction of the breather with the phonon bath. Their structure, although resembling in many aspects the nonlocal terms in the standard potential tunneling problems (see, e.g., [8,19]), is now somewhat more complicated. On one hand this is due to the fact that the integrations over the momenta have not been carried out. On the other hand the very formulation of the problem is different. There is an additional pair of conjugated coordinates J and χ, which is important when considering the phase space tunneling. Also we have an additional restriction $J(T/2)=J(-T/2)=J_0$, to be taken into account.

C. Adiabatic approximation

A direct calculation of the path integral seems hardly possible unless some approximations are used. In order to understand what sort of an approximation can be appropriate here, we need to analyze the equations of motion for the dimer coordinates and momenta that can be obtained by minimizing the action in Eq. (4.5):

$$\dot{y}-\frac{\partial H_d}{\partial\varphi}+\int_{-T/2}^{T/2}dt'\sqrt{A_L(t)A_L(t')}[K_L(t-t')\sin\ \psi_L(t,t')-L_L(t-t')\cos\ \psi_L(t,t')]$$

$$-\int_{-T/2}^{T/2}dt'\sqrt{A_R(t)A_R(t')}[K_R(t-t')\sin\ \psi_R(t,t')-L_{\alpha}(t-t')\cos\ \psi_R(t,t')]=0, \tag{4.7}$$

$$\dot{\varphi}+\frac{\partial H_d}{\partial y}-\int_{-T/2}^{T/2}dt'\sqrt{A_L(t')/A_L(t)}[K_L(t-t')\cos\ \psi_L(t,t')-L_L(t-t')\sin\ \psi_L(t,t')]$$

$$+\int_{-T/2}^{T/2}dt'\sqrt{A_R(t')/A_R(t)}[K_R(t-t')\cos\ \psi_R(t,t')-L_R(t-t')\sin\ \psi_R(t,t')]=0, \tag{4.8}$$

$$\dot{J}-2\int_{-T/2}^{T/2}dt'\sqrt{A_L(t)A_L(t')}[K_L(t-t')\sin\ \psi_L(t,t')-L_L(t-t')\cos\ \psi_L(t,t')]$$

$$-2\int_{-T/2}^{T/2}dt'\sqrt{A_R(t)A_R(t,)}[K_R(t-t')\sin\ \psi_R(t,t')-L_R(t-t')\cos\ \psi_R(t,t')]=0, \tag{4.9}$$

$$\dot{\chi}+\frac{\partial H_d}{\partial J}-\frac{1}{2}\int_{-T/2}^{T/2}dt'\sqrt{A_L(t')/A_L(t)}[K_L(t-t')\cos\ \psi_L(t,t')-L_L(t-t')\sin\ \psi_L(t,t')]$$

$$+\frac{1}{2}\int_{-T/2}^{T/2}dt'\sqrt{A_R(t')/A_R(t)}[K_R(t-t')\cos\ \psi_R(t,t')-L_R(t-t')\sin\ \psi_R(t,t')]=0. \tag{4.10}$$

First of all we observe that the isolated periodic orbits found in Sec. IV A are solutions of the equations of motion. By substituting one of these isolated orbits, corresponding to say the y_+ minimum, one obtains the nonlocal action terms in the form

$$S_{L,R}[y,\varphi,J,\chi]=A_{L,R}\int_{-T/2}^{T/2}dt\int_{-T/2}^{T/2}dt'\tilde{K}_{L,R}(t-t') \tag{4.11}$$

where the kernel reads

$$\tilde{K}_{L,R}(t)=\frac{1}{2}\sum_{\mu}\ (C_{\mu}^{L,R})^2\frac{\cos[\lambda_{\mu}^{L,R}(T/2-|t|)-\omega|t|]}{\sin\ \lambda_{\mu}^{L,R}T/2} \tag{4.12}$$

and $A_L=J_0/2+y_+$, $A_R=J_0/2-y_+$.

This kernel is similar to the kernels encountered in the standard configuration space tunneling problems (see, e.g., [8,19]) except for the additional term $\omega|t|$ in the argument of the cosine function. This term ensures a rapid convergency of the integral (4.6) regardless of the phonon density of states provided ω is large enough compared to $\lambda_\mu^{L,R}$, which can be achieved if $\gamma J_0 > 2C$, which is the condition for the very existence of the breather in our system. It should be mentioned, in particular, that the internal breather frequency ω in the kernel makes the logarithmic divergency of the action appearing in the so-called Ohmic case for particle tunneling, as described in [8], impossible.

The frequency ω characterizes the isolated periodic orbit. Any motion with smaller frequencies can be considered as slow and an adiabatic approximation may be appropriate in such a case. This holds in particular for the instanton solution (3.11) of equations (4.7)–(4.10) (if rewritten in the imaginary time) and such an adiabatic approximation may be used when analyzing the phase space tunneling problem as well. A more detailed discussion of the applicability of this adiabatic approximation is given in the next section.

The rapid convergency of the integrals in the nonlocal terms of the action ensures that the main contribution is coming from $t-t'$ being small. Thus the dependence of the dimer coordinates on t' can be approximately represented as

$$\begin{aligned} J(t') &= J(t) + \dot{J}(t)(t-t') + \cdots, \\ y(t') &= y(t) + \dot{y}(t)(t-t') + \cdots, \\ \varphi(t') - \varphi(t) &= \dot{\varphi}(t)(t-t') + \cdots, \\ \chi(t') - \chi(t) &= -\omega(t-t') + \delta\dot{\chi}(t)(t-t') + \cdots. \end{aligned} \tag{4.13}$$

This expansion is substituted into the action in the exponent of Eq. (4.5) and integration over t' is carried out in the limit $T \to \infty$. Keeping the leading terms of the expansion the adiabatic approximation for the action is obtained

$$\begin{aligned} S_{\mathrm{ad}} = \int_{-\infty}^{\infty} dt \{ & J(t)(\omega + M_0) - J(t)(1+M_1)\delta\dot{\chi}(t) \\ & - y(t)(1+M_1)\dot{\varphi}(t) - H_d[y(t), \varphi(t), J(t)] \}, \end{aligned} \tag{4.14}$$

where

$$M_0 = \sum_\mu \frac{C_\mu^2}{\lambda_\mu - \omega} \tag{4.15}$$

and

$$M_1 = \sum_\mu \frac{C_\mu^2}{(\omega - \lambda_\mu)^2}. \tag{4.16}$$

Now all the terms in the action (4.14) are local and it can be directly compared with the results obtained for the isolated dimer. Actually we have now to calculate the propagator (3.7) using this new action. First the integration over $\delta\chi(t)$ again yields only the paths with $J(t) \equiv J_0$. Then changing integration variables, $\tilde{t} = t/(1+M_1)$, in the remaining part of the action one obtains the propagator in the form (up to factors irrelevant to tunneling)

$$\begin{aligned} Z \sim \int \mathcal{D}[y(\tilde{t})] \int \mathcal{D}[\varphi(\tilde{t})] \exp\Bigg\{ & -\frac{i(1+M_1)}{\hbar} \\ & \times \int_{-\infty}^{\infty} d\tilde{t} [\mathbf{y}(\tilde{t})\dot{\varphi}(\tilde{t}) - H_d[y(\tilde{t}), \varphi(\tilde{t}), J(\tilde{t})]] \Bigg\}. \end{aligned} \tag{4.17}$$

The propagator (3.10) can be transformed into the propagator (4.17) by scaling the Planck constant $\hbar \to \hbar/(1+M_1)$. This means that the splittings of the quantum breather levels due to tunneling in the chain can be obtained from the splitting found for the isolated dimer just by the same scaling.

V. DISCUSSION

We have studied the tunneling of a localized breather excitation in a chain of particles due to quantum fluctuations. For this purpose we used an extended version of a dimer model. The original dimer model was recently investigated classically and quantum mechanically [12,13]. Assuming that the breather is mainly localized on one bond, we replaced all the bonds by harmonic ones, except for two of them, thus allowing for tunneling from one bond to the other under the influence of the remaining harmonic bonds.

For the isolated dimer, i.e., when the harmonic chains and their coupling to the dimer are removed, we have applied the path integral technique and reproduced the result for the tunneling splitting $\Delta E_n^{(0)}$ obtained earlier within a perturbative approach. This agreement has been achieved for the exponential factor, which represents the main contribution to $\Delta E_n^{(0)}$. Taking the interaction with the harmonic chains into account we have calculated the propagator by use of an adiabatic approximation. The result (4.17) allows us to find an equation for the probability amplitude of the breather tunneling in the chain if we know the probability amplitude for the isolated dimer. For example, we may use Eq. (1.10) in Ref. [12] (a more general derivation can be found in [13]) derived perturbatively for the isolated dimer. The quantum number $n = J/\hbar$ is the number of bosons that comprise the breather. It is the only parameter in this equation containing the Planck constant $\hbar$. Applying the above scaling one arrives at the amplitude for a breather tunneling in the chain,

$$\Delta E = \frac{2\tilde{n}C}{(\tilde{n}-1)!}\left(\frac{C}{\gamma}\right)^{\tilde{n}-1}, \tag{5.1}$$

where $\tilde{n} = J(1+M_1)/\hbar$. For large values of $\tilde{n}$ the Stirling formula results in

$$\Delta E \approx \frac{2\tilde{n}C}{\sqrt{\tilde{n}-1}} \exp\left\{ -(\tilde{n}-1)\ln\frac{(\tilde{n}-1)\gamma}{eC} \right\}. \tag{5.2}$$

It is readily seen that the interaction with the bath diminishes the exponential factor due to the increase of the $\tilde{n}$ with respect to n (M_1 is always positive). This is the same type of

behavior as predicted in [20] for the influence of the bath on the configuration space tunneling.

Here we comment again on the quality of our adiabatic approximation. The nonadiabatic corrections in the action (4.14) are proportional to the quantity M_1, Eq. (4.16), which for $\omega \gg \max\{\lambda_\mu\}=\omega_0+2C$ can be estimated as $M_1 \sim C^2/\omega^2 \ll 1$. Direct analysis of the adiabatic expansion (4.13) shows that the next order terms in the action (4.6) will contain additional powers of the ratio $\omega_{\rm inst}/\omega$. From Eq. (4.2) one finds that the breather frequency ω is always larger than γJ_0. Therefore, the frequency, $\omega_{\rm inst}=\gamma J_0/2\sqrt{1-4C^2/\gamma^2 J_0^2}$, typical of the instanton is smaller than the breather frequency at least by a factor of 2. It may become especially small near the bifurcation point, when $2C/\gamma J_0$ is close to one. Hence, we expect the adiabatic expansion to be quite reasonable if the instanton frequency $\omega_{\rm inst}$ is small enough compared to the breather frequency ω.

It has been shown for the configuration space tunneling that the behavior of the density of states of the harmonic bath for frequencies close to zero strongly influences this renormalization. In the Ohmic or sub-Ohmic case the coupling to the bath may lead to a suppression of tunneling [9]. This effect, however, does not occur for the phase space tunneling of the breather for our model Hamiltonian (2.2)–(2.7) even if the phonon density of states corresponds to the Ohmic case. The reason for this can be seen from the nonlocal kernel in adiabatic approximation, (4.12). Choosing T such that $T\omega/2=2\pi\nu$ with ν being a positive integer the argument of the cosine in Eq. (4.12) can be rewritten as $(\lambda_\mu^{L,R}-\omega)(T/2-|t|)$. Since the breather frequency $\omega>0$ must be larger than the upper edge $\max\{\lambda_\mu\}=\omega_0+2C$ of the phonon band, there will be a gap, meaning that $\lambda_\mu^{L,R}-\omega$ never becomes zero. Consequently, the coupling to the phonon bath results in an interaction between the instantons that decays exponentially with ''distance'' $|\tau-\tau'|$ (where τ is the position of an instanton) and not as a power law $\sim|\tau-\tau'|^{-2}$ as is the case for the Ohmic damping [9,8,19].

The occurrence of this gap is related to the fact that the breather itself already has its own nonzero frequency ω. Since this will also be true for breathers in quite different types of models, e.g., where no anharmonic terms with respect to the momenta exist, we may speculate that tunneling of a breather cannot be generally suppressed even in the Ohmic or sub-Ohmic cases.

Finally, we want to emphasize that the existence of many boson bound states has been obtained rigorously only for integrable models. Although our present calculation is not a proof of existence of bound states in the semiclassical limit, the finding that the tunneling in the dimer is reduced when considering an infinite chain, yields the right trend to connect these bound states to classical breather solutions.

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