

Discrete Quantum Breathers — What do we know about them?

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The knowledge about discrete quantum breathers, accumulated during the last two decades, is reviewed. "Prehistory" of the problem is described and some important properties differentiating localized and extended vibrational modes are outlined. The state of art of our understanding of the principal features of the quantum discrete breathers is presented.

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The idea of a localization of vibrational energy due to anharmonic effects was put forward independently several times, in different fields, under different names, aiming at different applications. One of the most popular name for such a localized state during the last decade is breather. Quantization of such localized excitations has been also under study for quite a long time. This paper reviews the field with a special emphasis on the results related to the quantum breathers. Among the problems touched upon are quantization of breathers, separation between the quantum breathers, corresponding to classically localized states, and phonons — extended states, dynamical properties of breathers. The amount of the results related to quantum breathers is not large and the best has been done to make a possibly complete coverage of the field.

I. INTRODUCTION

The idea of a possible localization of vibrational energy in a single highly excited local mode of an anharmonic discrete system was first discussed in chemical physics. The research in solid state was mainly concentrated on studying extended low energy vibrational

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excitations — phonons, which played important part in shaping thermodynamic and kinetic properties of crystals. Anharmonicity was considered mainly as an additional weak factor in an otherwise harmonic crystals. It usually yielded small corrections to physical quantities, which were mainly determined by the harmonic part of the vibration energy. Two exclusions are well known — thermal expansion and phonon thermal resistivity — when a nonzero result appears only due to the anharmonicity. However, even in these cases it was possible to consider only the lowest order perturbation terms.

The situation in chemistry has been different from the very beginning, since the typical processes such as chemical reactions, radiation and radiationless electronic transitions are necessarily accompanied by a release or absorption of a rather high energy, when anharmonic properties of molecular vibrations may fully reveal themselves. A tendency of the vibrational energy to localize on a single bond rather than to be equally distributed among numerous bonds available in molecules was discussed as early as in the 60s [1] (see also reviews [2, 3]). The attention at that time was largely concentrated on studies of radiationless transitions between electronically excited and ground states of the molecules. The fact that such a transition proceeds via a single highly excited anharmonic bond rather than over many weakly excited, and hence nearly harmonic bonds, can make a principal difference. For example the Franck-Condon factor, which is in fact the overlap of the vibrational wave function in two different electronic states and which controls the transition rate of the radiationless transitions, can, in principle, be calculated using a harmonic approximation. However, the neglect of anharmonicity for highly excited vibrational states may underestimate the transition rate by many orders of magnitude as demonstrated in reference [4], where the Franck - Condon factor was calculated for Morse oscillators.

Even if we go back to the mid-60s and 70s when the principal attention was concentrated on localization of vibrational energy on single molecular bonds, we realize that the story has actually begun much earlier. The idea that infrared absorption is localized in certain parts of molecules was clearly recognized at least as early as 1908 [5]. Quantum Morse oscillator was used to analyze some peculiar features of the infrared absorption in molecules in 1929 [6]. It became clear by that time that, for instance, the vibration energy in aromatic molecules, containing benzene rings is typically localized on one of the six stretching CH oscillators rather than distributed over the ring. In the early thirties Mecke et al [7–9] (more references to the works of this group can be found in review [10], see also [11]) started publishing his

series of papers on the subject. These important early achievements escaped, however, the attention of the people researching this field beginning from the 60s.

Returning to the 60s and 70s, we mention an extensive discussion of the properties of the so called "accepting" and "promoting" modes (see, e g. [12]). This discussion is in fact still ongoing. We may just pick up one of the most recent papers [13] considering the role of the promoting modes in radiationless transitions. The main idea is that the transfer of electronic energy of an excited molecule into vibrational excitations proceeds not via all available vibrational modes, but rather only a limited number of the modes take part in the process. There are only a few (possibly one) promoting modes, which are responsible for the transition between the excited and the ground electronic states of the molecule. There is also a limited number of accepting modes, which accept the rather high electronic energy released in the course of the transition. This approach is sound if such high excitations are stable enough and can exist during a sufficiently long time without decaying into low energy extended normal vibrations.

The role of anharmonic effects in molecular crystals was studied by Kranendok [14, 15], and later by Agranovich (see review [16] and references therein) whose attention was concentrated on coupled states of two phonons — biphonons. We shall see below that such states are just the simplest possible quantum breathers. An analogy of such biphonon states with two-magnon states [17–19] was also emphasized in [16].

A very interesting experimental indications favoring the existence of relatively stable highly excited vibrational states was reviewed in [20]. Dissociations of various molecules were induced by irradiation of powerful infrared lasers. Dissociation happens locally, only one or just a few bonds should be broken. About thirty infrared quanta are necessary to excite a bond high enough to break it. It is a direct indication that such highly excited vibrational states of the bond live sufficiently long in order to have enough time to accumulate the necessary number of photons.

The idea of a localization of anharmonic excitations was promoted by Ovchinnikov in 1969 [21] (see also review [22]). Two coupled anharmonic oscillators were considered and it was shown that the energy of a highly excited oscillator would not flow to the other one, so that the excitation energy remained localized on one of these two oscillators. It was also assumed that this property would hold for more complex systems consisting of many coupled oscillators. It was outlined (although not proven) in review [22] that these local

anharmonic oscillations in complex systems may be linearly stable and even the possible role of the Arnold diffusion was indicated.

More recently it was emphasized that localized anharmonic excitations in molecules could play a role of doorway states (see review [23]). The standard theories based on the Fermi golden rule assumed that the density of vibrational states in the molecule was the essential parameter determining the relaxation times of various excited states. However, the experiment clearly demonstrated that there was no direct correlation between the densities of states in various molecules and the relaxation times measured in these molecules. For example, an increase of the density of states by three orders of magnitude may be accompanied by a decrease of the lifetime of some states by a factor of two. That is where the idea of a doorway state enters. Actually the major part of the states contributing to the observed density of states have only a minor relevance to the relaxation process [24]. In fact this process proceeds via only one or maybe few highly excited localized states, which largely determine the relaxation rate. The connection between the doorway states and discrete quantum breathers was discussed in [25].

A possibility of a localization of vibrational excitation in an anharmonic chain was analyzed in [26]. This paper discussed the long wave limit where the originally discrete problem could be reduced to a continuous problem, e.g. to a sine-Gordon equation. Localized excitations for anharmonic crystals were introduced in references [27, 28]. Paper [29] reviews numerous aspects of the problem of classical breathers and discusses various techniques of their calculations.

Different authors call these types of excitation by different names: local modes, localized solitons, doorway states, intrinsic local modes, and, finally, discrete breathers. The latter name is most popular in the nonlinear dynamics community and it will be used below.

II. LOCAL AND EXTENDED MODES

A detailed analysis of the structure of the phase space allowing for a separation between local and normal (extended) modes and transitions between behaviors typical of each type of modes was carried out by Jaffe and Brumer [30]. They addressed the problem by restricting themselves to two bound anharmonic oscillators. This problem was also discussed in [31] where systems with a larger number of oscillators were discussed as well. The approaches

to both the local and normal modes are approximate schemes representing the hamiltonian of the system as

$$H = H_0 + V, \quad H_0 = \sum_j H_0^j(q_j, p_j)$$

where each term $H_0^j(q_j, p_j)$ depends only on the j -th pair of generalized coordinates, and the coupling between them is accounted for by the term V . If we choose the normal mode approach, these generalized coordinates are normal coordinates, which can be most easily obtained in the small amplitude limit. These are symmetry coordinates and they can be classified by means of the irreducible representations of the whole system. The local mode approach chooses displacement of an individual bond j from equilibrium as the coordinate q_j . Then the bond anharmonicity is directly included into the H_0^j term.

The choice between the approaches depends on the type of the problem addressed and the quality of the resulting zeroth order approximation (neglecting V). We are always interested in having possibly small corrections due to the coupling V . It is worth emphasizing that the treatment of the local modes in [30] is very close to the anticontinuum limit used by MacKay and Aubry [32] in order to give a mathematical proof of the classical discrete breather existence (see also [33]).

An insight to localized modes is provided by turning to the angle — action variables $\{\varphi_j, I_j\}$ with j enumerating the bonds. In the absence of V the phase space motion is restricted by certain tori determined by the conserving hamiltonian $H = \sum_j H_j(I_j)$. Then according to [30] we define the amplitude dependent frequencies $\omega_j = \frac{\partial H_j(I_j)}{\partial I_j}$. The behavior typical of a local mode shows up when the amplitudes of the different bonds differ strongly from each other, and hence the corresponding frequencies differ as well.

If the amplitudes, and hence the frequencies of different bonds coincide (say, $\omega_1 = \omega_2$) the 1:1 resonance takes place and a small perturbation yields a normal mode behavior. A commensurate ratio $n_1\omega_1 = n_2\omega_2$, with integer n_j may also lead to a resonance. This resonance is similar to the well known Fermi resonance between quantum oscillators. The discussion in [30] is limited largely to a dimer, i.e. two coupled anharmonic oscillators. In this case one can easily imagine 1:1 resonances at various excitation levels of the bonds. However, if we consider a system of many or even infinite number of bonds, then such a 1:1 resonance would require an equal and finite excitation of all the bonds. This would correspond to a large or even infinite accumulated excitation energy. Such a situation does

not seem to be generic and achievable in real physical systems. The exclusion is the case of small (infinitesimally small) excitations of the bonds, i.e. excitation of various phonon modes. This type of excitations will be usually implied below, when considering extended normal excitations.

One of the important conclusions of [30] is that the tori related to the local and to the normal mode types of motion cannot be deformed into each other by any continuous variations of the hamiltonian. These two types of tori are situated in different parts of the phase space. Varying the coupling or other parameters of the hamiltonian changes the shape of the separatrix between these two parts but never mix them. The corresponding bifurcation point was studied later by Scott et al [31].

III. QUANTUM BREATHER.

Let us try to understand what are the properties of the wave function of a quantum breather, which would allow us to distinguish it from the normal states. (The discussion in this section is based largely on the references [25, 33]). In classical mechanics we separate between normal (phonon) modes, which reflect the symmetry of the system and are extended over the whole system, and the local modes (breathers), when only a small number of neighboring sites are involved in the motion. This crystal-clear distinction becomes blurred when we turn to quantum mechanics.

Let us assume that we have a classical breather solution with the corresponding phase-space trajectory lying on a torus. We can obtain such a solution by exciting a motion of the j -th site of the lattice in the anticontinuum limit (without intersite interaction) and then gradually switching the intersite interaction on. This motion can be now quantized, resulting in a set of wave functions, $\Psi_{j,\alpha}(\{\mathbf{r}_i\})$ with α being quantum number. This step is not necessarily easy, and not always can be done analytically even approximately. However, there are cases when it is doable, at least numerically.

Now we have to recollect that an eigen function of a periodic hamiltonian must satisfy the Bloch theorem, which states that

$$\Psi(\{\mathbf{r}_j + \mathbf{a}\}) = e^{i\mathbf{k}\mathbf{a}}\Psi(\{\mathbf{r}_j\}). \quad (1)$$

Here \mathbf{a} is the lattice period, and \mathbf{k} is the wave vector. These functions are certainly ex-

tended, reflect the symmetry of the system and their classification can be carried out using the irreducible representations of the symmetry group of the system. But in the classical mechanics all these were just features typical of the normal modes, meaning that quantized breather states cannot be distinguished from the quantized normal (phonon) states, which also satisfy Bloch theorem (1), or, at least, they cannot be distinguished along the guidelines, used in classical mechanics (see discussion in Section 2).

Let us try to construct a quantum breather wave function in the form

$$\Psi_{\mathbf{k},\alpha}(\{\mathbf{r}_j\}) = \frac{1}{\sqrt{N}} \sum_{j'} e^{i\mathbf{k}\mathbf{r}_{j'}} \Psi_{j',\alpha}(\{\mathbf{r}_j\}) \quad (2)$$

where N is the number of sites in the lattice. Obviously this function satisfies the Bloch theorem (1) although it is constructed using only the site functions with a fixed value of α . This construction can be viewed as a tight binding approximation, often used when describing electron motion in a narrow band. The local functions $\Psi_{j',\alpha}(\{\mathbf{r}_j\})$, if orthogonalized, may play the role of the Wannier functions. In the anticontinuum limit they are just wave functions of the single bond excitations and remain rather close to them as long as the coupling parameter remains small enough.

A single phonon excitation, which in the classical mechanics is associated with a normal extended vibration, is obtained by quantizing the normal coordinates. Now an n phonon function should be considered. A multiphonon state is a symmetrized product of n , single phonon wave functions

$$\Psi_{\mathbf{k},n}(\{\mathbf{r}_j\}) = \widehat{P}_S \prod_{i=1}^n \varphi_{\mathbf{k}_i}(\{\mathbf{r}_j\}) \quad (3)$$

where \widehat{P}_S denotes the symmetrization of the product of functions. The structure of the multiphonon wave function (3) certainly differs from that of the quantum breather wave function (2). In principle, the corresponding wave function can be also represented in the form similar to (2). But the corresponding Wannier functions will strongly differ from the single bond excitations.

We can invert the question. Let us assume that we are given a function $\Psi_{\mathbf{k}}(\{\mathbf{r}_j\})$, which observes the Bloch condition (1), and we are asked to determine whether the given function represents a quantized breather or just a symmetrized product (or combination of such products) of single phonon excitations. In both cases the function is extended and may be classified according to the irreducible representations of the crystal group. It means that the approach used in [30] within the framework of the classical mechanics does not help.

On the other hand, the difference between the two states, the quantum breather (2) and the n phonon state (3), is physically quite clear. A quantum breather forms as a result of a coherent tunneling of a high excitation of a bond, whereas a normal multiphonon states correspond to independent motion of n low energy excitations extended over the whole crystal. Rather loosely we may say that in the quantum breather case all the "phonons", or better to say bosons, are always coupled together on a bond. As for the multiphonon state the phonons are not coupled, move independently and actually never meet each other. The probability that n independent phonons meet simultaneously on one of N bonds of the lattice can be estimated as N^{-n} .

We may now try to formalize this intuitive understanding. It is rather easy to do for such models as discrete nonlinear Schrödinger equation (DNLS) with the hamiltonian

$$H = \omega_0 \sum_i \hat{\Psi}_i^\dagger \hat{\Psi}_i + \frac{\gamma}{2} \sum_i \hat{\Psi}_i^\dagger \hat{\Psi}_i^\dagger \hat{\Psi}_i \hat{\Psi}_i + C \sum_i [\hat{\Psi}_i^\dagger \hat{\Psi}_{i+1} + \hat{\Psi}_i^\dagger \hat{\Psi}_{i-1}] \quad (4)$$

where the operator of the total number of boson excitation

$$\hat{B} = \sum_i \hat{\Psi}_i^\dagger \hat{\Psi}_i$$

commutes with the hamiltonian and the corresponding physical quantity conserves. Now the procedure, to be carried out with the given wave function, is to measure the probability of having n phonons in a site. The operator for such a probability can be defined as

$$\hat{B}^{(n)} = \sum_i \frac{1}{n!} \hat{\Psi}_i^{\dagger n} \hat{\Psi}_i^n \quad (5)$$

Calculating the expectation value, $\langle \hat{B}^{(n)} \rangle_{breather}$, of this operator for the quantum breather function (2) one gets exactly 1 in the anticontinuum limit, and a finite quantity, smaller than 1, for a finite coupling. The expectation value of this operator for the multiphonon function (3) is of the order of N^{1-n} and tends to zero in the thermodynamic limit ($N \rightarrow \infty$) for any $n \geq 2$. This procedure can be also applied to other hamiltonians, for which the number of boson excitations does not necessarily conserve. The most important property of a wave function, indicating that it represents a quantum breather state, is that the corresponding expectation value of the operator (5) remains finite in the thermodynamic limit.

The quantum breather states, $\Psi_{j, \alpha}(\{\mathbf{r}_j\})$, form a band, which may be called the breather band, generated from the α -th quantum state of an individual bond. In the weak coupling

limit the band spectrum in the one dimensional case is

$$E_\alpha(k) = t_{0\alpha} + 2(t_{0\alpha}S_\alpha + t_{1\alpha}) \cos ka \quad (6)$$

where $t_{0\alpha} = \langle \Psi_{j,\alpha} | H | \Psi_{j,\alpha} \rangle$, $S_\alpha = \langle \Psi_{j,\alpha} | \Psi_{j\pm 1,\alpha} \rangle$, and $t_{1\alpha} = \langle \Psi_{j,\alpha} | H | \Psi_{j\pm 1,\alpha} \rangle$.

The most important parameter here is t_1 , which gives the probability amplitude of a tunneling translation of a quantized local vibrational excitation by one lattice spacing. The problem of its calculation was addressed in several contexts. It seems that it is sufficient to consider two adjacent anharmonic bonds (a dimer), where in the classical case trajectories appear, which are not invariant under permutation of the bonds, meaning that one bond may be strongly excited whereas the other bond remains at a much lower degree of excitation. Quantum mechanics would allow a tunneling transition when the excitation energy is transferred from one bond to another.

An estimate for such tunneling probability was given in [22] for a transition between two Morse oscillators coupled by a bilinear interaction. An assumption was made that one oscillator is excited at a high quantum state n while the second one was in its ground state $n = 0$. Then the exchange of this excitation between the two oscillators was estimated by perturbation theory. A better estimate for the breather tunneling transition was presented in [34] for an integrable dimer was considered. The DNLS hamiltonian (4) with only two sites was considered, for which the tunneling probability is

$$\frac{2nC}{(n-1)!} \left(\frac{C}{\gamma} \right)^{n-1} \quad (7)$$

A more general equation when a tunneling exchange between two not equally excited bonds of the dimer take place, can be found in reference [35]. This tunneling probability is small, moreover, it decreases rapidly with the growth of the excitation number n .

Now a question may be asked: Is there any difference between the tunneling transfer of a vibrational excitation between the two bonds of a dimer and a similar tunneling in a lattice with macroscopically large number of sites? A difference may appear since the tunneling object interacts with extended normal oscillations — phonons, and the tunneling probability can be strongly renormalized by this interaction. The influence of interaction of a tunneling particle with extended excitations on its tunneling has been studied in many details, see, e.g., [36]. One of the most interesting phenomena predicted in these studies is a possibility of a tunneling suppression [37], which may take place in the so called Ohmic case, when the density of the extended excitations is linear.

This suppression is due to the behavior of the interaction of the tunneling particle with the continuum of extended states, which in the Ohmic case becomes divergent in the "infrared" limit. The question whether the same divergence may happen in the case of breather tunneling is addressed in [38]. The analysis carried out in this paper demonstrates that there is an important difference between the phase-space tunneling of a localized vibrational excitation and the real space tunneling of a particle. The local vibrational excitation is characterized by its own internal frequency, Ω , which interfere with the continuum of the extended excitations and leaves no room for the above "infrared" divergence.

Then an adiabatic approximation can be applied, assuming the internal motion to be more rapid than the motion associated with the "infrared part" of the spectrum of the extended normal vibrations. The final conclusion of [38] is that the tunneling probability t_1 can be obtained from (7) just by introducing a "renormalized" excitation number

$$\tilde{n} = n \left(1 + \sum_{\nu} \frac{C_{\nu}^2}{\Omega - \omega_{\nu}} \right)$$

instead of n , where C_{ν} is the coupling of the local excitation with extended excitations, characterized by the frequencies ω_{ν} .

An illuminating discussion of quantum breathers on a periodic one dimensional lattice was carried out in references [39, 40] (see also [11, 41]) using the example of the quantum DNLS. This model conserves the total number of bosons, so that using number state representation the quantum problem is reduced to diagonalization of finite size matrices, when considering a system with a finite number of sites N , and a finite number of bosons n .

In particular, the band energy was calculated in two interesting cases. The band energy of a two boson breather state in DNLS lattice for $N \rightarrow \infty$ and an arbitrary value of the anharmonicity versus coupling ratio, γ/C , is

$$E_2(k) = -\sqrt{\gamma^2 + 16C^2 \cos^2(ka/2)},$$

which converges to the form (6) in the limit of small C . The spectrum is also found in the limit of large anharmonicity γ and for an arbitrary n ,

$$E_n(k) = -\frac{1}{2}n(n-1)\gamma - \frac{2nC^{n-1}}{(n-1)!\gamma^{n-1}} \cos ka. \quad (8)$$

The first term in (8) is the energy of an individual bond with n bosons, whereas the second term can be, up to a numerical factor, obtained using equations (6) for the breather band energy and (7) for the tunneling amplitude in the NLS dimer.

A detailed discussion of two coupled phonons in molecular crystals, biphonons, was carried out in [16]. It is quite clear that two coupled phonons make just the minimal condition for a quantum breather. Several quantum breather bands were also obtained numerically in reference [42]. References [43, 44] consider a model, where the nonlinearity appear due to a strong coupling of Einstein modes with electrons, and analyze some properties of the n boson bands. The results were successfully applied to the interpretation of the Raman scattering data in mixed valence transition metal complexes [45].

Many of the above considerations reflect our expectations of the quantum breather behavior and are based on such general ideas as quantum levels and bands, Bloch theorem, phase space tunneling and so on. They are also confirmed by findings in papers referred to above. It is obvious that this approach works well in the anticontinuous limit ($C = 0$) when the onsite oscillators can be considered as independent. Then an excited state of an individual oscillator does not decay and the probability of tunneling of such an excitation to another site is zero. The Bloch type construction (2) is formally an eigenfunction of the whole hamiltonian. The question addressed by MacKay [46] was, does a small but finite coupling C introduce also a finite perturbation to this pattern, so that this perturbation does not depend on the number N of the lattice sites and, hence, does not diverge with N . The answer is positive and a proof is presented in the paper [46] that there is a certain, small but finite, range of the coupling parameter values where the above quantum breather properties hold.

The question, what limits this range from above, remains open from the rigorous mathematical point of view. However some physical arguments can be presented here. When gradually switching the coupling on, the breather band becomes broader and its "center of mass" shifts either upward or downward. This broadening, when comparable with the energy gap between the different breather bands, will certainly destroy the breather character of these bands. However, the event, which most probably happens earlier, is crossing of a pair of still narrow breather bands. This is illustrated in Figure III. Certainly the crossing should be made avoided when the symmetry requires it. Such crossings are usually associated with the so called chaos assisted tunneling [47, 48].

This picture reflects our optimistic expectations that a breather band survives quite a few crossings without losing its specific features. A support for our belief that this picture really holds, comes from studies [25, 49]. These papers consider a trimer as a system mimicking

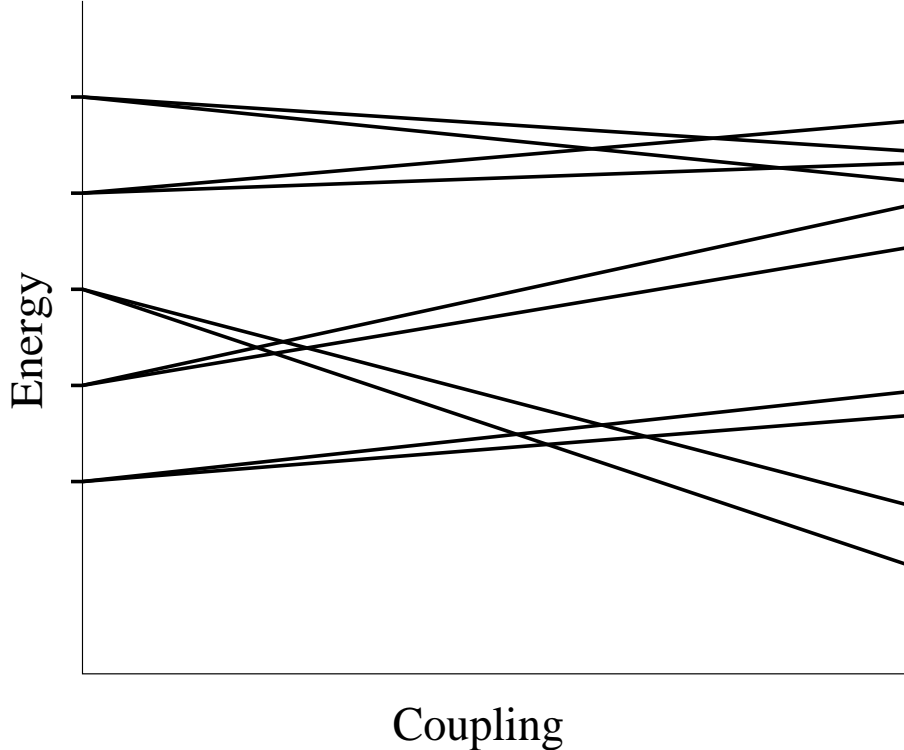


FIG. 1: This figure illustrates broadening and crossings of breather bands with increasing coupling parameter. Pairs of lines show boundaries of the breather bands, which change their energy, broaden and may cross each other with the increase of the coupling.

the behavior of a larger system. Tunneling pairs represent then the breather bands. The analysis carried out in these papers demonstrates that varying the parameters of the system leads to multiple crossings of these tunneling pairs. However, the pairs appear to be rather robust creatures, capable of surviving many crossings without losing their quantum breather identities. Certainly similar analysis for a really large system is necessary, but it requires a rapidly increasing (with the growing number of the systems sites) computer time and is still to be done.

IV. DYNAMICS OF A LOCALIZED QUANTUM EXCITATION

The picture of quantized breathers as described in the previous section is similar to that of quasiparticles moving in a band. Due to very small tunneling probability, which decreases exponentially for higher excitation levels, the width of this band is extremely small, or, in the other words, the effective mass of the quasiparticle is very large. Thinking about dynamics

of such an excitation, at least two aspects of it may be discussed.

First, a large tunneling time implies that the excitation stays predominantly at the same site of the lattice. An interaction of such a quantum state with available extended excitations may cause its decay. This issue is discussed in references [50, 51]. Highly excited local anharmonic excitations are assumed to exist and to be linearly stable. Then a second order coupling of the breather and phonon coordinates is, in principle, allowed (two phonon processes). Various regimes of the breather relaxation are considered with the conclusion that the relaxation may proceed not necessarily exponentially but rather with a possible emission of phonon bursts.

Second, if the decay time of a quantum breather appears to be long enough, then the breather can be thought about as a heavy particle moving or, better to say, diffusing in a narrow band. Various aspects of quantum diffusion of ordinary heavy particles, say, hydrogen interstitial atoms in crystals were studied (see review [52] and references therein, a description of the principle features of the quantum diffusion is also presented in the book [53]). The principal aim of these studies was to understand the low temperature behavior of the diffusion coefficient. The most important factor determining the diffusion is the interaction of the heavy particle with the phonons. At any reasonable temperature the typical phonon energy may be larger than the band width. Therefore a single phonon may easily destroy the resonance between two neighboring sites and hinder tunneling. Then the diffusion coefficient will decrease with the temperature. On the other hand two (or many) phonon processes may help the tunneling process and stimulate it, which results in a growth of the diffusion coefficient with the temperature. These two competing mechanisms may lead to a nonmonotonic low temperature dependence of the diffusion coefficient. Besides these phonon mechanisms governing the quantum diffusion of heavy particles, one should also take into account that defects, which inevitably appear in any real lattice, create stress fields around themselves and can relatively easy block the tunneling by breaking the resonances between the bonds.

All this being said about the quantum diffusion of a heavy particle and in spite of the obvious analogy between the quantum breathers and heavy particles, one should be cautious when transferring the knowledge available for heavy particles into the field of quantum breathers. An example of possible differences was indicated in our paper [38] where the absence of tunneling suppression for quantum breathers was demonstrated. It still remains

a topic for the future to study quantum diffusion of quantum breathers.

V. CONCLUSION

The reader can now see that the progress made till now in our understanding of quantum breathers is rather limited to say the least. It is worth mentioning here some more relevant references, especially the experimental ones. The authors of [54–57] observe breather modes in mixtures of 4-methyl-pyridine. They analyze their data by means of the quantum sine-Gordon equation. Breather excitations are also observed in Cu benzoate [58] by the electron spin resonance technique. The results for this quantum system are well interpreted by means of the classical sine-Gordon equation [59, 60]. Measurements [45], mentioned above, are most relevant to the current discussion since the discreteness appears to be important for their interpretation. The most recent publication [61] describes the observed slow relaxation in doped alkali-halides. The authors make use of the Fermi-Pasta-Ulam (FPU) model and introduce an entity, which they call "FPU soliton". In the context of their paper it is the same breather. It is interesting also to mention that some ideas related to quantum breathers find now application to such systems as coupled Bose-Einstein condensates [62], which are well described by the DNLS or Bose-Hubbard model.

We may now compare the flourishing field of classical discrete breathers, where dozens of papers are being published every year, studying many subtle details of breathers, their dynamics, their interactions with other breathers or with extended excitations, with the scarce information and a small amount of papers on the quantum discrete breathers accumulated during, say, last decade. One may ask a question: Why it is so? Why does the field of quantum breathers not attract much more attention. I present here my opinion, which may be at least part of the answer. In many cases a study of a certain breather related phenomenon (classical) is carried out in the following fashion. One chooses a model system, containing a certain amount of sites, large enough to be a good approximation for "infinite", runs a computer simulation for a time, which is long enough to be considered "infinite", and gets some results. This procedure plays a role similar to that of an experiment, which measures properties of the breather. Then one can try to apply various analytical methods in order to get an understanding of the observations, i.e. to make a theory.

This type of work became possible in the nineties of the last century when worksta-

tions started being easily accessible. Try now to imagine the same approach to a quantum breather. Classical breather requires a consideration of an isolated orbit in the phase space of the system. Quantum breather requires a consideration of a wave function or, say, of a Wigner distribution. It is quite clear that the amount of information to be crunched by the computer may be many orders of magnitude larger in the quantum case. This makes a real computer experiment on the scale similar to that regularly done for classical breathers, hardly possible, if the limitations of the currently available computers are taken into account, and strongly cripples our efforts to study quantum breathers. Shall we wait for the advent of new much more powerful computers, or may be some new bright ideas will clear the way? We'll see in the future.

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- [1] B.R. Henry and W. Siebrand, *J.Chem.Phys.*, **49**, 5369 (1968).
- [2] M.L. Sage and J. Jortner, *Advan.Chem.Phys.*, **47**, 293 (1981).
- [3] B.R. Henry, in: *Vibrational Spectra and Structure*, ed. J.R. Durig (Elsevier, Amsterdam, 1981) p.269.
- [4] A.A. Kovalev and B.I. Makshantsev, *Spectroscopy Letters*, **5**, 19 (1972).
- [5] W.W. Coblenz, (1908) *Supplementary Investigations of Infrared Spectra*. Washington, DC: Carnegie Inst. Publ.
- [6] J.W. Ellis, *Phys.Rev.* **33**, 27 (1929).
- [7] R. Mecke *Z.Phys.Chem. B* **17**, 1 (1932).
- [8] R. Mecke, *Z.Phys.* **99**, 217 (1936).
- [9] R. Mecke, *Z.Electrochem.* **54**, 38 (1950).
- [10] M. Quack, *Annu.Rev.Phys.Chem.* **41**, 839 (1990).
- [11] A. Scott, *Nonlinear Science*, Oxford University Press, NY (1999).
- [12] M.G. Prais, D.F. Heller, and K. Freed, *Chemical Physics*, **6**, 331 (1974).
- [13] D.C. Moule and E.C. Lim, *J.Chem.Phys.*, **19**, 9341 (1999).
- [14] J. van Kranendoonk, *Physica (Utrecht)* **25**, 1080 (1959).
- [15] J. van Kranendoonk and G. Karl, *Rev.Mod.Phys.* **40**, 531 (1968).
- [16] V.M. Agranovich and I.I. Lalov, *Uspekhi Fiz.Nauk* **146**, 267 (1985) [*Sov.Phys.Uspekhi* **28**,

- 484 (1965)]
- [17] H. Bethe, *Z.Phys.* **71**, 205 (1931).
 - [18] M. Wortis, *Phys.Rev.* **132**, 85 (1963).
 - [19] I. Hanus, *Phys.Rev.Lett.* **11**, 336 (1962).
 - [20] N. Bloembergen and E. Yablonovich, *Physics Today*, **31**, 23 (1978).
 - [21] A.A. Ovchinnikov, *Zh.Eksp.Teor.Fiz.*, **57**, 263 (1969) [*Sov.Phys. JETP* **30**, 147 (1970)].
 - [22] A.A. Ovchinnikov and N.S.Erikhman, *Sov.Phys. – Uspekhi* **25**, 738 (1982) [*Usp. Fiz. Nauk*, **138**, 289 (1982)].
 - [23] K.K. Lehmann, G. Scoles, B.H. Pate, *Annu.Rev.Phys.Chem.*, **45**, 241 (1994).
 - [24] S.A. Schofield, R.E. Wyatt, and P.G. Wolynes, *J.Chem.Phys.*, **105**, 940 (1996).
 - [25] S. Flach and V. Fleurov, *J.Phys.: Condens.Mat.*, **9**, 7039 (1997).
 - [26] A.M. Kosevich and A.S. Kovalev, *Sov.Phys.-JETP*, **40**, 891 (1974) [*ZhETF*, **67**, 1793 (1974)].
 - [27] A.J. Sievers and S.Takeno, *Phys.Rev.Lett.*, **61**, 970 (1988).
 - [28] S. Takeno, K. Kisoda, and A.J. Sievers, *Prog.Theor.Phys.Suppl.*, **94**, 242 (1988).
 - [29] S. Flach and C.R. Willis, *Phys.Rep.*, **295**, 181 (1998).
 - [30] C. Jaffe and P. Brumer, *J.Chem.Phys.*, **73**, 5646 (1980).
 - [31] A.C. Scott, P.S. Lomdahl, and J.C. Eilbeck, *Chem.Phys.Lett.*, **113**, 29 (1985).
 - [32] R.S. MacKay and S. Aubry, *Nonlinearity*, **7**, 1623 (1994).
 - [33] S. Aubry, *Physica D* **103**, 201 (1997).
 - [34] L. Bernstein, J.C. Eilbeck and A.C. Scott, *Nonlinearity*, **3**, 293, (1990).
 - [35] S.Aubry, S. Flach, K. Kladko, and E. Olbrich, *Phys.Rev.Lett.*, **76**, 1607 (1996).
 - [36] A.J. Leggett, S. Chakravarty, A.T.Dorsey, M.P.A. Fisher, A. Garg, and W. Zwerger, *Rev.Mod.Phys.*, **59**, 1, (1987).
 - [37] A.J. Bray and M.A. Moore, *Phys.Rev.Lett.*, **49**, 1546 (1982).
 - [38] V. Fleurov, R. Schilling, and S. Flach, *Phys.Rev. E*, **58**, 339 (1998).
 - [39] P.D. Miller, A.C. Scott, J. Carr, and J.C. Eilbeck, *Physica Scripta*, **44**, 509 (1991).
 - [40] A.C. Scott, J.C. Eilbeck, and H. Gilhøj, *Physica D*, **78**, 194 (1994).
 - [41] H. Feddersen, P.L. Christiansen, and M. Salerno, *Physica Scripta*, **43**, 353 (1991).
 - [42] W.Z. Wang, J.T. Gammel, A.R. Bishop and M.I. Salkola, *Phys.Rev.Lett.*, **76**, 3598 (1996).
 - [43] W.Z. Wang, A.R. Bishop, J.T. Gammel, and R.N. Silver, *Phys.Rev.Lett.*, **80**, 3284 (1998).
 - [44] N.K. Voulgarakis, G.Kalosakas, A.R. Bishop, and G.P.Tsironis, *Phys.Rev. B* **64**, 020301(R)

- (2001).
- [45] B.I. Swanson, J.A. Brozik, S.P.Love, G.F. Strous, A.P. Shreve, A.R. Bishop, W.Z. Wang, M.I. Salkola, *Phys.Rev.Lett.*, **82**, 3288 (1999).
 - [46] R.S. MacKay, *Physica A* **288**, 174 (2000).
 - [47] O. Bohigas, S. Tomsovic and D. Ullmo, *Phys.Rev.Lett*, **64**, 1479 (1990).
 - [48] O. Bohigas, S. Tomsovic and D. Ullmo, *Phys.Rep.*, **223**, 43 (1993).
 - [49] S. Flach, V. Fleurov and A. Ovchinnikov, *Phys.Rev. B* **63**, 094304 (2001).
 - [50] V. Hizhnyakov, *Phys.Rev. B*, **53**, 13981 (1996).
 - [51] V. Hizhnyakov and D. Nevedrov, *Phys.Rev. B* **56**, R2908 (1997).
 - [52] Yu. Kagan, *J.Low Temp.Phys.*, **87**, 525 (1992).
 - [53] V.I. Goldanskii, L.I.Trakhtenberg, and V.N. Fleurov, *Tunneling phenomena in chemical physics*. (New York: Gordon and Breach, 1989).
 - [54] F. Fillaux and C.J. Carlile, *Phys.Rev. B* **42**, 5990 (1990).
 - [55] F. Fillaux, C.J. Carlile, G.J.Kearley, *Phys.Rev. B* **44**, 12280 (1991).
 - [56] F. Fillaux, C.J. Carlile, G.J.Kearley, *Physica B* **226**, 241 (1996).
 - [57] F. Fillaux, C.J. Carlile, G.J.Kearley, *Phys.Rev. B* **58**, 11416 (1998).
 - [58] T. Asano, H. Nojiri, Y. Inagaki, J.P. Boucher, T. Sakon, Y. Ajiro and M. Motokawa, *Phys. Rev.Lett.*, **84**, 5880 (2000).
 - [59] M. Oshikawa and I. Affleck, *Phys.Rev.Lett.* **82**, 5136 (1999).
 - [60] I. Affleck and M. Oshikawa, *Phys.Rev.*, B **59**, 14376 (1999).
 - [61] L.S. Schulman, E. Mihokova, A. Scardinicchio, P. Facchi, M. Nikl, K. Polak, and B. Gaveau, *Phys.Rev.Lett.* **88**, 224101 (2002).
 - [62] R. Franzosi and V. Penne, *Phys.Rev. A* **65**, 013601 (2001).