Delocalization-Localization Transition due to Anharmonicity

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Analytical and numerical calculations for a reduced Fermi-Pasta-Ulam chain demonstrate that energy localization does not require more than one conserved quantity. Clear evidence for the existence of a sharp delocalization-localization transition at a critical amplitude A_c is given. Approaching A_c from above and below, diverging time scales occur. Above A_c, the energy packet converges towards a discrete breather. Nevertheless, ballistic energy transportation is present, demonstrating that its existence does not necessarily imply delocalization.

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One of the classical investigations of relaxation dynamics of macroscopic systems is to determine the time evolution of a perturbed equilibrium state. If this initial state converges to equilibrium, the system is called mixing, implying ergodicity, and it is nonmixing, otherwise. An important question is: Does there exist a sharp ergodicity breaking transition under variation of a physical control parameter like temperature or strength of perturbation?

Within a mode coupling theory for supercooled liquids, such a dynamical glass transition has been found, but its sharpness seems to result from the mode coupling approximations (for reviews see [1,2]). It is not our purpose to contribute to the theory of glass transition, but to study the influence of anharmonicity on the relaxational behavior at zero-temperature. In that case, the generic lowest energy state of a particle system is a crystal. One may ask a similar question as above: Does an initially localized energy excitation spread over the complete crystal, or not? In case of small excitation amplitudes, one can use the *harmonic* approximation. Then the time evolution of an initial configuration can be determined, exactly [3]. For one-dimensional harmonic lattices, the results are particularly simple [4,5]. Independent of the strength and size of the excitation, it always spreads over the full system, and energy transportation is ballistic, provided that there is no disorder. That *infinite* harmonic crystals are ergodic, in general, has been proven rigorously [6]. If the excitation amplitude increases, *anharmonicity* gets important.

Let us neglect any disorder, but taking anharmonic interactions into account. Discreteness of the lattice combined with anharmonicity allows for the existence of localized periodic vibrations, called discrete breathers (DB). For reviews, see Ref. [7]. Their existence suggests that under certain conditions a *localized* excitation may converge to a DB, whereby suppressing complete energy spreading. Indeed, numerical solutions of the discrete nonlinear Schrödinger equation (DNLS) [8] and references wherein, the Klein Gordon chain (KG) [9], and the β-Fermi-Pasta-Ulam chain (FPU) [10,11] demonstrate generation of DB and their role for slow energy relaxation. Particularly, the numerical results in Refs. [8,11] give evidence that DB generation from an initially localized excitation requires an excitation amplitude which is large enough. This has been supported by analytical studies of DNLS and its single impurity version [12]. Concerning analytical results, a little is known, only [13–15]. Recently, it was proven for a rather general DNLS (even including disorder) that the energy spreads incompletely, provided that the norm which is a measure of anharmonicity is large enough [15]. This proof is based on the existence of *two* conserved quantities, the energy and the norm.

The main questions which now arise are: Does energy localization need the existence of more than one conservation law? Is there a sharp transition between complete and incomplete energy spreading? If so, what are properties characterizing such a transition? To explore these questions is our main motivation. Let us consider, e.g., the β-FPU model. In case that the energy delocalizes completely, one can linearize the equation of motion at large times leading to the harmonic chain, which is exactly solvable. If it does not, it may converge to a DB. Since the amplitude of DB decays exponentially, one may linearize again, however, outside the center of the DB. Idealizing this situation, we consider a reduced FPU-chain with one anharmonic bond, only. The corresponding *classical* Hamiltonian for N particles with mass m and open boundary condition is as follows:

$$H = \sum_{n=1}^{N} \frac{1}{2m} p_n^2 + \frac{C}{2} \sum_{n=1,(n\neq M)}^{N-1} (x_{n+1} - x_n - a_n)^2 + V(x_{M+1} - x_M) \qquad (1)$$

where $C > 0$ is the elastic constant and a_n the equilibrium length of the n-th bond. $V(q)$ is chosen such that V has a single minimum at $q_{\min} = 0$ with $V''(q_{\min}) = C$. This rules out localized phonon modes of the linearized equation of motion. In addition, we will assume that $V''(q)$ is increasing with increasing $|q - q_{\min}|$. H is translationally invariant. After separation of c.o.m and introducing relative coordinates $q_n = x_{n+1} - x_n - a_n$ and their conjugate momenta π_n, the harmonic part of Eq. (1) can be transformed to normal coordinates $\{Q_\nu^L, P_\nu^L\}$ and $\{Q_\mu^R, P_\mu^R\}$ for the left $(1 \le n \le M-1)$ and right $(M+1 \le n \le N)$ harmonic part of the chain. Skipping the c.o.m.-energy, this yields

$$H = H_{\text{harm}} + H_{\text{anh}} + H_{\text{int}} \tag{2}$$

with $H_{\text{anh}} = \frac{1}{m}\pi_M^2 + V(q_M)$ the Hamiltonian for the isolated anharmonic bond, the harmonic Hamiltonian H_{harm}, and H_{int} containing the interaction of the anharmonic bond with the harmonic degrees of freedom (d.o.f.). Hamiltonian (2) is the only conserved quantity after separation of c.o.m. Since the equation of motion is linear in the harmonic d.o.f., these can be exactly eliminated. This leads for $N \to \infty$ and $M = \mathcal{O}(N)$ to the nonlinear integro-differential equation

$$\ddot{q}(\tau) + \frac{1}{2C}V'[q(\tau)] - \int_0^\tau d\tau' k(\tau-\tau')\frac{1}{C}V'[q(\tau')] = 0 \tag{3}$$

where the index M has been dropped for convenience. $Q_\nu^L(0) \equiv 0$, $P_\nu^L(0) \equiv 0$ and $Q_\mu^R(0) \equiv 0$, $P_\mu^R(0) \equiv 0$ were chosen as initial conditions. $\tau = \omega_0 t$ is a dimensionless time and $\omega_0 = 2(C/m)^{1/2}$ the upper phonon band edge. The lower edge is at zero, due to translation invariance. The memory kernel is given by $k(\tau) = -\dot{k}_1(\tau)$ where $k_1(\tau) = J_1(\tau)/\tau$ with J_n the Bessel function of order n. Having determined for given initial conditions $q(0)$ and $\dot{q}(0)$ a solution $q(\tau)$ of Eq. (3), one obtains the harmonic nearest-neighbor bond coordinates $q_n(\tau)$ from

$$q_n(\tau) = \int_0^\tau d\tau' G_{|M-n|}(\tau-\tau')\frac{1}{C}V'[q(\tau')], \qquad n \neq M \tag{4}$$

with the Green function $G_n(\tau) = 2nJ_{2n}(\tau)/\tau$. As initially localized excitation, we choose $q(0) = A$ and $\dot{q}(0) = 0$. Use of a "velocity excitation" $q(0) = 0$, $\dot{q}(0) = B$ will not change our results qualitatively. With this initial condition in mind, the conservation of the total energy implies that $|q(\tau)| < A$ for all $\tau > 0$.

As well known, elimination of a macroscopic number of d.o.f. induces dissipation. The frequency dependent damping constant $\gamma(\omega)$ follows from

$$\gamma(\omega) = \lim_{\varepsilon\to 0}\frac{1}{\omega}\Im[\hat{k}(\omega + i\varepsilon)] = \begin{cases}\sqrt{1-\omega^2}, & |\omega| < 1\\ 0, & |\omega| \ge 1\end{cases} \tag{5}$$

with ω measured in units of ω_0 and $\hat{k}$ the Laplace transform of $k(\tau)$. This exact result is obvious. For $|\omega| < 1$, i.e., for frequencies within the phonon band, the corresponding modes will be damped and consequently decay to zero, whereas all modes with frequency above that band will be undamped. If the anharmonic bond is isolated, i.e., the integral term in Eq. (3) is absent, $q(\tau)$ will perform periodic oscillations with frequency $\Omega_0(A)$, depending on the amplitude A. Because of $V''(q_{\min}) = C$, it follows for $A \to 0$ that $\Omega_0(A) \to 1/\sqrt{2}$ in units of ω_0. This frequency is within the phonon band. Since we have chosen a "hard" potential, i.e., $d\Omega_0(A)/dA > 0$, there will be a *critical amplitude* $A_c^{(0)}$ such that $\Omega_0(A)$ touches the upper phonon band edge:

$$\Omega_0(A_c^{(0)}) = 1. \tag{6}$$

Accordingly, one may speculate that for $A < A_c^{(0)}$, the initial excitation will completely delocalize and will converge to a breather for $A > A_c^{(0)}$. In the following, we will chose a symmetric potential $V(x)/C = \frac{1}{2}x^2 + \frac{1}{4}x^4$ for simplicity. x can be scaled such that the prefactor of the quartic term equals $1/4$. In that case, it is

$$\Omega_0(A) = \frac{\pi}{4}\sqrt{2 + A^2}/K[-A^2/(2 + A^2)] \tag{7}$$

with $K(m)$ the complete elliptic integral of first kind. Then, Eq. (6) yields

$$A_c^{(0)} \cong 1.16715. \tag{8}$$

In order to check the validity of our speculation above, we determine first the so-called limiting equation for the asymptotic solution $q_\infty(\tau) = \lim_{\Delta\to\infty} q(\tau + \Delta)$ [16]. The Laplace transform of Eq. (3) taking into account the initial conditions can be solved for the Laplace transform $\hat{q}(z)$ of $q(\tau)$ as function of $\widehat{q^3}(z)$. Transforming back to time regime yields

$$q(\tau) = AJ_0(\tau) - \int_0^\tau d\tau' J_1(\tau-\tau')q^3(\tau'), \tag{9}$$

which is equivalent to Eq. (3), as can be proven. For the pure harmonic chain, i.e., neglecting the nonlinear term, we obtain directly $q_{\text{harm}}(\tau) = AJ_0(\tau)$, as is well known. It is straightforward to derive the limiting equation

$$q_\infty(\tau) = -\int_{-\infty}^\tau d\tau' J_1(\tau-\tau')q_\infty^3(\tau'). \tag{10}$$

Since $q_\infty(\tau)$ is an asymptotic solution not possessing a relaxing component, its Fourier transform $\tilde{q}_\infty(\omega)$ can not have an absolutely continuous part $\tilde{q}_\infty^{(c)}(\omega)$. If it would, its contribution $q_\infty^{(c)}(\tau)$ to $q_\infty(\tau)$ would relax to zero for $\tau \to \infty$. Excluding a singular continuous component (which may occur for disordered systems at the mobility edge), $\tilde{q}_\infty(\omega)$ must have a discrete support, i.e., $q_\infty(\tau)$ is either constant, periodic, or quasiperiodic. If it is quasiperiodic, then there are at least two incommensurate frequencies ω_1 and ω_2. The anharmonicity generates Fourier modes with frequencies $m_1\omega_1 + m_2\omega_2$. There exists an infinite number of integer pairs (m_1, m_2) such that $m_1\omega_1 + m_2\omega_2$ is within the phonon band. Therefore, these modes are damped [cf. Eq. (5)] and converge to zero. Accordingly, consistent with our numerical results below, Eq. (10) has two kind of solutions, only: A static one $q_\infty^{\text{static}}(\tau) \equiv q_\infty$ and a periodic one $q_\infty^{\mathrm{periodic}}(\tau + \tau_0) \equiv q_\infty^{\mathrm{periodic}}(\tau)$ with $2\pi/\tau_0 > 1$ in order to avoid an overlap with the phonon frequencies $|\omega| \leq 1$. Substituting $q_\infty^{\mathrm{static}}(\tau) \equiv q_\infty$ into Eq. (10) yields the single solution $q_\infty^{\mathrm{static}}(\tau) \equiv 0$.

So far, we have argued that two types of asymptotic solutions exist, a static and a periodic one. In order to investigate the existence of a critical amplitude A_c, we solve Eq. (9) iteratively. With the asymptotic behavior of J_1, we arrive at

$$q(\tau) \cong A\sqrt{\frac{2}{\pi}}\Big[(\tau/\tau_s)^{-(1/2)}\sin\Big(\tau - \frac{\pi}{4}\Big) - (\tau/\tau_c)^{-(1/2)} \times \cos\Big(\tau - \frac{\pi}{4}\Big)\Big] \tag{11}$$

with relaxation times

$$\tau_\alpha(A) = [\sum_{n=0}^{\infty}(-1)^n \beta_n^{(\alpha)} A^{2n}]^2, \qquad \alpha = s, c. \tag{12}$$

$\beta_n^{(\alpha)}$ are given by n-fold integrals over products of J_1 and J_0. Equation (11) with $\tau_\alpha(A)$ from Eq. (12) is a formal result for $q(\tau)$ represented by a power series in A. It is a physical solution only if the infinite sums in Eq. (12) do exist. The critical value A_c is such that this is true for $A < A_c$. Then, it is

$$A_c = \min\{A_c^{(c)}, A_c^{(s)}\}, \qquad A_c^{(\alpha)} = \lim_{n\to\infty} A_n^{(\alpha)},$$
$$A_n^{(\alpha)} = |\beta_n^{(\alpha)}/\beta_{n+1}^{(\alpha)}|^{1/2}, \qquad \alpha = s, c. \tag{13}$$

An analytical calculation of these integrals seems impossible. Therefore, it is done numerically, which leads to $A_n^{(\alpha)}$ shown in Fig. 1 up to $n = 10$. For $n > 10$, the numerical errors become significant. This result gives evidence that A_c is close to $A_c^{(0)}$. For $A < A_c$, the asymptotic time dependence of $q(\tau)$ is similar to that of the harmonic solution $AJ_0(\tau)$, however, with a different phase and a *renormalized*

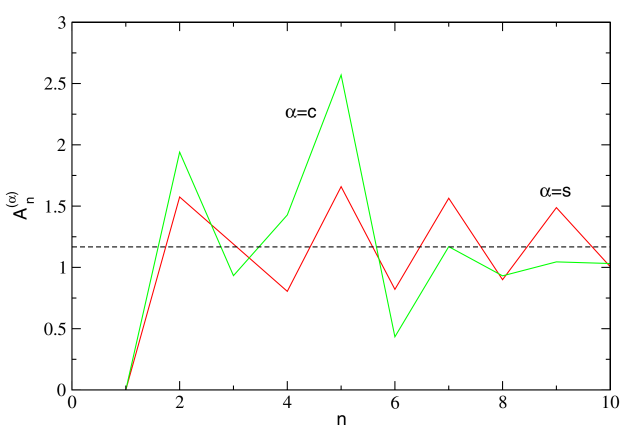

FIG. 1 (color online). n-dependence of $A_n^{(\alpha)}$ from Eq. (13) for $\alpha = s,\ c$. The dashed line represents $A_c^{(0)} \cong 1.16715$ [cf. Eq. (8)].

relaxation time $\tau_{\mathrm{rel}}(A) = \sqrt{\tau_s^2(A) + \tau_c^2(A)}$, which diverges at A_c. This behavior of $\tau_{\mathrm{rel}}(A)$ follows from the divergence of the alternating sums [cf. Eq. (12)] due to the quantitative difference of $\beta_n^{(\alpha)}$ for n even and n odd, which also leads to the "oscillations" of $A_n^{(\alpha)}$ in Fig. 1. According to Eq. (11), $q(\tau)$ decays by an inverse square root law, as also observed for the original β-FPU chain [10].

In order to check these results and to access $A > A_c$, we have solved Eq. (3) numerically up to $\tau_{\max} = 10^5$ using an integration step of $h = 0.05$. Figure 2 depicts $q^{\mathrm{env}}(\tau_i; A)$ for $\tau_i \approx 10^3$, 10^4 and 10^5 where $q^{\mathrm{env}}(\tau; A)$ is the envelope function of $|q(\tau)|$ for given A. With increasing τ_i, a clear sharpening of the transition is found at $A_c^{\mathrm{num}} \cong 1.181$, like for a second order phase transition with finite size effects. A_c^{num} differs from $A_c^{(0)}$ by about 1.2%. The frequency $\Omega^{\mathrm{num}}(A)$ close to $\tau_{\max}$ is shown in Fig. 2. For $A < A_c^{\mathrm{num}}$, we have $\Omega^{\mathrm{num}}(A) \cong 1$ and for $A > A_c^{\mathrm{num}}$, it is well approximated by $\Omega_0(A)$ for the isolated bond. However, for A above but close to A_c^{num}, the discrepancies are about 2%, whereas for $A \gg A_c^{\mathrm{num}}$, they disappear. Whether the small deviation of A_c^{num} and Ω^{num} from $A_c^{(0)}$ and $\Omega_0(A)$, respectively, is genuine or stems from numerical inaccuracy is unclear. Hence, it is not obvious that $A_c = A_c^{(0)}$. For $A > A_c^{\mathrm{num}}$, the initial excitation indeed converges to a DB with frequency $\Omega^{\mathrm{num}}(A)$. Figure 3 shows the numerically determined relaxation time $\tau_{\mathrm{rel}}(A)$ for $A < A_c^{\mathrm{num}}$, and for $A > A_c^{\mathrm{num}}$ the inverse modulation frequency $2\pi/\omega_{\mathrm{mod}}(A)$ of a modulation of the DB, which is observed numerically. For $\tau \to \infty$, the modulation amplitude decays to zero. τ_{rel} has been determined from the criterion $q^{\mathrm{env}}(\tau_{\mathrm{rel}}) = A/10$. Both τ_{rel} and $2\pi/\omega_{\mathrm{mod}}$ seem to diverge at A_c^{num} by a power law with an exponent ≈ 0.61 and ≈ 0.87, respectively, (see

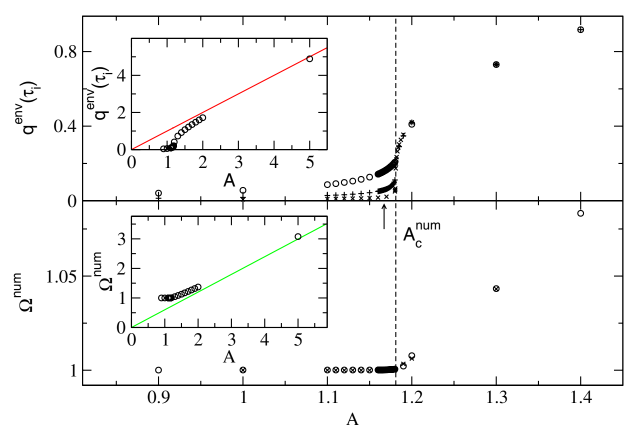

FIG. 2 (color online). Top panel: A-dependence of $q^{\mathrm{env}}(\tau_i)$ for $\tau_i \approx 10^3$ (circles), 10^4 (plus signs), and 10^5 (crosses) time units. The inset demonstrates the asymptotic behavior $q^{\mathrm{env}}(\tau_i) \sim A$ (solid line). Bottom panel: DB frequency $\Omega^{\mathrm{num}}(A)$ at $\tau_i \approx 10^5$ time units as function of A. The arrow indicates the critical value $A_c^{(0)}$ from Eq. (8) and the dashed line $A_c^{\mathrm{num}} \cong 1.181$. The inset shows the asymptotic A-dependence $\Omega(A) \sim A$ (solid line).

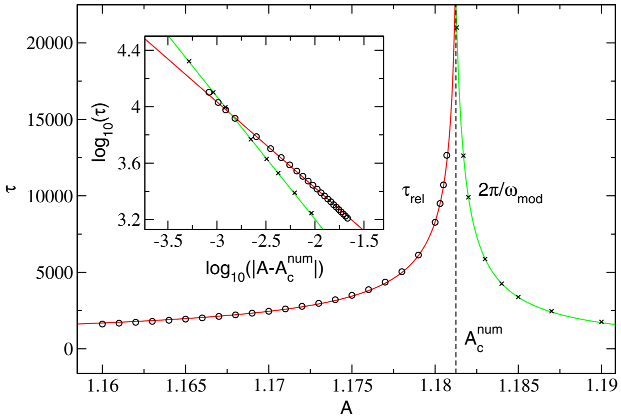

FIG. 3 (color online). Renormalized relaxation time τ_{rel} (circles) and modulation period $2\pi/\omega_{mod}$ (crosses) as function of A. The dashed line indicates $A_c^{num} \cong 1.181$. The solid lines represent power law fits of τ_{rel} and $2\pi/\omega_{mod}$ with exponents 0.61 and 0.87, respectively, which are supported by the log-log plots of the inset.

inset of Fig. 3). A power law divergence $\tau_{rel}(A) \sim (A_c - A)^{-\gamma}$ implies that $\beta_n^{(\alpha)} \sim (A_c)^{-n} n^{-(1-\gamma/2)}$ for $n \to \infty$. Whereas the exponential factor is strongly supported by our calculations, the validity of the power law part can not be checked due to the limitation $n \leq 10$.

Finally, we have analytically determined the moments $m_\ell^{(pot)}(\tau) = \sum_{n=1}^N (n-M)^\ell e_n^{(pot)}(\tau)$, $\ell = 1, 2, 3, \ldots$ of the potential energy profile $e_n^{(pot)}(\tau)$ in the thermodynamic limit. As a result, we find

$$m_\ell^{(pot)}(\tau) = \int_0^\tau d\tau_1 \int_0^\tau d\tau_2 K_\ell(\tau - \tau_1, \tau - \tau_2) \times \frac{1}{C} V'[q(\tau_1)] \frac{1}{C} V'[q(\tau_2)]. \tag{14}$$

Let us restrict to $\ell = 2$. $K_2(x, y)$ can be calculated analytically and expressed by $J_1(x \pm y)$ and $J_2(x \pm y)$. Taking into account the asymptotic expansion of J_n, we find $m_2^{(pot)}(\tau) \sim \tau^2$ for $\tau \to \infty$, for *all* A. Hence, the energy transportation is ballistic. This is expected since the transportation is within the half infinite left and right *harmonic* part of the chain. Using the profile of the kinetic energy will not change these results.

To summarize, based on combined analytical and numerical calculations of a reduced β-FPU chain where the anharmonicity is restricted to a single bond, we have presented clear evidence for the existence of a *critical* amplitude A_c which separates delocalization from localization. This demonstrates that a single conservation law is sufficient for such a transition. A_c^{num} differs slightly from $A_c^{(0)}$. Therefore, it is not clear whether A_c coincides with $A_c^{(0)}$ or not. Of course, no compelling arguments exist for their equality. In addition, the divergence of the iteration series is the mathematical origin of the transition at A_c and leads for $A < A_c$ to a renormalized (due to anharmonicity) relaxation time τ_{rel} which diverges at A_c. The numerical solution suggests a power law divergence with exponent smaller then one. Above A_c, it yields the convergence towards a DB with frequency very close to $\Omega_0(A)$ of the isolated bond. Finally, from the large τ behavior of the second moment $m_2(\tau)$, we find *ballistic* energy transportation for $A < A_c^{num}$ and $A > A_c^{num}$. This proves that a divergence of $m_2(\tau)$ is not necessarily an indication of complete energy spreading, as it has been assumed for DNLS [17], supporting the conclusion in [15].

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