Discreteness effects on soliton dynamics: A simple experiment

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We present a simple laboratory experiment to illustrate some aspects of the soliton theory in discrete lattices with a system that models the dynamics of dislocations in a crystal or the properties of adsorbed atomic layers. The apparatus not only shows the role of the Peierls–Nabarro potential but also illustrates the hierarchy of depinning transitions and the importance of the collective motion in mass transport. © *2000 American Association of Physics Teachers.*

I. INTRODUCTION

Since the discovery of solitary waves by J. Scott Russell[1] on his horse along the Edinburgh canal, and the seminal paper by Zabusky and Kruskal[2] explaining the recurrence phenomenon found by Fermi–Pasta–Ulam in a nonlinear chain of atoms, the soliton concept has been the starting point of very fruitful research: It has not only led to very important advances in applied mathematics but it is also an excellent tool for explaining the properties of various physical systems.[3]

The soliton concept is generally associated with continuous fields. For instance, the very interesting resource letter on solitons, recently published in the *American Journal of Physics*,[4] does not contain more than a few lines on discrete lattices despite the fact that many physical systems are intrinsically discrete, such as crystals or macromolecules. This is because, except for very few specific cases such as the Toda lattice, the discretized version of integrable partial differential equations that describes physical systems does not have true soliton solutions. However this does not mean that the soliton concept is useless for describing nonlinear excitations in discrete systems. Such systems can sustain approximate soliton solutions, and discreteness introduces new features such as soliton pinning or radiation of small amplitude waves. These effects are important for understanding some physical phenomena. For instance, it is because their width is of the same order as the lattice spacing that dislocations do not propagate freely in a crystal and radiate vibrational modes when they are forced to propagate by an external stress. This explains the familiar observation that when one successively bends and unbends a piece of iron wire many times it gets hot. Each plastic distortion moves dislocations that radiate vibrational waves in the solid, raising its temperature.

The present paper has a dual purpose. First we want to give a brief tutorial on quasisolitons in discrete systems using the example of the diffusion of atoms on a crystalline surface because, on the one hand, it allows a rather intuitive understanding of the phenomena and, on the other hand, it shows how collective effects can lead to new phenomena. Then we introduce a simple experiment, easily built in a physics laboratory, which illustrates some of the discreteness effects that cannot be shown with the soliton experiments that have been proposed earlier, such as water waves experiments (see the review by Segur in Ref. 3) or the chain of strongly coupled pendula proposed by A. C. Scott.[5]

II. A BRIEF TUTORIAL ON COLLECTIVE DIFFUSION

Before describing the apparatus and experimental results, let us recall some basic ideas on the diffusion of particles over a periodic potential under the effect of an applied force. The motion of a single particle can be easily analyzed if one considers only the low temperature situation where the thermal fluctuations can be neglected. In the absence of a driving force, the particle is trapped in a potential well. Applying a driving force is equivalent to tilting the potential and, above a critical angle α_0, the minimum disappears and the particle starts to slide on the washboard potential.[6]

Instead of a single particle let us now consider a chain of particles coupled by harmonic springs with an equilibrium length equal to the distance between the potential minima: This state is called a commensurate state. Its ground state is reached when all the particles are in the potential minima [Fig. 1(a)] and the situation is comparable to the case of a single particle: The motion induced by an external force will only start when the minima of the total potential (including the force term) have disappeared. If a defect is introduced in the chain, the situation becomes very interesting and is equivalent to creating a dislocation in a crystal. Consider for instance the case of a missing particle obtained by moving one-half of the chain by one unit, i.e., a kink in the particle positions. In the vicinity of the defect, the competition between the elastic energy of the springs and the substrate potential energy displaces the particles with respect to the minima of the potential [Fig. 1(b)]. As a result, the particles next to the defect are easier to move with an external force than a particle sitting at the bottom of the well. For a sinusoidal potential of period $a, V(x)=V_0[1-\cos(2\pi x/a)]$, when the coupling between the particles is strong, the position of the nth particle is $x_n=a[n+(2/\pi)\tan^{-1}\exp(n/l)]$, with $l=(a/2\pi)\sqrt{k/V_0}$ where k is the spring elastic constant.[5] No analytical solution for the structure of the defect is known in the case of weak coupling.

When the coupling between the particles is very *strong*, the defect is extended. The displacements of the particles vary progressively from zero to one lattice spacing across the defect. Consequently, there are particles at any level of the substrate potential, including on the maximum. This is the situation that is realized in the chain of strongly coupled pendula described by Scott.[5] In this quasicontinuum situation, it is easy to understand why the defect (or soliton in the terminology of nonlinear science) can move freely. When it is translated, some particles have to climb over the substrate potential barriers but simultaneously others move downward

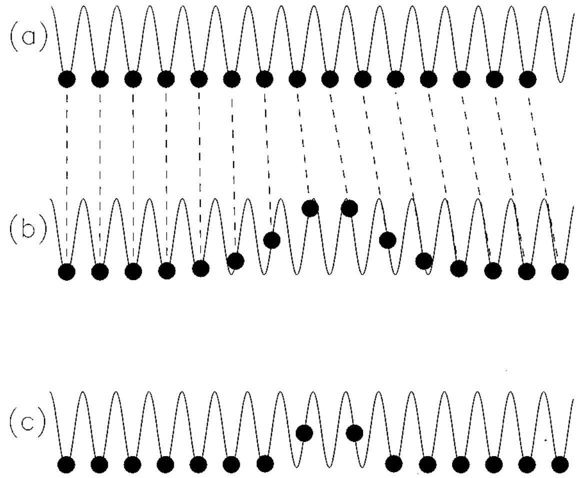

Fig. 1. Positions of a set of harmonically coupled particles subjected to a periodic potential. The springs connecting the particles (schematized by the thick line) have an equilibrium length equal to the period of the potential. (a) Ground state of the system. All particles are in the potential minima. $\theta=1$. (b) Excited state. The particles on the right half of the chain have been moved to the next potential well, creating a localized defect in the particle distribution. $\theta=1-1/N$. (c) The same excited state for a weaker coupling k (weaker connecting springs). The defect is narrower (i.e., the width l is smaller), and the atoms in the defect core are closer to the minima of the potential. The depinning force required to move the defect (c) is therefore higher than the depinning force in case (b). $\theta=1-1/N$.

in the potential and the overall translation does not require any energy. In a continuum model, the system is invariant under *any* translation and the free motion of the soliton is simply a manifestation of this translational symmetry (Goldstone mode).

In the *weakly* coupled situation that we consider here, the situation is different. The defect is highly localized and even though some particles are slightly displaced from the potential minima as in Fig. 1(c), the springs are not strong enough to maintain particles at the top of the substrate potential barriers. Now, in order to translate the defect, one has to move particles up on the substrate potential: There is a barrier to the free translation of the defect, which is well known in dislocation theory as the Peierls–Nabarro (PN) barrier. The weak coupling case appears therefore as a natural intermediate case between the case of individual particles which must overcome the full potential barrier of the substrate potential and the continuum case where the soliton is completely free to move. In this intermediate case, the defect moves as a *collective excitation* over an *effective potential*, the PN potential, which has the period of the lattice and an amplitude which is much lower than the individual potential barrier of the substrate. This analysis in terms of a collective object explains why the critical stress for the plastic deformation of a crystal is several orders of magnitude lower than the stress that would translate a full atomic plane above another.[7]

The case of atoms adsorbed on an atomic surface is even more interesting because usually the equilibrium distance b that the atoms would select if they were free is not commensurate with the period a of the crystalline substrate. As a result, the interaction forces compete with the substrate potential to determine the particle positions. The atomic layer minimizes the energy by letting the particles drop near the bottom of the substrate potential wells almost everywhere and compensating for the mismatch between a and b by creating local discommensurations which are very similar to the isolated defect described above for the commensurate case. The only difference is that, depending on the commensurability ratio, there is a hierarchy of defects with different shapes and different barriers. In the case of an irrational ratio, this hierarchy is complete and some defects have a vanishingly small PN barrier: In the discrete lattice (provided the coupling is not too weak[8]), a vanishingly small external force can cause mass transport in the system. The application of an external driving force to an interacting chain of atoms exhibits this *hierarchy of depinning transitions*.[9] For very low force, no motion can be detected. Then, the geometrical kinks (the discommensurations due to the concentration of particles related to the number of minima of the potential) start to move whereas the atoms remain static. For larger external forces, additional defects (*kink–antikink pairs*) are created, giving rise to an increase of the mobility. Finally, for high enough forces, all atoms move with the mobility of single Brownian particles.

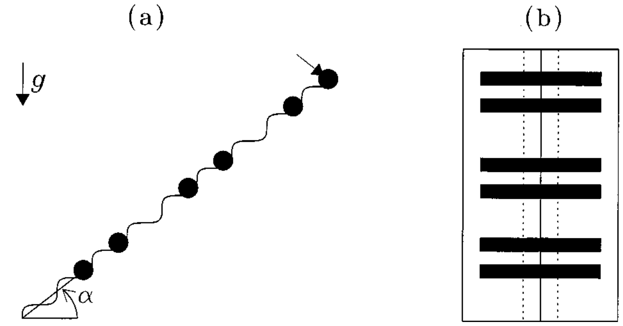

Fig. 2. Sketch of the experiment in the case $\theta=2/3$. The side view is presented in (a), whereas (b) presents the top view. In (a), the arrow g indicates the direction of the gravity field. The top arrow means that this cylinder is always kept fixed. In (b), the dotted lines represent the slot made in the plastic support in order to let the elastic, represented by the solid line, free.

III. EXPERIMENT

Let us now describe the experimental apparatus sketched in Fig. 2. The system under study is a chain of steel cylinders, each one 60 mm in length and 8 mm in diameter. The cylinders sit on a washboard potential cut in a block of plastic (approximate sine-shape potential). The height of the valleys is 10 mm and the lattice spacing is 20 mm. The cylinders are coupled to one another with an elastic string; the first cylinder is fixed whereas the other ones are free to move. In the example shown in Fig. 2, a 3-mm slot was made along the center of the plastic support [represented by the two dotted lines in Fig. 2(b)] in order to let the elastic move freely.

The concentration of cylinders, which determines the presence and structure of the discommensurations, is defined as $\theta=M/N$ where M is the number of cylinders and N the numbers of lattice spacings. The defects shown in Fig. 1(b) and (c) correspond to $\theta=15/16$ while Fig. 2 shows schematically the case $\theta=2/3$. In the experiment, the length b of the elastic strings is adjusted for each concentration by imposing the condition $\theta=a/b$, which means that in the absence of the substrate potential, the cylinders would be equally spaced in such a way that M cylinders would cover N lattice spacings, achieving the desired concentration.

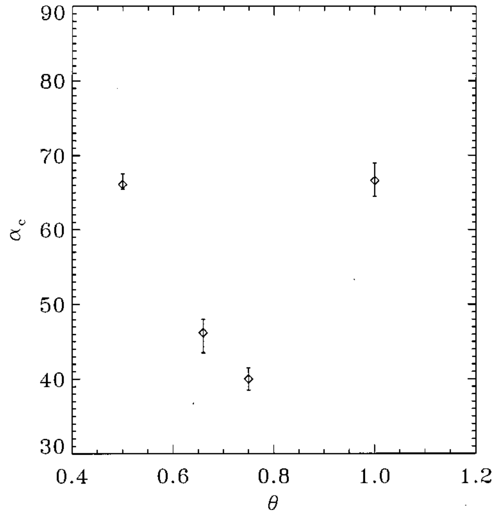

Fig. 3. Critical angle above which the initial concentration is unstable, giving rise to a moving kink soliton. The concentration is defined as the ratio between the number of cylinders and the number of sites.

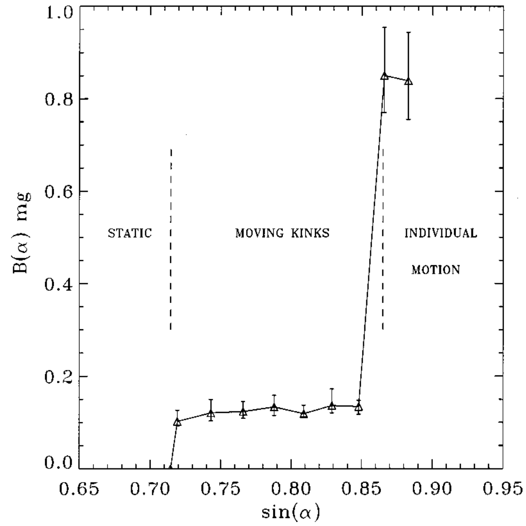

Fig. 4. Mobility in the case $\theta=2/3$, represented in Fig. 2, versus the external force, monitored by changing the angle α. The results illustrate the three different regions, and the hierarchy of depinning transitions.

The apparatus can be used to test the static and dynamical properties of this model system. First one can measure the depinning force which is required to move a lattice with a given concentration above the substrate. This is done by progressively inclining the system, i.e., increasing very slowly the angle α and determining the critical angle α_c above which the initial distribution of cylinders is unstable, i.e., above which at least one cylinder begins to slide. The results of this experiment are shown in Fig. 3. For $\theta=1/q$ (with $q=1,2,...$), the system has a trivial ground state with one cylinder at the bottom of the substrate potential well every q wells. In these cases, all cylinders start to move simultaneously. As discussed above, these commensurate cases should be the hardest to depin and this is confirmed by the experiment. Moreover the behavior should not depend on the number of empty wells that might separate two cylinders, i.e., we expect the same critical angle for $q=1$ or $q=2$. This is confirmed by the results shown in Fig. 3. When $\theta=p/q$ is a rational number with $q>p, q\neq 1$, such as $\theta=2/3$ shown in Fig. 2, the ground state involves defects, and Fig. 3 shows that their cooperative motion (cases $\theta=2/3, \theta=3/4$) occurs for lower angles than the individual motion. This illustrates therefore the depinning hierarchy, the Peierls–Nabarro barrier being lower than the substrate barrier. Figure 3 also shows that the PN barrier depends on the commensurability ratio which governs the structure of the kink defects;[9,10] higher order rational numbers result in a lower PN barrier: $\alpha_c(2/3)>\alpha_c(3/4)\Rightarrow E_{\mathrm{PN}}(2/3)>E_{\mathrm{PN}}(3/4)$. With a system as small as the one we are using we cannot study other rationals such as 3/5, 5/8, 8/13 that should lead to lower barriers. A truly incommensurate case, leading to a vanishing PN barrier,[8] corresponds to an irrational ratio and therefore it cannot be obtained in an experiment since M and N are necessarily integers. This case can however be approached by rational numbers with numerators and denominators chosen in a Fibonacci sequence,[11] but it would require a model much longer than the one we have built.

The second class of experiments that can be performed tests the dynamical properties of the system by measuring the mobility of the defect as a function of the applied force. This is done by artificially holding the defect above the critical angle α_c while the potential is tilted, and then letting it go. When the constraint is released, the defect slides on the washboard potential. Using a high speed charge-coupled device (CCD) camera to record the fast motion, we measure the time Δt for the propagation of the defect over n lattice spacings.

Since the velocity is $\langle v\rangle=na/\Delta t$ and the external force is due to gravity, $F=mg\sin(\alpha)$, the mobility is by definition

$$B(\alpha)=\langle v\rangle/F=\frac{na/\Delta t}{mg\sin(\alpha)}. \tag{1}$$

The results, obtained for the concentration $\theta=2/3$ sketched in Fig. 2, are plotted in Fig. 4: They clearly show a plateau corresponding to the kink-running state, obtained when only the defect moves, leading to the first contribution to mass transport. The final transition to the sliding state, where all cylinders slide on the washboard potential, is reached for higher external forces.

IV. CONCLUSION

In this brief report, we have presented a simple teaching experiment stressing the kink concept in a discrete system. One is able to illustrate different theoretical ideas in a simple way using this experiment. The Peierls–Nabarro potential, usually presented in the context of dislocation theory, and its role are not only clearly emphasized but one shows that it is a function of the concentration,[8] i.e., for atoms adsorbed on a crystal, it varies with the coverage. Moreover, this experiment explains the recently developed idea about two-dimensional diffusion of atoms.[9] One easily detects a hierarchy of depinnings: First the defects (kinks or antikinks) are moving, then for higher forces, we have the individual motion. The present apparatus is too short to illustrate experimentally the existence of a hysteresis phenomenon in the force driving the diffusion:[9] The chain starts to slide for a force F_1 but stops only when the force has been lowered below $F_2<F_1$ because, once the motion has been initiated, the kinetic energy allows the particles, or the defect, to overcome a small potential barrier. It would be very interesting to

build a much longer chain, so that few defects could coexist and of course interact. The critical angle of the different concentration regions would also be different.

This experiment has however some important differences from the physical problem of atomic diffusion. The elastic strings apply a force to the cylinders only when they are extended (not in compression) and the unavoidable solid friction has no simple equivalent at the microscopic level. It is therefore important not to overemphasize these results. Nevertheless, as recent very nice experiments in Josephson junction arrays[12] have confirmed discreteness effects on soliton-like structures (see the review by Peyrard in Ref. 3), we think that the present experiment, conceptually and materially more appropriate for teaching purposes, could be an excellent tool to present the soliton concept in the framework of discreteness to nonspecialists.

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WESTERN CIV

Anyone who became convinced that modern cosmology was peculiarly Western, and who did care about objective truth, might reasonably conclude that Western civilization is superior to all others in at least one respect, that in trying to understand what you can see in the sky on a starry night, Western astronomers got it right.

Steven Weinberg, ''Before the Big Bang,'' New York Review of Books, June 12, 1997.