The Commensurate Incommensurate Transition

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I. INTRODUCTION

In condensed matter physics there are many successful models of phase transitions between a more ordered and less ordered state. Break a continuous symmetry and you've got yourself a cpmtomipus phase transition. Roughly speaking the transition occurs when the symmetry breaking potential term becomes the dominant one in the free energy and the system 'contracts' in phase space - decreasing entropy but more than compensating by the lowered energy. However, what happens when you have two types of potential energies favoring different system configurations; how do you describe the transition between two (or more) different types of order? The question is broad enough to have no general answer. Yet speaking phenomenologically we can say that often, as the different orders compete, the system develops new and interesting structure. Possibly the simplest example of this type of effect occurs is in the 1-D Frenkel-Kontorova (FK) model which is the primary topic of this paper. Like many 1-D models its virtue lies in its solvability which allows us to see in detail how the system develops its novel structure; and crucially to get a flavor for how approximation schemes such as perturbation theory and variational approaches either fail or succeed to reveal the full structure.

II. THE FK MODEL

The FK model is so elegantly simple that most physicists could write it down by simply looking at the picture:(1)

But since my aversion to repetition is weaker than my desire for clarity, I will also describe the system in words. As for notation, I will largely use the conventions contained in Pokrovsky and Talapov's book[2] on the subject. Indeed I should acknowledge that this

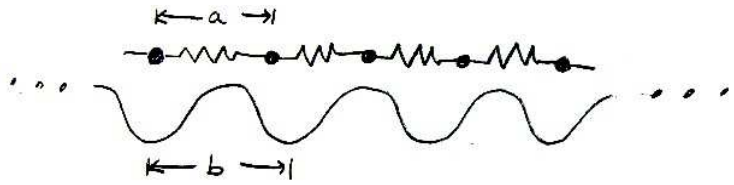

FIG. 1: This says it all

FIG. 2: With a small interaction the degeneracy is lifted

paper is largely based on their excellent treatment of the subject.

The system is composed of an infinite number of point particles at positions $..., x_1, x_2, x_3, ...$ These particles interact harmonically with their nearest neighbor with an equilibrium spacing of a. All the atoms also experience a periodic cosine potential of period b; we could consider a more general periodic potential but the case of only one mode is sufficient to illustrate the relevant physics. The discussion will primarily be restricted to classical particles in one dimension at $T = 0$ (the only T at which transitions occur in 1D without long range interaction), though in the penultimate section we will briefly comment on various other generalizations. Thus, the primary question I will ask is: Given the form of the potential energy, what is the lowest energy configuration of particles?

Let us first consider the case when the potential energy is given by only a harmonic interaction between neighbors then $U_{harm} = \frac{\lambda}{2}\sum_n (x_{n+1} - x_n - a)^2$. For this form of the potential the minimum energy configuration is easily seen to be $x_n = na$. Now lets consider the case when the external potential is dominant and has the form $U_{ext} = \gamma \sum_n (1 - \cos(2\pi x_n/b)$. If the interaction term is exactly zero then we would have the unphysical situation that any configuration with the atoms randomly distributed at the equivalent minimums would all be a ground state. However, with any vanishingly small interaction that is repulsive at short distances and attractive at long distances (compared to b) this degeneracy is broken and $x_n = nb$ becomes the unique ground state.(2)

Thus both ground states are of the form $x_n = n\tilde{a}$. The question then becomes when both terms in the potential energy are important what is the ground state? Naively we would expect that the system configuration to also have the same form, however we will find out

that in fact the 'interplay' between the two terms generates more structure than either term does by itself. In my opinion this is one of the clearest examples of the dictum, "more is different."

But how do we move forward? Well, to simplify our lives we first minimize the number of symbols we will have to write down by defining our length and energy scales via $b = 2\pi$ and $\lambda = (2\pi)^{-2}$; we include here factors of 2π so we don't have to write them later; though I'm afraid this might case some confusion. Now we simply solve the stationary state equations for the potential energy $\delta U = 0$. Which generates an infinite number of second order difference equations:

$$2x_n - x_{n+1} - x_{n-1} + \gamma \sin(x_n) = 0 \tag{2.1}$$

Solving this set of equations will now occupy us for the next three sections. Note that a does not appear in these equations. Remember though that this is just an equation for a stationary solution and like a second order differential equation it has two free parameters. To find the global minimum you have to compute how the total energy depends on these two parameters and then minimize with respect to these variables. This last step will prove to be highly non-trivial in the general case.

III. PERTURBATION THEORY

Lets begin by trying to use perturbation theory to solve the equations. Namely, lets assume that the external potential is a small perturbation of the harmonic ground state. We do this via $x_n = n(a + \alpha) + u_n$ where α and u are both small. This is a nonstandard perturbation since it allows configurations of particles that are not arbitrarily close to the configuration being expanded about. However in principle this should work since what is important is not that the change in configuration be small, but that the change in the coordinates that describe the configuration be small. Meaning typically you need the perturbing (and perturbed) potentials to be linear (quadratic) in the small change in coordinates.

In our case we can show that the perturbing potential is not linear in α (though it is almost constant) as follows: Assuming the u_n to be negligible the energy per particle for the external potential is given by

$$u = \gamma \lim_{n\to\infty} \frac{1}{n} \sum_n (1 - \cos((a + \alpha)n)) \tag{3.1}$$

We can already begin to see the importance of commensurability because the sum in this equation can be rewritten as $\sum_n \cos(2\pi n(a+\alpha)) = Re(\sum_n (e^{i2\pi(a+\alpha)})^n)$ from which we can be see that if $(a+\alpha) = 2\pi M$ or $(a+\alpha)/b = M$ where M is an integer, then the sum is $\sim N$ otherwise it is zero. Thus in principle if we stay far away from these danger points the perturbation in α should work though it would be a rather trivial calculation because to first order the perturbation is invariant of α. However, this is my point: the difference equations from which the perterbation make no reference to the scale a other than by the fact that we inserted by hand in our perametrization of the state we were peturbing about. And in fact we find that the peterbation is invarrient to α and thus to a. How can we have competition between length scales if our equations ignore one of them?

To answer this question we have to develop the calculation a little further. So for the moment we forget or troubles by ignoring the α dependance and concentrating on the u_n perturbations. We treat them by decomposing them into their fourier components $u_n =: \int \frac{dk}{2\pi a} e^{ikan} u(k)$ and analyzing the kth component of the difference equation we find after a bit of delta function trickery, we have to first order

$$u(k) = -i\gamma \frac{\delta(k^2-1)}{2(1-\cos(ka))} = 0 \tag{3.2}$$

Clearly all $u(k)$ components are zero except for $k = \pm 1$. We see again commensuration issues in this formula because if a is nearly equal to an integer multiple of b perturbation theory will not work because $|u| \ll 1$ is no longer valid. As an aside physically this divergence comes from the fact that if the periods almost line up, there is a strong tenancy to just compress the whole string of springs a little and line everything up exactly. (In fact it turns out its best to compress the springs in lumps which we will see leads to the formations of solitons). Otherwise, where perturbation is valid we see that perturbation creates not a net compression but a simple periodic modulation of the positions to take advantage of the local conditions of the potential.(3)

Let us now return to our concerns about the missing a scale. We saw it caused the theory to break down, but we already saw that. What about where it is valid? To answer this question we have to calculate the decrease of the energy per particle due to the perturbation. However we also restore the $/alpha$ dependance to see if varring it can lower the energy. After a few steps of algebra:

$$u = \frac{1}{2}\alpha^2 - \frac{\gamma^2}{2(1-\cos(a+\alpha))} \tag{3.3}$$

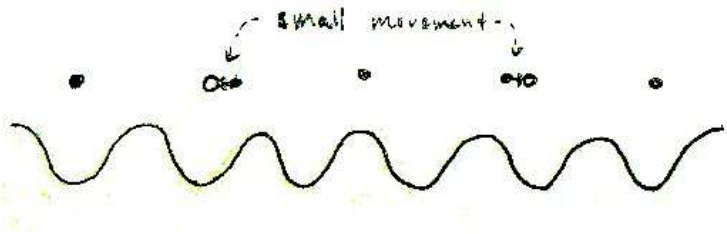

FIG. 3: The text reads 'small movement.'

What we now see by inspection that $\alpha = 0$ is no longer the energy minimum (assuming the above calculation is self consistent). But the important point is that the physics certainly does care about the scale a. And here is the central point: even though the difference equation mysteriously drops the scale a and thus its solutions don't depend on it this doesn't mean that the physics is invariant of a, because solving the difference equations is only part of the problem's solution since solving the difference equations still leaves you with two free parameters. The second part of the problem is using the minimumization of the energy to determine how to fix these free parameters, and its at this second, just a crucial step that the a scale becomes important. Perhaps, I've overemphasized this point. I only do so because it caused me a lot of confusion. The moral of the story is: solving the difference equations is interesting but it is only half of the problem.

IV. CONTINUUM APPROXIMATION

In the previous section we saw that perturbation theory broke down when a and b were nearly equal. However, we will now develop an approximation that is valid precisely in this regime. Define $a = b + \delta$ we need both $\delta \ll 1$ and $\gamma \ll 1$ which is well defined if we recall our definition of units at the end of the second section. The first thing to note is that since $\sin(an + u_n) = \sin((2\pi + \delta)n + u_n)$ we can write the difference equations as

$$u_{n+1} - 2x_n + x_{n-1} = \gamma \sin(\delta n + u_n) \tag{4.1}$$

Since δ is small the sine term doesn't vary much explicitly with n and secondly since γ is small we know that u_n is only a slowly varying function of n. Thus we can make a continuum approximation $u_{n+1} - u_n \cong du/dn =: u'$, likewise for the second derivative. It is conventional

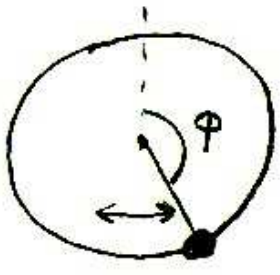

FIG. 4: The Mechanical Analogue

to define $\phi(n) := \delta n + u_n$. Thus the potential takes the form.

$$U = \int dn(\frac{1}{2}(\phi' - \delta)^2 + \gamma \sin(\phi) \tag{4.2}$$

Calculating $\delta U/\delta\phi = 0$ or considering the continuum limit of the difference equations we derive the following equation of motion:

$$\phi'' = \gamma sin(\phi) \tag{4.3}$$

This is the equation of motion of a pendulum with n playing the role of time. Thus to describe its solution I will use a mechanical analogy, since in my opinion the best explanations find the shortest distance between what you understand and what you don't. Importantly given the sign of the right hand side we are effectively measuring the angle of the pendulum from vertical.(4)

As we have discussed there are two constants of motion. Both can be understood in our analogy: One as the total 'energy' (I use quotes to distinguish from the real physical potential energy of the configuration of particles) of the pendulum which I will parameterize as $E := \frac{1}{2}\phi'^2 - \gamma\cos(\phi)$. The other is the arbitrary choice of the origin for time. A pendulum has two very distinct types of motion one is oscillation back and forth at the bottom of a potential well; the other is when the energy is large and the pendulum spins around and around. These two types of motion are effectively described in terms of a phase space diagram.(5) When inspecting figure(5) it is important to note that for configurations of the 'occilate' type ϕ is on average zero so this phase is commensurate. For the 'spin' type configuration ϕ' is on average positive which means that average period will be can be incommensurate with a. This is the main billing: The Commensurate-Incommensurate Transition!

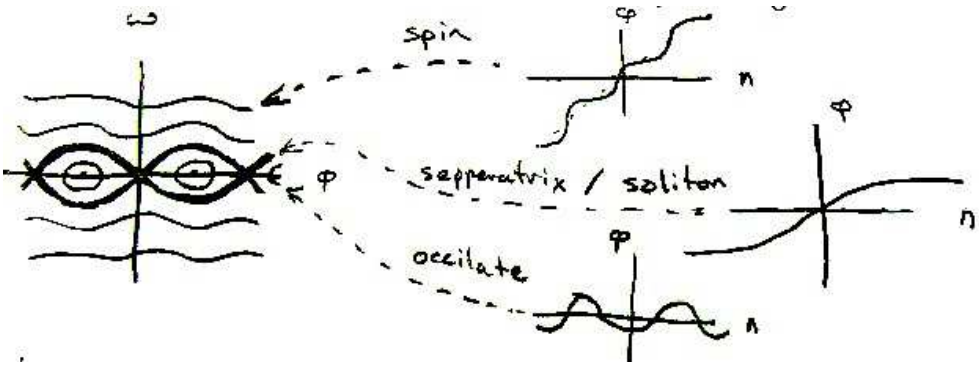

FIG. 5: Left: The phase space diagram of the mechanical analogue. Right: The corresponding real configurations showing the deviation from na as a function of n.

At the risk of pedantry lets mention again that every possible equation of motion is an extremal configuration. We've solved the difference equations. However we have yet to consider step two: figuring out which one is the global minimum. To do so we we must plug the configurations (indexed by their 'energy') into the configurational energy expression. The result is:

$$U(E) = \int dn[\frac{1}{2}(\phi_E(n)' - \delta)^2 - \gamma\cos(\phi_E(n))] \tag{4.4}$$

Note that each configuration is also indexed by its choice of time origen. Thus the above equation confirms by simple inspection that indeed the potential energy is invariant under this index. Physically this means that the translations of the structure seen in figure (5) are zero modes. Note that in the incommensurate phase these modes will have a non-zero net mass current.

The question now becomes for what values of γ and δ do we get the three different structures stated above: Spinning / Seperatrix / Oscillate; for lack of better terms. As the terminology suggests our strategy is the determine the condition for the *seperatrix* to be the ground state configuration, which will then *sepperate* the two types of configurations and thus define the CI transition. The soliton configuration is distinguished by having $E = 2\gamma =: E_s$ since for exactly this energy the pendulum takes an infinite amount of time to start at the top, fall, and re-approach the top asymptotically. To determine the condition for a single soliton to form we can compute its configurational energy - if its found to be negative, we know that solitons will populate the system until their interactions limit their density. To decide if a soliton has a negative energy we calculate its energy relative to the

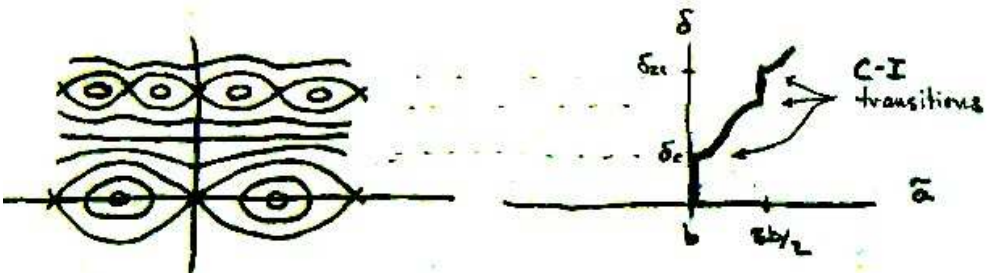

FIG. 6: Left: The phase space diagram of the mechanical analogue. Right: The corresponding real configurations showing the average particle spacing $\tilde{a}$ as a function of δ.

commensurate phase. After simplifying, using the relation $\phi' dn = d\phi$ and computing the resulting integral we arrive at

$$U(E_s) = -\delta + \frac{4}{\pi}\sqrt{\gamma} \tag{4.5}$$

Thus when $\delta_c \sim \sqrt{\gamma}$ we have a transition to the incommensurate phase. A more through treatment would expand $U(E - E_c)$ to forth order in an order parameter and see the standard uniform ϕ^4 transition, though since I'm not sure what in this case is the order parameter to do so is by default beyond the scope of this review.

Though we have observed the commensurate - incommensurate transition for $a = b + \delta$ a similar transition occurs for when $a = (M/N)b + \delta$. It is possible to derive an analogous energy equation

$$U_2 \sim \int dn[\frac{1}{2}(\phi' - h)^2 + \eta\cos(N\phi)] \tag{4.6}$$

Only for this case while $h \sim \delta$, $\eta \sim \gamma^N$. This means the transition will occur after $\delta_{2c} \sim \gamma^{N/2}$. If should be noted as a heuristic argument that since for small x, $\sum_n nx^n$ is finite and proportional to x, we can prove that for small γ the commensurate regions do not occupy all of the δ interval. We can further understand how this effects our original phase diagram in the following schematic way. Assume besides $a = b + \delta$ the only other important resonance is $a = 3b/2 + \delta_2$. When ω gets of order $b/2$ we effectively have to atoms spaced together at a distance $a \sim 3b/2$; Or said another way $a = 3b/2 + \delta_2$ which is the requirement for U_2 to be a good approximation. Thus around $\omega = b/2$ above the U structure we see in fig. (5) we get a copy of the same structure - only smaller and with half the period. Graphically we have.(6) As γ gets larger the commensurate regions δ_c get larger filling out more of the diagram till we are presented with a phase diagram labeled devil's staircase.(7)

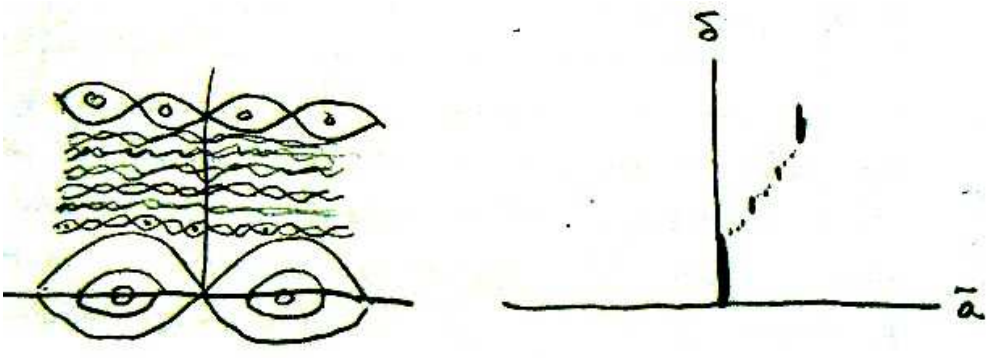

FIG. 7: In the limit that the δ interval is completely covered in commesurate regions we reach the devils staircase; here shown on its side.

V. EXACT SOLUTION

Even though the continuous approximation framework is the most effective way to think about the C-I transition it is only an approximation. For general δ and γ it will break down and the problem has to be approached directly using the method developed by Aubry [1]. The key step is motivated by the usefulness of the phase space concept in the continuum case. What we do is transform our second order equations for our extremal condition into first order equations via the definition $\omega_n := \phi_{n+1} - \phi_n$. The resulting equations are

$$\omega_{n+1} = \omega_n + \gamma \sin(\omega_n + \phi_n) \tag{5.1}$$

$$\phi_{n+1} = \omega_n + \phi_n \tag{5.2}$$

This mapping from a 2-D space onto a 2-D space is continuous but non-linear. We imagine starting with some initial position and move along the configuration chain by repetedly applying the transformation map.(8) Now consider how any continuous line connecting the first two points is transformed.(9) The general strategy to restrict your line so that it is as differentiable as possible at the successive mapping points. Once this is done you develop structures as close as possible to those found in the continuous approximation. In particular you would like to find a seperatix between trajectories with that on average increase with n (incommensurate) and those that are on average constant (commensurate). However in this chaotic landscape the seperatrix can have a complicated, and even self intersecting form.(10) Further, the dynamics of the evolution map are chaotic; meaning roughly that if two points

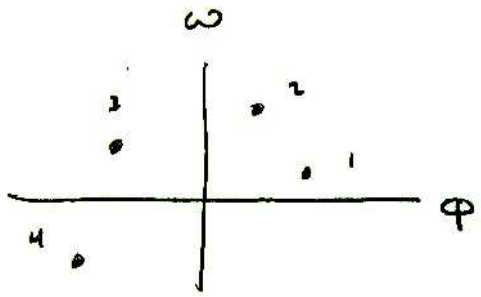

FIG. 8: Schematic of how the mapping could evolve sequentially.

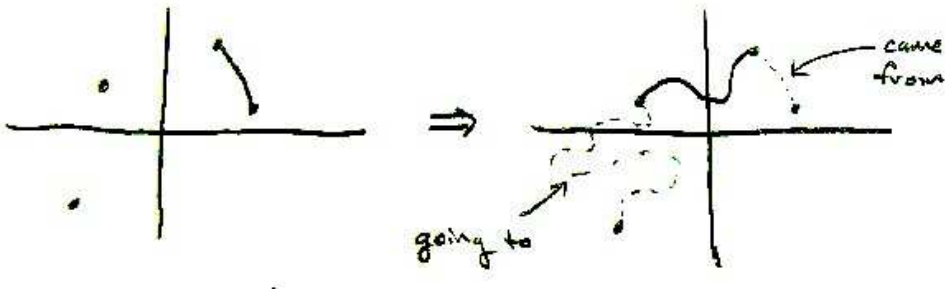

FIG. 9: A line connecting points 1 and 2, will get mapped to a line connecting points 2 and 3 and thus form one continuous line.

are a small distance ϵ from each other, after N applications of the transformation the two points are typically found a distance $\epsilon e^{\lambda N}$ where λ is a positive exponent. Or said verbally the system is very sensitive to initial conditions. In particular searching through the possible solutions to find the global minimum is a seemingly intractable task - further it is a difficult question to determine if there are zero modes like in the continuum approximation or if the solitons are pinned.

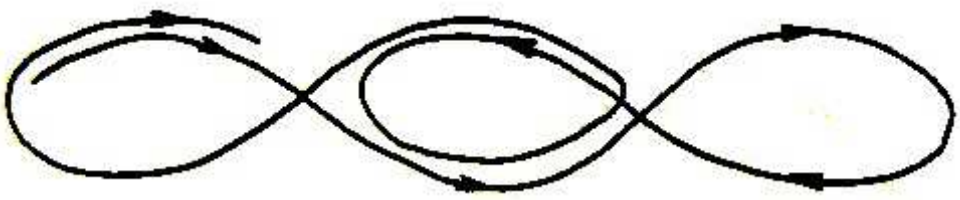

FIG. 10: Schematic of self-intersecting seperatrix. Taken from Pokrovsky[2].

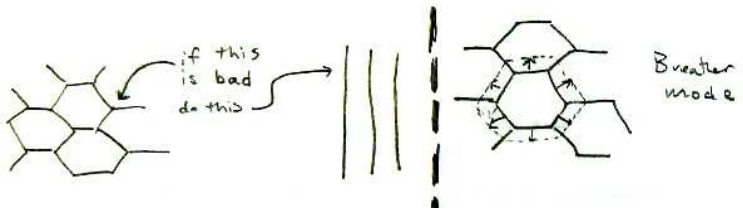

FIG. 11: Left: If soliton intersection energy is too high the linear regiem is favored. Right: An example of a breather mode.

VI. EXTENSIONS

Now that we have a good feel for the 1-D model and the kind of structures that can develop when two different types of order compete lets consider some generalizations. First of all this model has obvious extensions to higher dimensions, non-zero temperatures, quantum systems, and different types of interactions; all of which have been extensively developed. In this section I will mention in passing some points related to these issues that I find particularly interesting.

A. 2D C-I Transition

In 2D when such systems undergo the commensurate-incommensurate transition they likewise can develop soliton structure, that can be either honeycombed or linear depending on wether domain wall intersections are unfavorable. Also of interest the honeycomb structure has a near degenerate breathing mode.(11)

Rather unfortunately such phases are typically unstable to the spontaneous creation of vortices and are consequently simply incommensurate liquids.[4] Theoretical issues aside - there is a voluminous record of experiments that have explored for example the ordering of nobel gasses absorbed on substrates, though we do not have the space to detail it here. For a typical example of this type of scholarship I include a reference to a conference proceedings largely devoted to such issues.[5]

B. Quantum Solitons

The generalizations of classical field equations that support topological structures (such as the one we have been discussing) to a quantum setting implies a rather interesting idea that it is possible to quantize your field, not about a uniform state, but about topological one. There are still the usual boson modes but the field still retains the zero modes of the topological excitations. There are some severe restrictions on these theories (Derrick's theorem[6], however if I may be so bold as to wildly speculate I believe that if dislocations turn out to be explanation for a bulk supersolid effect, it is likely that this type of mathematical structure will be central.

C. The ANNNI Model

Finally it should be noted that these concepts are hardly confined to systems of particles on a periodic substrate. In particular if a ferromagnet has a competing axial anti-ferromagnet next neighbor interaction, in the axial direction the system can break up into ferromagnetic regions with the domain walls playing the same role as the solitons in the FK model, and undergoing the same type of C-I transition.[3]

VII. CONCLUSION

In conclusion we have seen that competition between a harmonic interaction and periodic potential can lead to very interesting topological structures. In particular we showed that it was in the very region where perturbation theory (our usual tool to head us in the right direction) that these interesting structures form. Further we saw that in the general case the structure of the system was so chaotic it was difficult to even understand if the concept of a soliton was even useful.

So what does this model mean for the general problem of transitions between competing orders. On one hand it is very exciting because it leaves you with the distinct impression that beautiful topological structures of walls, dislocations or kinks will proliferate through the system turning otherwise normal dynamics incredibly rich and fascinating. Yet on the other hand it leaves you feeling that it might all be a little pointless because if it can get so complicated so easily in even such a simple system will in real life will such systems ever be

understandable?

A way forward could be to look at the problem in a more geometric framework. If you pay attention to the metric and resulting topologies you are defining on both your space of potentials as well as your configuration space you may be able to show how in general useful topological structures form. Secondly in the other direction I believe that it may be true that these types of problems simply are unsolvable. Computer science has proven that not all true statements can be proven and have even defined numbers that exist but can be computed. It is perhaps time for physicist to put to serious intellectual effort into figuring out what the fundamental limits on our ability to logically construct theories. Are the some physical concepts that it is truly impossible not to calculate but rather to construct a theory about?

I guess these ideas of irreducible complexity and course grained emergent understanding are bound up together, and as a community we may be gathering together the tools that will allow us to say something interesting about the nature of physical understanding. Then again, if our understanding is indeed limited by complexity what makes us thing we can understand complexity.

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