Modeling Qunatum Fields with Discretized Anharmonic Oscillators

Zach Lamberty
Department of Physics, University of Notre Dame, Notre Dame, Indiana, 46556
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In this paper we have attempted to model various interactions in Quantum Field Theory (QFT) as interactions between point particles in a discretized field. In order to make this concept more tangible to undergraduate students, we have developed a mechanical analog consisting of coupled an harmonic oscillators. Our first application of this method was to model a one-dimensional chain string of oscillators experiencing simple harmonic oscillation in a massive potential. By constructing a very explicit model for these interactions, we are able to approach many of the subtle aspects of quantum field theory from a standpoint that ought to be more familiar to a typical undergraduate student. Having thus made the connection between the classical analog and a discrete quantum field, we constructed models of more complicated fields and potentials in a more abstract quantum field theory framework. The models dealt with can be divided into Klein-Gordon-type potentials in discretized one and two dimensional fields, next-order perturbations to these same potentials, and a next-order perturbation to the potential set in an expanding universe. The higher order perturbation models also have applications outside of quantum field theory, particularly in Higgs-based descriptions of the early universe and in hysteresis phenomena in solid state physics. Throughout all of our studies, we utilized the numerical and graphical software program Mathematica (TM) to generate visual representations of the physical realities in these scenarios. We hope that the visualizations aid in the understanding of these and similar quantum field effects.

I. WHY QUANTUM FIELD THEORY?

As the name suggests, quantum field theory is based on the idea that all "quantum" interactions can be described via interactions propagated through some special field. While this may seem like too far of a leap from our old friend quantum mechanics, it is actually perfectly analogous to the approach taken with a theoretical cousin, electromagnetism. I say cousin because both theories describe the propagation and interaction of certain particles (fundamental particles in one, charge-bearing particles and photons in the other) which are often thought of as having both wave- and particle-like natures. Where one falters while the other is unscathed is in the realm of general relativity. Because of Einstein's famous $E = mc^2$ relation, general relativity predicts that given enough energy, mass can be created out of nowhere. The primary equation in quantum mechanics is Shrödinger's equation, and any introductory quantum mechanics student knows that equation is unable to handle creation or annihilation. There is an obvious conflict between these two theories. Fortunately, quantum mechanics's cousin has already been through this conflict, and come out on the other side. It is the description of photons as excitations in an quantized electromagnetic field that provides for creation and annihilation operators, and subsequently a reconciliation with general relativity. Therefore, it is very natural to assume such a quantized field exists for quantum particles; our task is then to describe it as best we can.

This is the end to which this project is aimed, but what is unique about this project is the road it takes to get there. We desired to develop a program whereby undergraduate students could approach some of the more foreign notions of quantum field theory. Because of this, the main focus of this project was to develop an analogy between the abstract notions of quantum field theory and a scenario which is certainly more familiar with the average undergraduate student, that of a system of couple anharmonic oscillators. Hopefully, intuition and familiarity which have already been gained in undergraduate classical mechanics courses will transfer to the initially less tangible quantum field theories. What we cover cover along the way are the two fundamental ideas behind all of our models: the relativistic equation of motion and field quantization. A quick note: we assume throughout the reader is familiar with the notions of Lagrangian dynamics and field discretization. If one should happen not to be, or if he or she is looking for a fuller derivation of any equations cited here, we advise he or she look into the full version of this paper located here[1].

II. A MECHANICAL ANALOG: THE QUANTUM MATTRESS

A. Coupled Oscillators, or: a second (crash) course in classical mechanics

As we mentioned above, it is useful for a student encountering the ideas of quantum field theory for the first time to begin with a more accessible analog. For that reason, one should analyze this first example in great detail. Once the quantum field ideas have been introduced, we will make the jump to the abstract.

To start off, we model this "quantum mattress," in one dimension. Using the mechanical model we lay out here, one finds it to be a good representation of a discretized field in a massive potential. The model consists of a system of $n+1$ particles arranged as in figure (1). Each has a mass M and

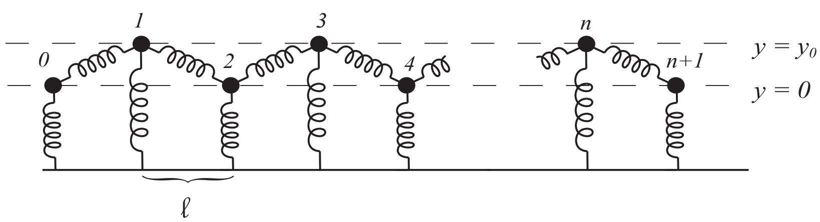

FIG. 1: The classical approximation of a quantum field.

is spaced a horizontal distance ℓ from each other, all with their own spring attached to a common baseline and springs coupling them to their two nearest neighbors. We assume that all motion is in the y direction, *i.e.* the particles are not moving (appreciably) in the x direction. Furthermore, all vertical (coupling) springs have spring constant K_v (K_c) and the same equilibrium length, respectively[2].

The system is known to be in equilibrium when all of the y_j with j even are at a height of $y = 0$ and the odd j at a height of $y = y_0$. We will denote by $\widetilde{y}_j$ the distance of the particle y_j from its respective equilibrium position. We also assume that the particles do not oscillate too far from equilibrium, i.e. $\widetilde{y}_j \ll y_0, \ell$. Under these assumptions, it is an exercise of basic classical dynamics to see that the equation of motion for the individual particles is given by

$$\ddot{\widetilde{y}}_j = -\frac{K_v}{M}\left[\widetilde{y}_j + \frac{1}{4}\left(\cos^2\theta_{eq} - 4\frac{K_c}{K_v}\sin^2\theta_{eq}\right)(\widetilde{y}_{j+1} - 2\widetilde{y}_j + \widetilde{y}_{j-1})\right]. \tag{1}$$

[1] http://www.nd.edu/ rlambert/LEPPStuff/fullpaper.pdf

[2] It is not necessary to *assume* that the equilibrium lengths are the same for the coupled springs; in fact it can quite easily be shown to be mandatory by considering the requirement that the particles move only in the y direction

B. What this Model Can Tells Us

It is interesting to note at this point how the equation of motion compares to the famous Klein-Gordon equation, the equation that one would obtain with the Euler-Lagrange relations for a potential $V(\phi) = \frac{m^2}{2}\phi^2$, $\partial_t{}^2\phi - \partial_x{}^2\phi + m^2\phi = 0$.

Clearly, our equation of motion can be related to this discretized version of the Klein-Gordon equation by the aforementioned discretization of the scalar field along with the relations

$$\frac{c^2}{\bar{\lambda}^2} \rightarrow \frac{K_v}{M} = \omega^2, \qquad \frac{c^2}{\Delta x^2} \rightarrow \frac{K_v}{4M}\left(\cos^2\theta_{eq} - 4\frac{K_c}{K_v}\sin^2\theta_{eq}\right).$$

Notice how this relationship establishes a direct connection between physically meaningful quantities in classical mechanics and apparently similar quantities in quantum mechanics. In many instances, we establish a one-to-one correspondence between familiar concepts and behaviors in classical mechanics and analogous effects in quantum field theory. For example, a disturbance in this ball and spring model would correspond to a disturbance in the quantum field–*i.e.* a particle. What we can glean from this mechanical model should tell us something qualitative about quantum field theory.

Thus we simulate a "particle collision" by superimposing two bumps in our model with opposite speeds. Indeed, the first test of whether or not our model accurately describes a quantum field is whether or not it propagates these wave packets undisturbed towards each other through our field. As can be seen by the visualization found here[3], this is exactly what happens. The two bumps are analogous to two massless particles (*i.e.* photons) colliding in quantum field theory. For a linear potential, the solutions add linearly. Therefore, colliding particles move through each other. To better describe what happens, we need to increase the complexity of the model by introducing non-linear terms to see what happens in a collision.

As seen in section (II B), our model is very successful in propagating two bumps towards each other, passing them through one another, and letting them continue on their way. We would like for our model to take into account how the two particles interact with each other, and to this end we introduce a slight perturbation. This amounts to changing the potential from $V(\phi) = \frac{m^2}{2}\phi^2$ to $V(\phi) = \frac{m^2}{2}\phi^2 - \frac{\xi}{4}\phi^4$. Accordingly, the equation of motion becomes $\partial_t{}^2\phi - \partial_x{}^2 - m^2\phi + \xi\phi^3$.

We could go back into the derivation for our mechanical model and accept terms of higher order in $\widetilde{y}$, or we may simply add the $\xi\phi^3$ term to the equation of motion and manipulate the value of ξ. We chose to do the later.

We would expect that this non-linear interaction would change the way colliding particles interact, but we also don't want it to affect them when they are not yet "colliding." For this reason we tweak our model to only include these non-linear interactions when the particles are literally colliding, *i.e.* when they are on top of each other. Furthermore, to ensure that energy and momentum are conserved (we are treating this perturbation as an interaction between parts of the model, rather than as the result of some extraneous force), the values of the amplitudes after the collision are scaled by appropriate factors to conserve those two quantities. The result is a scenario in which two particles come towards each other and pass through each other as before, but in the process create extra disturbances which follow in their wake. This can be seen as a manifestation of the energy generated by the collision, and represents the probabilities of particle creation in such a collision. A full video of a non-linear collision can be found here[4].

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[3] http://www.nd.edu/∼rlambert/LEPPStuff/Mathematica/1D/2WavesNatSpeed.GIF

[4] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/1Dnonlinear/2WavesNatSpeedNL.GIF

C. What it Can't: Practical Limitations

In spite of our best intentions, it turns out this model begins to break down in two dimensions. The reason for this is simply that the intuitive picture of a particle —*i.e* a propagating wave packet—is not a solution to the two dimensional wave equation. Rather than propagate in one direction, it instead spreads out radially. This isn't representative of any sort of flaw in the theory, but rather a flaw in our intuition. What we have shown is not that these particles don't exist, but merely that an illuminating visualization such as the one found in the one-dimensional case is not going to be made in the two dimensional case.

Having essentially maximized the usefulness of our mechanical analog, one might be tempted to think the project is over, and in a sense it is. Here one must abandon the familiarity of classical dynamics in favor of the more abstract yet more useful framework of quantum field theory. In that sense, this is only the halfway point in a development of an introductory glance at quantum field modeling. What we turn to next has aspects of much of our previous study, most notably a similar potential to the non-linear case study. We hope that any reader having fully followed the classical mechanic analog will feel comfortable knowing that the ideas and equations of the abstract quantum field theory are essentially the same as those previously encountered. The sections to follow ought to now be more accessible than they were at the start of the project.

III. A MORE ABSTRACT MODEL: SOLITONS

It is clear by now that there are many situations of interest in quantum field theory which will simply be inaccessible via this mechanical system analogy. The analogies we have presented thus far will pop up from time to time, but they can't really paint the complete picture, so to speak. Therefore, to proceed anywhere further we should make the jump from the familiar classical-mechanics example into the now-barely-familiar quantum field theory approach.

A. Solitons in Minkowski Space

One very interesting potential which has application in string theory and solid state physics is the "double well" potential

$$V(\phi) = -\frac{m}{2}\phi^2 + \frac{\lambda}{4}\phi^4 + \frac{m^4}{4\lambda},$$

(where the additional constant is an offset potential to ensure a minimum potential of 0). String theorists will note that this is simply the real-valued version of the "Mexican hat" or "wine bottle" potentials. In Minkowski space-time this yields an equation of motion of $\partial_t\phi^2 - \partial_x{}^2 - m^2\phi + \lambda\phi^3 = 0$. This potential is plotted out in figure (2). As we would expect, there are three extrema. What is crucially different about this potential when compared to the massive or electromagnetic potential is that the extrema at $\phi = 0$ is *unstable*. Therefore a particle will not find equilibrium there, but instead will oscillate towards the two symmetric potential wells at values $\pm m/\sqrt{\lambda}$ until it finds equilibrium. What makes this potential special is that the two minima are equally likely, so it is more or less random which of the two a particle will end up at.

The fact that these two potentials are equally attractive leads to a very interesting result. This potential will only sustain fields for which the aforementioned equation of motion is satisfied. Obviously, the ground state for such a setup is one in which all the particles are either in the left or the right potential well, but those can be accurately modeled by harmonic oscillators; the ϕ^4 dependence in the potential becomes slightly trivial in that instance. Another possible (and

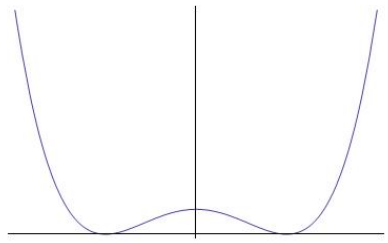

FIG. 2: $V(\phi) = -\frac{m^2}{2}\phi^2 + \frac{\lambda}{4}\phi^4 + \frac{m^4}{4\lambda}$

significantly more interesting) situation is one in which about half of the particles are in one well, about half in the other, and a very small number essentially jumping from the low value to the high value. Mathematically this can be represented by the function

$$\phi(x;t) = \frac{m}{\sqrt{\lambda}} \tanh \frac{m\gamma(x+vt)}{\sqrt{2}}, \quad \text{where } \gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

(we will not derive this equation, but the reader ought to check to ensure it satisfies the equation of motion). The solution will evolve in time by simply moving either left or right at speed v as can be seen here[5].

To fall back on our mechanical analogy temporarily, this is akin to assuming a system of coupled springs with two equilibrium positions. The springs on the left are in the first equilibrium, and those on the right in the second. To remain coupled, there must be some finite region of transition, and that is what the jump in the soliton. This is what is called a **domain wall**, a region which separates two regions of nearly constant, differing field values. For those who are familiar with ferromagnets, think about the domain walls separating regions of opposite magnetic field. More importantly for our present discussion, in some string-base grand unified theories it is believed solitons were formed in the early universe as part of the cooling and expanding process.

In those GUTs which predict them, solitons are formed as a consequence of the expansion of the universe. In times close to the big bang, the universe is divided into many separate causally connected regions, due to the fact that the effects traveling at the speed of light haven't had enough time to impact neighboring regions. Those regions which are causally connected tend to settle into one of the two potential wells, but not both. Thus we have neighboring regions that can be at opposite field values which, as the universe expands, will soon be coming into contact with each other. Such a situation would be described mathematically by two soliton solutions colliding, annihilating each other, and leaving behind a sinusoidal distribution. Indeed, this is exactly what we see in our models. Before we can show this, however, a word on how these models were created.

B. Solitons in an Accelerating Universe

It is essential for any early-universe approximation to take into account expansion, and this is usually done by considering the **Hubble parameter**, given by

$$H(t) = \frac{\dot{a}(t)}{a(t)}.$$

[5] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Propagating/1Soliton.GIF

This Hubble parameter is incorporated as part of the metric in general relativity (for a full derivation see [1]), and subsequently the equation of motion becomes $\ddot{\phi} - \overrightarrow{\nabla}^2\phi + 3H(t)\dot{\phi} + V'(\phi) = 0$.

One reasonable assumption is that the acceleration scales as t^p. Supposing we choose some time t_0 after the big bang to be the starting point for our model, we obtain a value of the Hubble parameter of $H(t) = p/(t + t_0)$. In this equation p can take on any value, but most cosmological models use either $\frac{1}{2}$ or $\frac{2}{3}$. For the purposes of our visualizations we used $p = \frac{2}{3}$, but the fact of the matter is that the models will be qualitatively equivalent for any positive value of p.

Now, consider the case of acceleration in one dimension with the potential listed above,

$$V(\phi) = -\frac{m^2}{2}\phi^2 + \frac{\lambda}{4}\phi^4 + \frac{m^4}{4\lambda}.$$

In this case the equation of motion takes the form $\partial_t{}^2\phi - \partial_x{}^2\phi + 3H(t)\partial_t\phi - m^2\phi + \lambda\phi^3 = 0$.

Clearly, as time goes by the effect of the Hubble parameter on the equation of motion will greatly decrease. For the purposes of our model we chose the value of our constants so that at the start of our simulation $H \gg m$, at some point the two values became roughly equivalent, and towards the end $H < m$. Because of this, our models all experience a stabilizing frictional force to begin with, a middle period during which they move rapidly towards one of the two equilibrium values, and a final phase in which they oscillate around their equilibrium value as they did in the non-accelerating scenario.

There are a couple of ways one could go with this equation of motion, depending on what sort of initial field disturbances one would like to consider. We started our inquiry by examining what would happen if the field were initially completely random and had no x dependence. In this case, the spatial derivatives drop out of the equation of motion, and we have $\partial_t{}^2\phi - 3H(t)\partial_t\phi - m^2\phi + \lambda\phi^3 = 0$. More than anything, this model would test the time-evolution predictions pertaining to the new Hubble parameter. To this end we generated a number of visualizations. The first[6] movie is a representation of 200 particles given random initial potentials and allowed to move independently of each other. A second[7] movie was generated from 20 particles, and a visual representation of those particles as they move along the potential well can be seen here[8]. This last movie is particularly illuminating as far as the changing effects of the Hubble parameter are concerned. Unfortunately, this is about the most information that can be extracted from these models, so we should move to more complicated versions.

In order to better approximate the real situation, we re-introduce x dependence to our field and regain the original equation of motion. Furthermore, if we provide adequate inter-particle spacing (*i.e.* the space between neighboring particles is on the order of ct_0, the distance between causally connected regions), we can assume each particle represents an individual causally connected region. Thus, the evolution of this system in time can be though of as a fitting model for the collision of many domain walls in the early universe. What we would expect to see initially in this instance is similar to what happened in the no-x-dependence scenario, with random values initially being pulled towards their closest equilibrium point. However, as was the case before, this equation ought to approximate the non-accelerating universe at large t. Therefore we would expect to see the formation of soliton solutions in those regions where phase transitions are necessary, and that these solitons ought to either be propagating towards each other or already colliding. This is, in fact, exactly what we see. Note particularly this[9] movie which shows a video of a 90-particle

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[6] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Hubble/1D/delphi0/NoSpace200.GIF
[7] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Hubble/1D/delphi0/NoSpaceFull20.GIF
[8] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Hubble/1D/delphi0/NoSpaceFull20movie.GIF
[9] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Hubble/1D/delphiNOT0/PeriodicFull90.GIF

distribution. Note in particular how two solitons collide and essentially neutralize each other in the center of the distribution just as we had hoped.

Having developed an interesting picture of the one dimensional situation, we would like to see how the scenario shapes up in two dimensions. We make most of the same assumptions as before—an initially random distribution for a field which has both an x and y dependence, and initial values of our constants which allow us to think of each individual point as initially being a separate causally connected region of the early universe. We allow the Hubble parameter to move through the same values as before. In this case we expect two-dimensional solitons (which are essentially two-dimensional walls) to be generated, move towards each other, and interact.

We created three video representing these effects, a three-dimensional plot[10], a contour plot[11], and a density plot[12].

IV. CONCLUDING REMARKS

As mentioned before, the fullest version of this paper, all the videos linked here and a number more, and the Mathematica notebooks which were used to generate them can all be found online[13]. It is our hope that this project can be utilized as an educational tool for undergraduate students who would be experiencing quantum field theory for the first time. We believe it would be a very useful and appropriate exercise particulary for a computationally-based course or a modern laboratory for undergraduate students.

V. ACKNOWLEDGEMENTS

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[1] Carroll, Steve. *Spacetime and Geometry: An Introduction to General Relativity*, Benjamin Cummings, 2003

[2] Zee, A. *Quantum Field Theory in a Nutshell*

[3] Thornton, Stephen and Jerry Marion. *Classical Dynamics of Particles and Systems*, Brooks Cole, 2003

[10] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Hubble/2D/603Dplot.GIF

[11] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Hubble/2D/60ContourPlot.GIF

[12] http://www.nd.edu/ rlambert/LEPPStuff/Mathematica/Solitons/Hubble/2D/60DensityPlot.GIF

[13] http://www.nd.edu/ rlambert/LEPPStuff/