The Klein-Gordon field and its variational principle.

Klein-Gordon field

The simplest relativistic classical field is the Klein-Gordon field. To begin with we can think of the Klein-Gordon field as simply a function on spacetime, also known as a *scalar field*, $\varphi\colon \mathbf{R}^4 \to \mathbf{R}$. Introduce coordinates $x^\alpha = (t, x, y, z)$ on $\mathbf{R}^4$. The field equation – known as the *Klein-Gordon equation* – is given by

$$\Box\varphi - m^2\varphi = 0, \tag{2.1}$$

where $\Box$ is the wave operator (or "d'Alembertian"),

$$\Box\varphi = -\frac{\partial^2\varphi}{\partial t^2} + \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2} = -\frac{\partial^2\varphi}{\partial t^2} + \nabla^2\varphi = -\varphi_{,tt} + \varphi_{,xx} + \varphi_{,yy} + \varphi_{,zz}, \tag{2.2}$$

and m is a parameter known as the *mass* of the Klein-Gordon field. (Here we are using units in which $\hbar = c = 1$. It is a nice exercise to use put things in terms of SI units.) You can see that the Klein-Gordon (KG) equation is just a simple generalization of the wave equation, which it reduces to when $m = 0$. In quantum field theory the corresponding Klein-Gordon field is characterized by "particles" with rest mass m and no other structure (*e.g.,* no spin, no electric charge, *etc.* .) So the Klein-Gordon field is physically (and mathematically, too) the simplest of the relativistic fields that one can study.

If you like you can view the Klein-Gordon equation as a "toy model" for the Maxwell equations. The quantum electromagnetic field is characterized by "photons" which have vanishing rest mass, no electric charge, but they do carry intrinsic "spin". Coherent states of the quantum electromagnetic fields containing many, many photons are well approximated by "classical" electromagnetic fields satisfying the Maxwell equations. Likewise, you can imagine that coherent states involving many "Klein-Gordon particles" (sometimes called scalar mesons) are well described by a classical scalar field satisfying the Klein-Gordon equation.

The KG equation originally arose in an attempt to give a relativistic generalization of the Schrödinger equation. The idea was to let φ be the complex-valued wave function describing a spinless particle of mass m. But this idea didn't quite work out as expected (see below for a hint as to what goes wrong). Later, when it was realized that a more viable way to do quantum theory in a relativistic setting was via quantum field theory, the KG equation came back as a field equation for a quantum field whose classical limit is the KG equation above. The role of the KG equation as a sort of relativistic Schrödinger

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equation is not completely destroyed in the quantum field theoretic picture, however. The story is too long to go into in this course, but we will give a hint as to what this last sentence means in a moment.

Solving the KG equation

Let us have a closer look at the KG equation and its solutions. The KG equation is a linear PDE with constant coefficients. One standard strategy for solving such equations is via Fourier analysis. To this end, let us suppose that φ is sufficiently well behaved* so that we have the following Fourier expansion of φ at any given value of t:

$$\varphi(x) = \left(\frac{1}{2\pi}\right)^{3/2} \int_{\mathbf{R}^3} d^3k\, \hat{\varphi}_{\mathbf{k}}(t)\, e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{2.3}$$

where $\mathbf{k} = (k_x, k_y, k_z) \in \mathbf{R}^3$, and

$$\hat{\varphi}_{-\mathbf{k}} = \hat{\varphi}^*_{\mathbf{k}}, \tag{2.4}$$

since φ is a real valued function. The KG equation implies the following equation for the Fourier transform $\hat{\varphi}_{\mathbf{k}}(t)$ of φ:

$$\ddot{\hat{\varphi}}_{\mathbf{k}} + (k^2 + m^2)\hat{\varphi}_{\mathbf{k}} = 0. \tag{2.5}$$

This equation is, of course, quite easy to solve. We have

$$\hat{\varphi}_{\mathbf{k}}(t) = a_{\mathbf{k}} e^{-i\omega_k t} + b_{\mathbf{k}} e^{i\omega_k t}, \tag{2.6}$$

where

$$\omega_k = \sqrt{k^2 + m^2}, \tag{2.7}$$

and $a_{\mathbf{k}}$, $b_{\mathbf{k}}$ are complex constants for each $\mathbf{k}$. The reality condition (2.4) on φ implies that

$$b_{\mathbf{k}} = a^*_{-\mathbf{k}}, \tag{2.8}$$

so that φ solves the KG equation if and only if it takes the form

$$\varphi(x) = \left(\frac{1}{2\pi}\right)^{3/2} \int_{\mathbf{R}^3} d^3k\, \left(a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_k t} + a^*_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega_k t}\right). \tag{2.9}$$

PROBLEM: *Verify (2.4)–(2.9).*

* "Sufficiently well behaved" could mean for example that, for each t, $\varphi \in L^1(\mathbf{R}^3)$ or $\varphi \in L^2(\mathbf{R}^3)$.

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Let us pause and note something familiar here. Granted a little Fourier analysis, the KG equation is really just an infinite collection of uncoupled "harmonic oscillator equations" for the real and imaginary parts of $\hat{\varphi}_k(t)$ with "natural frequency" ω_k. Thus we can see quite explicitly how the KG field is akin to a dynamical system with an infinite number of degrees of freedom. Indeed, if label the degrees of freedom with the Fourier wave vector $\mathbf{k}$; each degree of freedom is a harmonic oscillator. It is this interpretation which is used to make the (non-interacting) quantum Klein-Gordon field: each harmonic oscillator is given the usual quantum mechanical treatment.

A small digression: one particle wave functions

From our form (2.9) for the general solution of the KG equation we can take a superficial glimpse at how this equation is used as a sort of Schrödinger equation in the quantum field theory description. To begin, we note that $\varphi = \varphi^+ + \varphi^-$, where

$$\varphi^+ := \left(\frac{1}{2\pi}\right)^{3/2} \int_{\mathbf{R}^3} d^3k \, a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_k t}, \tag{2.10}$$

and

$$\varphi^- := \left(\frac{1}{2\pi}\right)^{3/2} \int_{\mathbf{R}^3} d^3k \, a^*_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega_k t} \tag{2.11}$$

are each complex-valued solutions to the KG equation. These are called the *positive frequency* and *negative frequency* solutions of the KG equation, respectively. Let us focus on the positive frequency solutions. They satisfy the KG equation, but they also satisfy the stronger equation

$$i\frac{\partial \varphi^+}{\partial t} = \sqrt{-\nabla^2 + m^2}\varphi^+, \tag{2.12}$$

where the square root operator is defined via Fourier analysis to be*

$$\sqrt{-\nabla^2 + m^2}\varphi^+ := \left(\frac{1}{2\pi}\right)^{3/2} \int_{\mathbf{R}^3} d^3k \, \omega_k a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_k t} .tag$$

Thus the positive frequency solutions of the KG equation satisfy a Schrödinger equation with Hamiltonian

$$H = \sqrt{-\nabla^2 + m^2}. \tag{2.13}$$

This Hamiltonian can be interpreted as the kinetic energy of a relativistic particle (in the reference frame labeled by spacetime coordinates (t, x, y, z)). It is possible to give a relativistically invariant normalization condition on the positive frequency wave functions so that one can use them to compute probabilities for the outcome of measurements made

* The domain of this operator will necessarily be limited to a subspace of functions.

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on the particle. Thus the positive frequency solutions are sometimes called the "one-particle wave functions".

In a quantum field theoretic treatment, the (normalizable) positive frequency solutions represent the wave functions of KG particles. What about the negative frequency solutions? There are difficulties in using the negative frequency solutions to describe KG particles. For example, you can easily check that they satisfy a Schrödinger equation with a *negative* kinetic energy, which is unphysical. Moreover, the relativistic inner product with respect to which one can normalize the positive frequency solutions leads to a *negative* norm for the negative frequency solutions. This means that the negative frequency part of the solution to the KG equation cannot be used to describe the quantum mechanics of a single particle. In quantum field theory (as opposed to quantum mechanics), the negative frequency solutions are interpreted in terms of the possibility for destruction of particles. Quantum field theory, you see, allows for creation and destruction of particles. But now we are going too far afield...

Variational Principle

In physics, fundamental theories always arise from a variational principle. Ultimately this stems from their roots as quantum mechanical systems. For us, the presence of a variational principle is a very powerful tool for organizing the information in a field theory. Presumably you have seen a variational principle or two in your life. I will not assume you are particularly proficient with the calculus of variations – one of the goals of this course is to make you better at it – but I will assume that you are familiar with the basic strategy of a variational principle.

So, consider *any* map $\varphi\colon \mathbf{R}^4 \to \mathbf{R}$ (not necessarily satisfying any field equations) and consider the following integral

$$S[\varphi] = \int_{\mathcal{R}\subset\mathbf{R}^4} d^4x\, \frac{1}{2}\left(\varphi_{,t}^2 - (\nabla\varphi)^2 - m^2\varphi^2\right). \tag{2.14}$$

The region $\mathcal{R}$ can be anything you like at this point, but typically we assume

$$\mathcal{R} = \{(t,x,y,z)|\, t_1 \le t \le t_2,\ -\infty < x,y,z < \infty\}. \tag{2.15}$$

We restrict attention to fields such that $S[\varphi]$ exists. For example, we can assume that φ is always a smooth function of compact spatial support. The value of the integral, of course, depends upon which function φ we choose. We say that $S = S[\varphi]$ is a *functional* of φ. We will use this functional to obtain the KG equation by a variational principle. When a functional can be used in this manner it is called the *action functional* for the field theory.

The variational principle goes as follows. Consider an arbitrary one-parameter family of fields, $\varphi = \varphi_\lambda$. As a random example, we might have

$$\varphi_\lambda = \cos(\lambda(t+x))\, e^{-(x^2+y^2+z^2)}. \tag{2.16}$$

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You should think of φ_λ as defining a curve in the "space of fields".* We can evaluate the functional S along this curve; the value of the functional defines an ordinary function of λ, again denoted S:

$$S(\lambda) := S[\varphi_\lambda]. \tag{2.17}$$

We now define a *critical point* of the action functional $S[\varphi]$ to be a "point in the space of fields", that is, a field, say $\varphi_0 = \varphi_0(x)$, which defines a critical point of $S(\lambda)$ for any curve passing through φ_0.

This way of defining a critical point is a natural generalization to the space of fields of the usual notion of critical point from multi-variable calculus. Recall that in ordinary calculus a critical point (x_0, y_0, z_0) of a function f is a point where all the first derivatives of f vanish,

$$\partial_x f(x_0, y_0, z_0) = \partial_y f(x_0, y_0, z_0) = \partial_z f(x_0, y_0, z_0) = 0. \tag{2.18}$$

This is equivalent to the vanishing of the rate of change of f along any curve through (x_0, y_0, z_0). To see this, define the parametric form of a curve $\vec{x}(\lambda)$ passing through $\vec{x}(0) = (x_0, y_0, z_0)$ via

$$\vec{x}(\lambda) = (x(\lambda), y(\lambda), z(\lambda)) \tag{2.19}$$

with $\lambda = 0$ corresponding to the point p on the curve,

$$(x(0), y(0), z(0)) = (x_0, y_0, z_0). \tag{2.20}$$

The tangent vector $T(\lambda)$ to the curve at the point $\vec{x}(\lambda)$ has Cartesian components

$$\vec{T}(\lambda) = (x'(\lambda), y'(\lambda), z'(\lambda)), \tag{2.21}$$

and the rate of change of a function $f = f(x, y, z)$ along the curve at the point $\vec{x}(\lambda)$ is given by

$$\vec{T}(\lambda) \cdot \nabla f\Big|_{\vec{x}=\vec{x}(\lambda)} = x'(\lambda)\partial_x f(\vec{x}(\lambda)) + y'(\lambda)\partial_y f(\vec{x}(\lambda)) + z'(\lambda)\partial_z f(\vec{x}(\lambda)). \tag{2.22}$$

Now it should be apparent that the vanishing of the rate of change of f along *any* curve passing through a point p is equivalent to the vanishing of the gradient of f at p, which is the same as the vanishing of all the first derivatives of f at p.

It is this interpretation of "critical point" in terms of vanishing rate of change along any curve that we generalize to the infinite-dimensional space of fields.

We shall show that the critical points of the functional $S[\varphi]$ correspond to functions on spacetime which solve the KG equation. To this end, let us consider a curve that passes

* The space of fields is the set of all allowed functions on spacetime. It can be endowed with enough structure to view it as a smooth manifold whose points are the allowed functions. The curve in the example (2.16) passes through the point $\varphi = e^{-(x^2+y^2+z^2)}$ at $\lambda = 0$.

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through a putative critical point at, say, $\lambda = 0$. This is easy to arrange. For example, let $\hat{\varphi}(\lambda)$ be any curve. Define φ_λ via

$$\varphi_\lambda = \hat{\varphi}_\lambda - \hat{\varphi}_0 + \varphi. \tag{2.23}$$

If $\varphi_{\lambda=0} \equiv \varphi$ is a critical point, then

$$\delta S := \left(\frac{dS(\lambda)}{d\lambda}\right)_{\lambda=0} = 0. \tag{2.24}$$

We call δS the *first variation of the action*; its vanishing is the condition for a critical point. Computing δS explicitly, we find

$$\delta S = \int_{\mathcal{R}} d^4x \, \left(\varphi_{,t}\delta\varphi_{,t} - \nabla\varphi\cdot\nabla\delta\varphi - m^2\varphi\delta\varphi\right), \tag{2.25}$$

where the function $\delta\varphi$ – the *variation of* φ – is defined by

$$\delta\varphi := \left(\frac{d\varphi(\lambda)}{d\lambda}\right)_{\lambda=0}. \tag{2.26}$$

The critical point condition means that $\delta S = 0$ for all variations of φ, and we want to see what that implies about the critical point φ.

To this end we observe that $\delta\varphi$ is a completely arbitrary function (aside from regularity and boundary conditions to be discussed below). To see this, for any function ψ consider the curve

$$\varphi_\lambda = \varphi + \lambda\psi, \tag{2.27}$$

so that

$$\delta\varphi = \psi. \tag{2.28}$$

To make use of the fact that $\delta S = 0$ must hold for arbitrary $\delta\varphi$ we integrate by parts in δS:

$$\begin{aligned} 0 = \dot{S} = \int_{\mathcal{R}} d^4x \, \left(-\varphi_{,tt} + \nabla^2\varphi - m^2\varphi\right)\delta\varphi \\ + \left[\int_{\mathbf{R}^3} d^3x \, \varphi_{,t}\delta\varphi\right]_{t_1}^{t_2} - \int_{t_1}^{t_2} dt \int_{r\to\infty} d^2S \, \mathbf{n}\cdot\nabla\varphi\delta\varphi \end{aligned} \tag{2.29}$$

Here the last two terms are the boundary contributions from $\partial\mathcal{R}$. For concreteness, I have assumed that

$$\mathcal{R} = [t_1, t_2]\times\mathbf{R}^3. \tag{2.30}$$

The last integral is over the "sphere at infinity" in $\mathbf{R}^3$, with $\mathbf{n}$ being the outward unit normal to that sphere.

If you need a little help seeing where (2.29) came from, the key is to write

$$\varphi_{,t}\delta\varphi_{,t} - \nabla\varphi\cdot\nabla\delta\varphi = \partial_t(\varphi_{,t}\delta\varphi) - \nabla\cdot(\nabla\varphi\delta\varphi) - \varphi_{,tt} + \nabla^2\varphi. \tag{2.31}$$

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The first term's time integral is easy to perform, and the second term's spatial integral can be evaluated using the divergence theorem.

To continue with our analysis of (2.29), we make the following two assumptions regarding the boundary conditions to be placed on our various fields. First, we note that φ, and φ_λ, and hence $\delta\varphi$, must vanish at spatial infinity ($r \to \infty$ at fixed t) in order for the action integral to converge. Further, we assume that φ and $\delta\varphi$ vanish as $r \to \infty$ fast enough so that in δS the boundary integral over the sphere at infinity vanishes. Second, we fix two functions

$$\phi_1, \phi_2 : \mathbf{R}^3 \to \mathbf{R}$$

and we assume that at t_1 and t_2, for any allowed φ – not just the critical point,

$$\varphi|_{t_1} = \phi_1, \quad \varphi|_{t_2} = \phi_2. \tag{2.32}$$

The functions ϕ_1 and ϕ_2 are fixed but arbitrary, subject to the asymptotic conditions as $r \to \infty$. Now, for our one parameter family of fields we also demand

$$\varphi_\lambda|_{t_1} = \phi_1, \quad \varphi_\lambda|_{t_2} = \phi_2, \tag{2.33}$$

which forces

$$\delta\varphi|_{t_1} = 0 = \delta\varphi|_{t_2}. \tag{2.34}$$

With these boundary conditions, we see that the assumption that φ is a (smooth) critical point implies that

$$0 = \int_{\mathcal{R}} d^4x \left(-\varphi_{,tt} + \nabla^2\varphi - m^2\varphi\right) \delta\varphi \tag{2.35}$$

for any function $\delta\varphi$ subject to (2.34) and the asymptotic conditions just described. Now, it is a standard theorem in calculus that this implies

$$-\varphi_{,tt} + \nabla^2\varphi - m^2\varphi = 0 \tag{2.36}$$

everywhere in the region $\mathcal{R}$.

This, then, is the variational principle for the KG equation. The critical points of the KG action, subject to the two types of boundary conditions we described (asymptotic conditions as spatial infinity and initial/final boundary conditions), are the solutions of the KG equation.

Getting used to δ. Functional derivatives.

We have already introduced the notation for δ, known colloquially as a "variation". For any quantity F built from the field φ, and for any one parameter family of fields φ_λ, we define

$$\delta F := \left(\frac{dF}{d\lambda}\right)_{\lambda=0}. \tag{2.37}$$

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A couple of important properties of δ are: (i) that it is a linear operation obeying Leibniz rule (it is a derivation); (ii) variations commute with differentiation, *e.g.,*

$$\delta(\varphi_{,\alpha}) = \frac{\partial}{\partial x^\alpha}\delta\varphi \equiv \delta\varphi_{,\alpha}. \tag{2.38}$$

We have just computed the *first variation* of the KG action:

$$\delta S[\varphi] = \int_{\mathcal{R}} d^4x \, \left(\varphi_{,t}\delta\varphi_{,t} - \nabla\varphi\cdot\nabla\delta\varphi - m^2\varphi\delta\varphi\right). \tag{2.39}$$

By definition, if the first variation of a functional $S[\varphi]$ can be expressed as

$$\delta S[\varphi] = \int_{\mathcal{R}} d^4x \, F\,\delta\varphi, \tag{2.40}$$

then we say that S is *differentiable* and that

$$F \equiv \frac{\delta S}{\delta\varphi} \tag{2.41}$$

is the *functional derivative* of the action. For a differentiable functional $S[\varphi]$, then, we write

$$\delta S[\varphi] = \int_{\mathcal{R}} \frac{\delta S}{\delta\varphi}\delta\varphi. \tag{2.42}$$

We have seen that, with our choice of boundary conditions, the KG action is differentiable and that

$$\frac{\delta S}{\delta\varphi} = -\varphi_{,tt} + \nabla^2\varphi - m^2\varphi$$

In general, the idea of variational principles is to encode the field equations into an action so that they arise as the equations

$$\frac{\delta S}{\delta\varphi} = 0.$$

The Lagrangian

Following the pattern of classical mechanics we introduce the notion of a *Lagrangian* L, which is defined as

$$L = \int_{\mathbf{R}^3} d^3x \, \frac{1}{2}\left(\varphi_{,t}^2 - (\nabla\varphi)^2 - m^2\varphi^2\right), \tag{2.43}$$

so that

$$S[\varphi] = \int_{t_1}^{t_2} dt\, L. \tag{2.44}$$

In classical mechanics, the Lagrangian is a function of the independent variables, the dependent variables (the "degrees of freedom"), and the derivatives of the dependent variables.

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In field theory we have, in effect, degrees of freedom labeled by spatial points. We then have the possibility of expressing the Lagrangian as an integral over space (a sum over the degrees of freedom). In the KG theory we have that

$$L = \int_{\mathbf{R}^3} d^3x\, \mathcal{L}, \tag{2.45}$$

where

$$\mathcal{L} = \frac{1}{2}\left(\varphi_{,t}^2 - (\nabla\varphi)^2 - m^2\varphi^2\right) \tag{2.46}$$

is the *Lagrangian density*. The Lagrangian density depends at a point (t, x, y, z) on the values of the field φ and its derivatives at (t, x, y, z) via a particular formula, which we write as

$$\mathcal{L} = \mathcal{L}(\varphi, \partial\varphi). \tag{2.47}$$

We say that $\mathcal{L}$ is a *local function of the field*. Theories like the KG theory which admit an action which is a spacetime integral of a local Lagrangian density are called *local field theories*.

Let us note that the Lagrangian for the KG theory can be viewed as having the same structure as that for a finite dimensional dynamical system in non-relativistic Newtonian mechanics, namely, $L = T - U$, where T can be viewed as a kinetic energy for the field,

$$T = \int_{\mathbf{R}^3} d^3x\, \frac{1}{2}\varphi_{,t}^2 \tag{2.48}$$

and U plays the role of potential energy:

$$U := \int_{\mathbf{R}^3} d^3x\, \frac{1}{2}\left((\nabla\varphi)^2 + m^2\varphi^2\right). \tag{2.49}$$

Evidently, we can view $\frac{1}{2}\varphi_{,t}^2$ as the kinetic energy density, and view $(\nabla\varphi)^2 + m^2\varphi^2$ as the potential energy density.

The Euler-Lagrange equations

We have seen that the Lagrangian density $\mathcal{L}$ of the KG theory is a local function of the KG field. We can express the functional derivative of the KG action purely in terms of the Lagrangian density. To see how this is done, we note that

$$\begin{aligned} \delta\mathcal{L} &= \varphi_{,t}\delta\varphi_{,t} - \nabla\varphi\cdot\nabla\delta\varphi - m^2\varphi\delta\varphi \\ &= \left(-\varphi_{,tt} + \nabla^2\varphi - m^2\varphi\right)\delta\varphi + \frac{\partial}{\partial x^\alpha}V^\alpha, \end{aligned} \tag{2.50}$$

where $x^\alpha = (t, x, y, z)$, $\alpha = 0, 1, 2, 3$, and we are using the Einstein summation convention,

$$\frac{\partial}{\partial x^\alpha}V^\alpha \equiv \sum_\alpha \frac{\partial}{\partial x^\alpha}V^\alpha. \tag{2.51}$$

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Here

$$V^0 = \varphi_{,t}\delta\varphi, \quad V^i = -(\nabla\varphi)^i\delta\varphi. \tag{2.52}$$

The term involving V^α is a four-dimensional *divergence* and leads to the boundary contributions to the variation of the action via the divergence theorem. Assuming the boundary conditions are such that these terms vanish, we see that the functional derivative of the action is computed by (1) varying the Lagrangian density, and (2) integrating by parts to move all derivatives of the field variations into divergences and (3) throwing away the divergences.

We now give a slightly more general way to think about this last computation. First, we view the formula giving the definition of the Lagrangian as a function

$$\mathcal{L} = \mathcal{L}(\varphi, \varphi_{,\alpha}), \tag{2.53}$$

where now, formally, φ and $\varphi_{,\alpha}$ are just a set of 5 variables upon which the Lagrangian density depends. From this point of view the field φ does not depend upon x^α and neither does $\varphi_{,\alpha}$. Recalling that the field variation is really a differentiation process, we can define the variation of the Lagrangian via

$$\begin{aligned}\delta\mathcal{L} :&= \frac{\partial\mathcal{L}}{\partial\varphi}\delta\varphi + \frac{\partial\mathcal{L}}{\partial\varphi_{,\alpha}}\delta\varphi_{,\alpha} \\ &= \left(\frac{\partial\mathcal{L}}{\partial\varphi} - D_\alpha\frac{\partial\mathcal{L}}{\partial\varphi_{,\alpha}}\right)\delta\varphi + D_\alpha V^\alpha,\end{aligned} \tag{2.54}$$

where

$$V^\alpha = \frac{\partial\mathcal{L}}{\partial\varphi_{,\alpha}}\delta\varphi, \tag{2.55}$$

and we have introduced the *total derivative*

$$D_\alpha F(\varphi, \varphi_{,\alpha}) = \frac{\partial F}{\partial\varphi}\varphi_{,\alpha} + \frac{\partial F}{\partial\varphi_{,\beta}}\varphi_{,\alpha\beta}. \tag{2.56}$$

The total derivative just implements the ordinary derivative when we are viewing the local functions of the fields as ordinary functions in multi-variable calculus. In other words, if we imagine substituting a specific field, that is, a specific function $\varphi(t, x, y, z)$ into one of our formulas, rendering the formula as a specific function of (t, x, y, z), then the formula involving the total derivative just reduces under the same procedure to the derivative of the resulting function of (t, x, y, z) with respect to the spacetime coordinates. Put yet differently, the total derivative simply implements the spacetime coordinate derivative via the chain rule on functions of functions, *e.g.,* $\mathcal{L}(\varphi(x)), \frac{\partial\varphi(x)}{\partial x^\alpha})$. The reason I have to say all these things is that sometimes we want to manipulate a formula $\mathcal{L}(\varphi, \partial\varphi)$ for the Lagrangian using the ordinary rules of multivariable calculus, *e.g.,* define $\frac{\partial\mathcal{L}}{\partial\varphi}$, so that we

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are viewing the Lagrangian as a function of 5 variables. But sometimes we want to consider the particular function of (t, x, y, z) we get by substituting a field into the formula for the Lagrangian. Hopefully this is not too confusing. Let us return now to the main line of the current discussion.

Evidently, given our boundary conditions, we can write the functional derivative of the action in terms of the *Euler-Lagrange derivative* of (or *Euler-Lagrange expression* for) the Lagrangian density, which is defined as

$$\mathcal{E}(\mathcal{L}) := \frac{\partial \mathcal{L}}{\partial \varphi} - D_\alpha \frac{\partial \mathcal{L}}{\partial \varphi_{,\alpha}}. \tag{2.57}$$

We have

$$\frac{\delta S}{\delta \varphi} = \mathcal{E}(\mathcal{L}) = -\varphi_{,tt} + \nabla^2 \varphi - m^2 \varphi, \tag{2.58}$$

and the KG field equation is the *Euler-Lagrange equation* of the Lagrangian density $\mathcal{L}$:

$$\mathcal{E}(\mathcal{L}) = 0. \tag{2.59}$$

PROBLEM: Compute the Euler-Lagrange derivative of the KG Lagrangian density and explicitly verify that the Euler-Lagrange equation is indeed the KG equation.

PROBLEM: Consider a Lagrangian density that is a divergence:

$$\mathcal{L} = D_\alpha W^\alpha, \tag{2.60}$$

where

$$W^\alpha = W^\alpha(\varphi). \tag{2.61}$$

Show that

$$\mathcal{E}(\mathcal{L}) \equiv 0. \tag{2.62}$$

Jet Space

To keep the presentation of Lagrangians and Euler-Lagrange derivatives tractable, I have specialized it somewhat based upon the simplicities of the KG equation. Here I will provide without proof a more general formalism. First, it is no problem to consider the case where the Lagrangian is a (local) function of the spacetime location, the fields, and the derivatives of the fields to any finite order. We write

$$\mathcal{L} = \mathcal{L}(x, \varphi, \partial\varphi, \partial^2\varphi, \ldots, \partial^k \varphi). \tag{2.63}$$

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Viewed this way, the Lagrangian is a function on a large but finite-dimensional space consisting of the spacetime points, and space of possible values of the fields and their derivatives to some finite order. This space is called the *jet space* for the field theory. If we vary $\mathcal{L}$ and "integrate by parts" so that all derivatives of $\delta\varphi$ appear inside divergences, then we have the *Euler-Lagrange identity*:

$$\delta\mathcal{L} = \mathcal{E}(\mathcal{L}) + D_\alpha V^\alpha, \tag{2.64}$$

where the general form for the Euler-Lagrange derivative is given by

$$\mathcal{E}(\mathcal{L}) := \frac{\partial\mathcal{L}}{\partial\varphi} - D_\alpha\frac{\partial\mathcal{L}}{\partial\varphi_{,\alpha}} + D_\alpha D_\beta\frac{\partial^2\mathcal{L}}{\partial\varphi_{,\alpha\beta}} - \cdots + (-1)^k D_{\alpha_1}\cdots D_{\alpha_k}\frac{\partial^k\mathcal{L}}{\partial\varphi_{,\alpha_1\cdots\alpha_k}}, \tag{2.65}$$

and, where the general form of the total derivative operator on a function

$$F = F(x, \varphi, \partial\varphi, \partial^2\varphi, \ldots, \partial^k\varphi), \tag{2.66}$$

is given by

$$D_\alpha F = \frac{\partial F}{\partial x^\alpha} + \frac{\partial F}{\partial\varphi}\varphi_{,\alpha} + \frac{\partial F}{\partial\varphi_{,\beta}}\varphi_{,\alpha\beta} + \cdots + \frac{\partial^k F}{\partial\varphi_{,\alpha_1\cdots\alpha_k}}\varphi_{,\alpha\alpha_1\cdots\alpha_k} \tag{2.67}$$

PROBLEM: Obtain a formula for the vector field V^α appearing in the boundary term in the Euler-Lagrange identity.

From the total derivative formula, it follows that divergences have trivial Euler-Lagrange derivatives

$$\mathcal{E}(D_\alpha V^\alpha) = 0. \tag{2.68}$$

This reflects the fact that the Euler-Lagrange derivative corresponds to the functional derivative in the case that the action functional is differentiable. In particular, the Euler-Lagrange derivative ignores all terms on the boundary of the domain of integration of the action integral.

To make contact between jet space and the usual calculus of variations one evaluates jet space formulas on a specific function $\varphi = \varphi(x)$, via

$$\varphi = \varphi(x), \quad \varphi_{,\alpha} = \frac{\partial\varphi(x)}{\partial x^\alpha}, \quad \varphi_{,\alpha\beta} = \frac{\partial^2\varphi(x)}{\partial x^\alpha\partial x^\beta}, \quad \ldots. \tag{2.69}$$

In this way formulas defined as function on jet space become formulas involving on the spacetime. A good framework for doing all this is to view jet space as a fiber bundle over spacetime. A particular KG field defines a cross section of that fiber bundle which can be used to pull back various structures to the base space.

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Functional Derivatives and Euler-Lagrange equations

The functional derivative of an action can be computed by restricting attention to field variations of compact support not including $\partial\mathcal{R}$, and computing

$$\delta S := \int_{\mathcal{R}} \frac{\delta S}{\delta \varphi}\delta\varphi. \tag{2.70}$$

The idea here is that the boundary terms that may arise by an integration by parts vanish since the variations (and all their derivatives) vanish on the boundary. From this point of view, the Euler-Lagrange derivative just computes the functional derivative when the action is a *local functional*, that is, when the action is the integral of a local Lagrangian density. By the same token, the Euler-Lagrange equations on a function φ are the necessary conditions δS to vanish. They are also sufficient conditions to make $\delta S = 0$ if you restrict attention to variations of compact support.

PROBLEM: Consider the Lagrangian (density)

$$\mathcal{L} = \frac{1}{2}\varphi(\Box - m^2)\varphi. \tag{2.71}$$

Compute the Euler-Lagrange equation of this Lagrangian and show that it yields the KG equation. Show that this Lagrangian density differs from our original Lagrangian density for the KG equation by a divergence.

Miscellaneous generalizations

There are a number of possible ways that one can generalize the KG field theory. Here I briefly mention a few generalizations that often arise in physical applications. The easiest way to describe thems is in terms of modifications of the Lagrangian density.

External "sources"

It is useful for some purposes to consider an inhomogeneous version of the KG equation. This is done by adding a term to the Lagrangian representing the interaction of the KG field with a prescribed "source", which mathematically is a given function $j(t, x, y, z)$. We have

$$\mathcal{L} = \frac{1}{2}(\varphi_{,t}^2 - (\nabla\varphi)^2 - m^2\varphi^2) - j\varphi. \tag{2.72}$$

The Euler-Lagrange (EL) equations are then

$$0 = \mathcal{E}(\mathcal{L}) = (\Box - m^2)\varphi - j. \tag{2.73}$$

The slickest way to solve this KG equation with sources is via Green's functions.

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This is a "toy model" of the Maxwell equations for the electromagnetic field in the presence of sources (electric charges and currents). Note that we have here an instance of a Lagrangian that, viewed as a function on jet space, depends upon the spacetime point (t, x, y, z) (via $j = j(t, x, y, z)$). In quantum field theory, the presence of a source will lead to particle production/annihilation via a transfer of energy-momentum (to be defined soon) between the field and the source.

Self-interacting field

The KG equation is linear; physically this corresponds to a "non-interacting" field. One way to see this is recall the interpretation of the KG field as a collection of (many!) oscillators. System of coupled oscillators obey linear equations. When quantized the oscillator states can be interpreted in terms of particle observables. In such an interpretation the particles propagate freely. This is why the KG field we have been studied is often called the "free" or "non-interacting" KG field.

One can of course modify the classical KG theory in a variety of ways to make it non-linear, that is, one can introduce "interactions". The simplest way to do this is to add a "potential term" term to the Lagrangian so that we have

$$\mathcal{L} = \frac{1}{2}(\varphi_{,t}^2 - (\nabla\varphi)^2 - m^2\varphi^2) - V(\varphi), \tag{2.74}$$

where V is a differentiable function of one variable. From the oscillator point of view such a term represents anharmonic contributions to the potential energy. The field equations are

$$0 = \mathcal{E}(\mathcal{L}) = (\Box - m^2)\varphi - V'(\varphi) = 0. \tag{2.75}$$

Provided V is not just a quadratic function, the field equation is non-linear.* Physically this corresponds to a "self-interacting" field. Of course, one can also add a source to the self-interacting theory.

A good example of a scalar field potential is the "double well potential", which is given by

$$V(\varphi) = -\frac{1}{2}a^2\varphi^2 + \frac{1}{4}b^2\varphi^4. \tag{2.76}$$

PROBLEM: Consider self-interacting KG fields with the potential (2.76). Characterize the set of solutions in which $\varphi = constant$ in terms of the values of the parameters m, a and b.

* Can you guess the interpretation of a quadratic potential?

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KG in arbitrary coordinates

We have presented the KG equation, action, Lagrangian, *etc.* using what we will call *inertial Cartesian coordinates* (t, x, y, z) on spacetime. Of course, we may use any coordinates that we like to describe the theory. It is a straightforward – if somewhat painful – exercise to transform the KG equation into any desired coordinate system. As a physicist we view the result as a new – but equivalent – representation of the KG field equation. Note however that, mathematically speaking, when you change coordinates in general you do get a *different* differential equation as the "new" KG equation. For example, in inertial Cartesian coordinates the KG equation is linear with constant coefficients. If you adopt spherical polar coordinates for space – defining *inertial spherical coordinates*, then the new version of the KG equation will still be linear but it will have variable coefficients. While this distinction may is to some extent just a matter of point of view, there are real consequences to the fact that the equation changes in different coordinate systems. We shall discuss this more later.

It is possible to give an elegant geometric prescription for computing the Lagrangian and field equations for any coordinate system. We proceed as follows. Introduce the *spacetime metric* g via

$$g = -dt \otimes dt + dx \otimes dx + dy \otimes dy + dz \otimes dz. \tag{2.77}$$

The metric is a symmetric tensor of type $\binom{0}{2}$. It defines a scalar product between tangent vectors at each point of spacetime. The metric has an inverse g^{-1} which is a symmetric tensor of type $\binom{2}{0}$,

$$g^{-1} = -\frac{\partial}{\partial t} \otimes \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \otimes \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \otimes \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \otimes \frac{\partial}{\partial z}. \tag{2.78}$$

Components of these tensors in the inertial Cartesian coordinates are the same, given by the familiar diagonal matrix:

$$g_{\alpha\beta} := g(\frac{\partial}{\partial x^\alpha}, \frac{\partial}{\partial x^\beta}) = g^{\alpha\beta} := g^{-1}(dx^\alpha, dx^\beta) = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.79}$$

It is not hard to check that the KG Lagrangian density can be expressed in terms of the metric by

$$\mathcal{L} = -\frac{1}{2}\sqrt{-\det(g)}\left(g^{-1}(d\varphi, d\varphi) + m^2\varphi^2\right). \tag{2.80}$$

This formula is geometric and we know how to compute it in any given coordinate system. Although we won't prove it, it is not too hard to show that the EL equations of the Lagrangian density, in any given coordinates, do yield the KG equation transformed to the chosen coordinates. (This is not obvious, but must be proved!)

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Let me take a moment to spell out how to transform the Lagrangian in terms of an explicit (but arbitrary) coordinate system. Call the old coordinates $x^\alpha = (t, x, y, z)$. Call the new coordinates $\hat{x}^\alpha$. Of course we will have an invertible transformation between the two coordinate systems. With the usual abuse of notation we will write

$$x^\alpha = x^\alpha(\hat{x}), \quad \hat{x}^\alpha = \hat{x}^\alpha(x). \tag{2.81}$$

The metric in the new coordinates has components

$$\hat{g}_{\alpha\beta}(\hat{x}) = \frac{\partial x^\gamma}{\partial \hat{x}^\alpha}\frac{\partial x^\delta}{\partial \hat{x}^\beta} g_{\gamma\delta}(x(\hat{x})). \tag{2.82}$$

Note that, while the original metric components formed a diagonal array of constants, the new metric components will, in general, form some 4×4 symmetric array of functions. One should now compute the inverse metric components,

$$\hat{g}^{\alpha\beta}(\hat{x}) = \frac{\partial \hat{x}^\gamma}{\partial x^\alpha}\frac{\partial \hat{x}^\delta}{\partial x^\beta} g^{\gamma\delta}(x(\hat{x})). \tag{2.83}$$

Equivalently, one can compute $\hat{g}^{\alpha\beta}(\hat{x})$ by finding the matrix inverse to $\hat{g}_{\alpha\beta}(\hat{x})$. Next, you have to compute

$$\det(\hat{g}) = \det(\hat{g}_{\alpha\beta}(\hat{x})), \tag{2.84}$$

and, finally, you can compute the Lagrangian

$$\hat{\mathcal{L}}(\hat{x}, \phi, \varphi) = -\frac{1}{2}\sqrt{-\det(\hat{g}(\hat{x}))}\left(\hat{g}^{\alpha\beta}(\hat{x})\frac{\partial\varphi}{\partial\hat{x}^\alpha}\frac{\partial\varphi}{\partial\hat{x}^\beta} + m^2\varphi^2\right). \tag{2.85}$$

At this point I want to try to nip some possible confusion in the bud. Note that, while we have a geometric prescription for computing the KG Lagrangian in any coordinates, it is not a good idea to think that there is but one KG Lagrangian for all coordinate systems. Strictly speaking, different coordinate systems will, in general, lead to different Lagrangians. This comment is supposed to be completely analogous to the previously mentioned fact that, while we can compute "the KG equation" in any coordinate system, each coordinate system leads, in general, to a different PDE. Likewise, we have different functions $\mathcal{L}(x, \varphi, \partial\varphi)$ in different coordinates. For example, in Cartesian coordinates $\mathcal{L}$ is in fact independent of x, which need not be true in other coordinates.

Coordinates are convenient for computations, but they are more or less arbitrary, so it is always a good idea to have a coordinate free formulation of any important structure, *e.g.,* the KG field theory. It is possible to phrase this whole discussion in a completely coordinate-free way. Let us just sketch this. We consider $\mathbf{R}^4$ equipped with a flat metric g of Lorentz signature. (This means that in any coordinates the eigenvalues of the metric component matrix have the signs (-+++). This is a coordinate independent requirement.)

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We introduce a scalar field $\varphi\colon \mathbf{R}^4 \to \mathbf{R}$ and a parameter m. Let $\epsilon(g)$ be the volume 4-form defined by the metric. We define the KG Lagrangian as a 4-form via

$$\mathcal{L} = -\frac{1}{2}\left(g^{-1}(d\varphi, d\varphi) + m^2\varphi^2\right)\epsilon(g). \tag{2.86}$$

The Lagrangian is to be viewed as a function on the jet space of the KG field. This function is defined using a choice of metric. Our discussion concerning the fact that different coordinates imply different Lagrangians (and EL equations) can be stated in coordinate free language as follows. Consider a diffeomorphism

$$f\colon \mathbf{R}^4 \to \mathbf{R}^4. \tag{2.87}$$

The diffeomorphism defines a new metric $\hat{g}$ by pull-back:

$$\hat{g} = f^* g. \tag{2.88}$$

We can define a new Lagrangian using this new metric.

$$\hat{\mathcal{L}} = -\frac{1}{2}\left(\hat{g}^{-1}(d\varphi, d\varphi) + m^2\varphi^2\right)\epsilon(\hat{g}). \tag{2.89}$$

This metric is flat and can equally well be used to build the KG theory. The EL equations arising from $\hat{\mathcal{L}}$ ($\mathcal{L}$) are the KG equations defined using $\hat{g}$ (g). The relation between the solution spaces of these two equations is that there is a bijection between the spaces of smooth solutions to each equation. The bijection between solutions φ to the EL equations of $\mathcal{L}$ and the solutions $\hat{\varphi}$ to the EL equations of $\hat{\mathcal{L}}$ is simply

$$\hat{\varphi} = f^*\varphi. \tag{2.90}$$

KG on any spacetime

A *spacetime* is defined as a pair (M, g) where M is a manifold and g is a Lorentzian metric.* We will always assume that everything in sight is smooth, unless otherwise indicated. Physically, we should take M to be four-dimensional, but this is not required mathematically and we shall not do it here. It is possible to generalize the KG field theory to any spacetime, but the generalization is not unique. Here I just mention two of the most popular possibilities.

First, we have the *minimally coupled KG theory*, defined by the Lagrangian

$$\mathcal{L}_1 = -\frac{1}{2}\left(g^{-1}(d\varphi, d\varphi) + m^2\varphi^2\right)\epsilon(g). \tag{2.91}$$

* This means that at each point $x \in M$, there exists a basis e_α for T_xM such that $g(e_\alpha, e_\beta) = \mathrm{diag}(-1, 1, 1, 1, \cdots, 1)$. By contrast, a Riemannian metric uses a positive definite metric so that the components of the metric at a point can be rendered as $\mathrm{diag}(1, 1, 1, 1, \cdots, 1)$.

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Of course, this is formally the same as our flat spacetime Lagrangian. The term "minimal coupling" has a precise technical definition, but we will not bother to discuss it. It amounts to making the most straightforward generalization from flat spacetime to curved spacetime as you can see here.

A second possibility is the *curvature coupled KG theory*, defined by the Lagrangian

$$\mathcal{L}_2 = -\frac{1}{2}\left[g^{-1}(d\varphi, d\varphi) + (m^2 + \xi R(g))\varphi^2\right]\epsilon(g), \tag{2.92}$$

where $R(g)$ is the scalar curvature of the metric and ξ is a parameter. The resulting theory is usually described with the terminology "non-minimally coupled".

If the spacetime is $(\mathbf{R}^4, g)$, with g a flat metric, then both of these Lagrangians reduce to one of the possible Lagrangians in flat spacetime that we discussed in the previous subsection. So, both can be considered possible generalizations to curved spacetimes.

Finally, let me mention a subtle issue for those of you who are ready to make sense of such things. I emphasize that all of these Lagrangians require the specification of a metric for their definition. If you change the metric then, strictly speaking, you are using a different Lagrangian (viewed, say, as a function on jet space). This is why, in a precise technical sense one does *not* use the adjectives "generally covariant" or "diffeomorphism invariant" to describe the KG field theories introduced above. If these Lagrangians had this property, then under a redefinition of the KG field via a diffeomorphism $f\colon M \to M$,

$$\varphi \to f^*\varphi, \tag{2.93}$$

the Lagrangian should not change. Of course, in order for the Lagrangian to stay unchanged (say, as a function on jet space) one must also redefine the metric by the diffeomorphism,

$$g \to f^*g. \tag{2.94}$$

But, as we already agreed, the Lagrangian changes when you use a different metric. The point is that the metric is not one of the fields in the KG field theory and you have no business treating them as such. Now, if the metric itself is treated as a field (not some background structure), subject to variation, EL equations, etc., then the Lagrangians we have written *are* generally covariant. Of course, we no longer are studying the KG theory, but something much more complex, *e.g.,* there are now 11 coupled non-linear field equations instead of 1 linear field equation. We will return to this issue again when we discuss what is meant by a symmetry.

PROBLEMS

1. Verify (2.4)–(2.9).

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2. Compute the Euler-Lagrange derivative of the KG Lagrangian density and explicitly verify that the Euler-Lagrange equation is indeed the KG equation.

3. Consider a Lagrangian density that is a divergence:

$$\mathcal{L} = D_\alpha W^\alpha,$$

where

$$W^\alpha = W^\alpha(\varphi).$$

Show that

$$\mathcal{E}(\mathcal{L}) \equiv 0.$$

4. Obtain a formula for the vector field V^α appearing in the boundary term in the Euler-Lagrange identity.

5. Consider the Lagrangian (density)

$$\mathcal{L} = \frac{1}{2}\varphi(\Box - m^2)\varphi.$$

Compute the Euler-Lagrange equation of this Lagrangian and show that it yields the KG equation. Show that this Lagrangian density differs from our original Lagrangian density for the KG equation by a divergence.

6. Consider self-interacting KG fields with the potential (2.76). Characterize the set of solutions in which $\varphi = constant$ in terms of the values of the parameters m, a and b.

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