Notes on quantizing the massive scalar field

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1 From coordinates to fields

Consider the familiar simple harmonic oscillator. It has the Lagrangian

$$\mathcal{L}(x,\dot{x}) = T - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2.$$

From mechanics, we know the equations of motion for this system are revealed by taking the functional derivative of the action $S = \int \mathcal{L}(x,\dot{x})\,\mathrm{d}t$ and setting it equal to 0 (i.e. finding an extremal trajectory of the action). Doing so reveals

$$\begin{aligned}
\frac{\delta S[x(t)]}{\delta x(t)} &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\Big(\int_a^b \frac{1}{2}m(\dot{x}+\varepsilon\dot{\eta})^2 - \frac{1}{2}k(x+\varepsilon\eta)^2\,\mathrm{d}t - \int_a^b \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2\,\mathrm{d}t\Big)\\
&= \lim_{\varepsilon\to 0}\Big(\int_a^b m\dot{x}\dot{\eta} - kx\eta\,\mathrm{d}t + \mathcal{O}(\varepsilon)\Big)\\
&= -\int_a^b (m\ddot{x}+kx)\eta\,\mathrm{d}t\\
&= 0
\end{aligned}$$

which implies $m\ddot{x} = -kx$, as we expect.[1] More generally we have

$$\begin{aligned}
\frac{\delta S[x(t)]}{\delta x(t)} &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\Big(\int_a^b \mathcal{L}(x+\varepsilon\eta,\dot{x}+\varepsilon\dot{\eta})\,\mathrm{d}t - \int_a^b \mathcal{L}(x,\dot{x})\,\mathrm{d}t\Big)\\
&= \lim_{\varepsilon\to 0}\Big(\int_a^b \frac{\partial\mathcal{L}}{\partial x}\eta + \frac{\partial\mathcal{L}}{\partial\dot{x}}\dot{\eta}\,\mathrm{d}t + \mathcal{O}(\varepsilon)\Big)\\
&= \int_a^b \Big(\frac{\partial\mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}}\Big)\eta\,\mathrm{d}t
\end{aligned}$$

which shows that valid trajectories must satisfy

$$\frac{\partial\mathcal{L}}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{x}} = 0.$$

This can immediately be generalized to a system with multiple coordinates,

$$\frac{\partial\mathcal{L}}{\partial q^a} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\dot{q}^a} = 0.$$

What is the equivalent principle for a covariant field $\phi(x)$? We know that a relativistic system must treat both temporal and spatial derivatives similarly, so the Lagrangian for such a field will have dependencies on ϕ and $\partial_\mu\phi$. By similar considerations, the action must be promoted to an integral over spacetime. Finding the extrema of this new action yields

[1] In the above series of steps, $\eta(t)$ is an arbitrary function that vanishes at the endpoints of the integral. It perturbs the action from the true path $x(t)$.

$$\begin{aligned}
\frac{\delta S[\phi(x)]}{\delta\phi(x)} &= \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\Big(\int_\Gamma \mathcal{L}(\phi+\varepsilon\varphi, \partial_\mu\phi+\varepsilon\partial_\mu\varphi)\,\mathrm{d}^4x - \int_\Gamma \mathcal{L}(\phi,\partial_\mu\phi)\,\mathrm{d}^4x\Big)\\
&= \lim_{\varepsilon\to 0}\Big(\int_\Gamma \frac{\partial\mathcal{L}}{\partial\phi}\varphi + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\partial_\mu\varphi\,\mathrm{d}^4x + \mathcal{O}(\varepsilon)\Big)\\
&= \int_\Gamma \Big(\frac{\partial\mathcal{L}}{\partial\phi} - \partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\Big)\varphi\,\mathrm{d}^4x\\
&= 0
\end{aligned}$$

or[2]

$$\frac{\partial\mathcal{L}}{\partial\phi} - \partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)} = 0.$$

This is the covariant form of the Euler-Lagrange equation. We have found it by assuming the action principle holds for fields.

2 The massive scalar field

Consider the relativistic classical field described by[3]

$$\begin{aligned}
\mathcal{L}(\phi,\partial_\mu\phi) &= \frac{1}{2}\partial_\mu\partial^\mu\phi - \frac{1}{2}m^2\phi^2\\
&= \frac{1}{2}\dot{\phi}^2 - \frac{1}{2}(\nabla\phi)\cdot(\nabla\phi) - \frac{1}{2}m^2\phi^2
\end{aligned}$$

where, by analogy to the Lagrangian of the simple harmonic oscillator, we identify $\frac{1}{2}\dot{\phi}^2$ with the kinetic energy of the field and $\frac{1}{2}(\nabla\phi)\cdot(\nabla\phi) + \frac{1}{2}m^2\phi^2$ with its potential energy. Recognizing that the Hamiltonian should be described by the sum of both quantities, we define the momentum conjugate to ϕ to be[4]

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\phi}}.$$

With this definition, we have

$$\mathcal{H}(\phi,\pi) = \pi\dot{\phi} - \mathcal{L}(\phi,\partial_\mu\phi),$$

which is a nice generalization of the Hamiltonian to fields.

The Euler-Lagrange equation for this system is

$$(\partial_\mu\partial^\mu + m^2)\phi(x) = 0.$$

We may Fourier transform this to find

$$\frac{1}{(2\pi)^4}\int \mathrm{d}^4k\,(-k_\mu k^\mu + m^2)\tilde{\phi}(k)e^{-ik_\mu x^\mu} = 0.$$

For this to hold true,

$$\tilde{\phi}(k) = 2\pi\delta(m^2 - k_\mu k^\mu)f(k)$$

for some $f(k)$. This is encouraging, as this constraint simply encodes the relativistic relationship between mass, energy, and momentum.

[2] As an aside, we can easily deal with vector and tensor fields by tacking an index onto ϕ.

[3] In many ways this is the first classical field one would suggest: the first term is the simplest way to construct a Lorentz scalar out of $\partial_\mu\phi$, and the second represents a potential dependent on the absolute value of the field. The factor of m^2 is there to make the units work out (where $\hbar = c = 1$). It is conveniently labeled to suggest mass, as it turns out the quanta of this field have a mass m.

[4] From this definition, we can see that an 'upstairs' index in ϕ gets converted to a 'downstairs' index in π. The converse holds true, too.

Writing $k_\mu k^\mu = k_0^2 - \mathbf{k}^2$, we see that

$$2\pi\delta(\mathbf{k}^2 + m^2 - k_0^2)f(k) = \frac{2\pi}{2k_0}\Big(\delta\big(k_0 - \sqrt{\mathbf{k}^2+m^2}\big) + \delta\big(k_0 + \sqrt{\mathbf{k}^2+m^2}\big)\Big)f(k_0, \mathbf{k})$$

where we have used

$$\delta(f(x)) = \sum_{\{a|f(a)=0\}} \frac{\delta(x-a)}{|f'(a)|},$$

treating k_0 as the independent variable. Substituting $\tilde{\phi}(k)$ into the Fourier expansion for $\phi(x)$ gives

$$\phi(x) = \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3\mathbf{k}}{2\omega}\Big(f(\omega,\mathbf{k})e^{-i\omega t}e^{i\mathbf{k}\cdot\mathbf{x}} + f(-\omega,\mathbf{k})e^{i\omega t}e^{i\mathbf{k}\cdot\mathbf{x}}\Big),$$

where we have defined $\omega = \sqrt{\mathbf{k}^2+m^2}$. Traditionally, one then makes the exchange $\mathbf{k} \to -\mathbf{k}$ in the second term to tidy up the notation

$$\phi(x) = \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3\mathbf{k}}{2\omega}\Big(a_\mathbf{k}e^{-i\omega t}e^{i\mathbf{k}\cdot\mathbf{x}} + b_\mathbf{k}e^{i\omega t}e^{-i\mathbf{k}\cdot\mathbf{x}}\Big),$$

where $a_\mathbf{k} = f(\omega,\mathbf{k})$ and $b_\mathbf{k} = f(-\omega,-\mathbf{k})$. In fact, this can be constrained further if $\phi(x)$ is real. In this case, $\phi(x) = \phi^*(x)$ and so

$$\phi(x) = \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3\mathbf{k}}{2\omega}\Big(a_\mathbf{k}e^{-i\omega t}e^{i\mathbf{k}\cdot\mathbf{x}} + a^*_\mathbf{k}e^{i\omega t}e^{-i\mathbf{k}\cdot\mathbf{x}}\Big),$$

3 From classical to quantum

We would like to quantize this field. For single particle quantum mechanics, the quantization process involves promoting q and p to operators—all other operators can be constructed from these. The position operators q^a and their conjugate momenta p_a obey the commutation relation

$$[q^a, p_b] = i\delta_{ab}.$$

Inspired by this, we do the same for fields. That is, $\phi(x) \to \hat{\phi}(x)$, $\pi(x) \to \hat{\pi}(x)$, $a_\mathbf{k} \to \hat{a}_\mathbf{k}$, and $a^*_\mathbf{k} \to \hat{a}^\dagger_\mathbf{k}$. Our new commutation relation is

$$[\hat{\phi}(t,\mathbf{x}), \hat{\pi}(t,\mathbf{y})] = i\delta^{(3)}(\mathbf{x}-\mathbf{y})$$

with $[\hat{\phi}(x), \hat{\phi}(y)] = [\hat{\pi}(x), \hat{\pi}(y)] = 0$, i.e. the field commutes with its conjugate momenta unless they are at the same point in space and time. In that case, their commutator is proportional to i.

For the classical massive scalar field $\pi = \dot{\phi}$, and so we have

$$\hat{\phi}(x) = \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3\mathbf{k}}{2\omega}\Big(\hat{a}_\mathbf{k}e^{-i\omega t}e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{a}^\dagger_\mathbf{k}e^{i\omega t}e^{-i\mathbf{k}\cdot\mathbf{x}}\Big)$$
$$\hat{\pi}(y) = -\frac{i}{(2\pi)^3}\int \frac{\mathrm{d}^3\mathbf{k'}}{2}\Big(\hat{a}_\mathbf{k'}e^{-i\omega t}e^{i\mathbf{k'}\cdot\mathbf{y}} - \hat{a}^\dagger_\mathbf{k'}e^{i\omega t}e^{-i\mathbf{k'}\cdot\mathbf{y}}\Big)$$

Imposing the new commutation relation amounts to the condition that

$$[\hat{\phi}(t,\mathbf{x}), \hat{\pi}(t,\mathbf{y})] = -\frac{i}{(2\pi)^6}\iint \frac{\mathrm{d}^3\mathbf{k}\,\mathrm{d}^3\mathbf{k'}}{4\omega}[\hat{a}_\mathbf{k}, \hat{a}_\mathbf{k'}]e^{-i2\omega t}e^{i\mathbf{k}\cdot\mathbf{x}+i\mathbf{k'}\cdot\mathbf{y}} - [\hat{a}_\mathbf{k}, \hat{a}^\dagger_\mathbf{k'}]e^{i\mathbf{k}\cdot\mathbf{x}-i\mathbf{k'}\cdot\mathbf{y}}$$