KLEIN-GORDON EQUATION FOR FIELDS; DERIVATION FROM THE LAGRANGIAN

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Reference: References: Robert D. Klauber, *Student Friendly Quantum Field Theory*, (Sandtrove Press, 2013) - Chapter 3, Problem 3.4.

We originally arrived at the Klein-Gordon equation

$$\left(\square^2+\mu^2\right)\phi=0 \tag{1}$$

by converting the relativistic energy equation

$$E^2=p^2+m^2 \tag{2}$$

to quantum operator form. The function ϕ that is a solution of this equation is a relativistic quantum *state*, that is, it's the relativistic analogue of the state Ψ that is the solution of the Schrödinger equation. ϕ can represent a relativistic quantum particle in the same way that Ψ represents a non-relativistic quantum particle.

To get a field theory, that is, a theory where $\phi(x)$ represents a field value and the four-vector x is a set of labels of points in space-time (rather than the spatial coordinates x^i representing the position of a particle), we need to go back to the classical field theory and convert it to a quantum theory. The Euler-Lagrange equations for a classical field are

$$\frac{\partial\mathcal{L}}{\partial\phi^r}-\frac{\partial}{\partial q^\mu}\left(\frac{\partial\mathcal{L}}{\partial\phi^r_{,\mu}}\right)=0 \tag{3}$$

where ϕ^r is the rth field, q^μ is the μth coordinate in spacetime and $\mathcal{L}$ is the Lagrangian (strictly, the Lagrangian density). At this point, most sources I've seen magically produce $\mathcal{L}$ seemingly out of thin air, although some books (such as Klauber) mention that the Lagrangian does come out of classical field theory. I may delve into this at some point, but in order not to slow things down too much, I'll just quote the Lagrangian here:

$$\mathcal{L}_0^0=K\left(\partial_\alpha\phi\partial^\alpha\phi-\mu^2\phi^2\right) \tag{4}$$

The superscript 0 on $\mathcal{L}_0^0$ indicates that we're dealing with a *scalar* field (as opposed to a field with spin) and the subscript 0 indicates that it's a *free* field (no potential terms). K is a constant. The Legendre transformation gives the Hamiltonian density for the field as

$$\mathcal{H}_0^0 = \pi_0^0 \dot{\phi} - \mathcal{L}_0^0 \tag{5}$$

where the conjugate momentum is, from 4

$$\pi_0^0 = \frac{\partial \mathcal{L}_0^0}{\partial (\partial_0 \phi)} = \frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}} = 2K\dot{\phi} \tag{6}$$

Therefore

$$\begin{aligned} \mathcal{H}_0^0 &= 2K\dot{\phi}\dot{\phi} - K\left(\partial_\alpha \partial^\alpha \phi - \mu^2 \phi^2\right) &(7)\\ &= K\left(\dot{\phi}\dot{\phi} + \nabla\phi \cdot \nabla\phi + \mu^2\phi^2\right) &(8)\end{aligned}$$

At this point, there's a bit of (informed) hand-waving, where we realize that since the wave function Ψ in Schrödinger quantum mechanics is a complex function, it's most likely that ϕ in field theory is also complex. However, if we wish to retain the meaning of the Hamiltonian as the energy density, it must be real, so we need to combine ϕ and $\phi^\dagger$ in such a way as to give a real Hamiltonian and Lagrangian. We can do this by noticing that ϕ and its derivatives always appear in squared terms in 4 and 8, which suggests replacing these terms by products of a term with its complex conjugate. So we try (taking $K = 1$)

$$\begin{aligned} \mathcal{L}_0^0 &= \partial_\alpha \phi^\dagger \partial^\alpha \phi - \mu^2 \phi^\dagger \phi &(9)\\ &= \dot{\phi}^\dagger \dot{\phi} - \nabla\phi^\dagger \cdot \nabla\phi - \mu^2 \phi^\dagger \phi &(10)\end{aligned}$$

Calculating the Hamiltonian is a bit trickier, for we need to realize that with a complex field, we actually have *two* fields, since the real and imaginary parts are two separate functions. In fact, the way this is handled is to treat ϕ and $\phi^\dagger$ as the separate fields. Then our original notation for the Hamiltonian is

$$\mathcal{H}_0^0 = \pi_r \dot{\phi}^r - \mathcal{L}_0^0 \tag{11}$$

where there is a sum over r, the index specifying which field we're talking about. Here, this becomes

$$\mathcal{H}_0^0 = \pi_0^0 \dot{\phi} + \pi_0^{0\dagger} \dot{\phi}^\dagger - \mathcal{L}_0^0 \tag{12}$$

From 6 and 10 we have

$$\pi_0^0 = \frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}} = \dot{\phi}^\dagger \tag{13}$$

$$\pi_0^{0\dagger} = \frac{\partial \mathcal{L}_0^0}{\partial \dot{\phi}^\dagger} = \dot{\phi} \tag{14}$$

$$\mathcal{H}_0^0 = \dot{\phi}^\dagger \dot{\phi} + \dot{\phi}\dot{\phi}^\dagger - \left[\dot{\phi}^\dagger \phi - \nabla\phi^\dagger \cdot \nabla\phi - \mu^2 \phi^\dagger \phi\right] \tag{15}$$

$$= \dot{\phi}\dot{\phi}^\dagger + \nabla\phi^\dagger \cdot \nabla\phi + \mu^2 \phi^\dagger \phi \tag{16}$$

Using 10 in 3 we get, for $\phi^r = \phi$:

$$\frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial q^\mu}\left(\frac{\partial \mathcal{L}}{\partial \phi_{,\mu}}\right) = -\mu^2 \phi^\dagger - \partial_0\left(\partial^0 \phi^\dagger\right) + \partial_i\left(\partial^i \phi^\dagger\right) = 0 \tag{17}$$

$$\left(\partial_\mu \partial^\mu + \mu^2\right)\phi^\dagger = \left(\Box^2 + \mu^2\right)\phi^\dagger = 0 \tag{18}$$

Taking $\phi^r = \phi^\dagger$ gives the conjugate equation

$$\left(\partial_\mu \partial^\mu + \mu^2\right)\phi = \left(\Box^2 + \mu^2\right)\phi = 0 \tag{19}$$

This is the Klein-Gordon equation, but the crucial difference is that the function ϕ here is a *field* rather than the function ϕ in our earlier solution, which represented a state of a particle or superposition of particles. In the former solution, ϕ was a direct analogue of the non-relativistic wave function Ψ; in our present case, it represents the value of the quantum field at each point q^μ in spacetime.

However, the two solutions are *mathematically* equivalent, so they must have the same solution, which we can write as

$$\phi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a(\mathbf{k})\, e^{-ikx} + \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} b^\dagger(\mathbf{k})\, e^{ikx} \tag{20}$$

$$\equiv \phi^+ + \phi^- \tag{21}$$

$$\phi^\dagger(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} a^\dagger(\mathbf{k})\, e^{ikx} + \sum_{\mathbf{k}} \frac{1}{\sqrt{2V\omega_{\mathbf{k}}}} b(\mathbf{k})\, e^{-ikx} \tag{22}$$

$$\equiv \phi^{\dagger +} + \phi^{\dagger -} \tag{23}$$

[Take care to distinguish between the $+$ and $\dagger$ symbols in the superscripts.] We've written the coefficient a and b using lowercase rather than the uppercase we used for the particle theory, as they turn out to be operators rather than simply numerical constants.

We can work out the constant μ in 19 in traditional units by applying this equation to one component of the solution. Since 20 is a sum of terms, each of which is a solution, we can look at just one term, say $\phi_{\mathbf{k}}=\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a(\mathbf{k})e^{-ikx}$. Then

$$\left(\partial_{\mu}\partial^{\mu}+\mu^{2}\right)\phi_{\mathbf{k}}=\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a(\mathbf{k})\left(\partial_{\mu}\partial^{\mu}+\mu^{2}\right)e^{-ikx} \tag{24}$$

$$=\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a(\mathbf{k})\left((-i)^{2}k_{\mu}k^{\mu}+\mu^{2}\right)e^{-ikx} \tag{25}$$

$$=\frac{1}{\sqrt{2V\omega_{\mathbf{k}}}}a(\mathbf{k})\left(-k_{\mu}k^{\mu}+\mu^{2}\right)e^{-ikx} \tag{26}$$

So we must have

$$\mu^{2}=k_{\mu}k^{\mu} \tag{27}$$

In cgs units, the 4-vector for spacetime is

$$x^{\mu}=[ct,\mathbf{x}] \tag{28}$$

The four-vector k^{μ} must be

$$k^{\mu}=\left[\frac{E_{\mathbf{k}}}{c\hbar},\frac{\mathbf{p}_{\mathbf{k}}}{\hbar}\right] \tag{29}$$

[We get this by multiplying by factors of c and $\hbar$ to make the product $k_{\mu}x^{\mu}$ dimensionless, as it must be since it is an exponent. Remember that the dimensions of $\hbar$ in cgs are (energy) $\times$ (time).]

So

$$k_{\mu}k^{\mu}=\frac{1}{\hbar^{2}}\left(\frac{E_{\mathbf{k}}^{2}}{c^{2}}-p_{\mathbf{k}}^{2}\right) \tag{30}$$

Using the relativistic relation $E^{2}=p^{2}c^{2}+m^{2}c^{4}$ we get

$$k_{\mu}k^{\mu} = \frac{1}{\hbar^{2}}\left(p_{\mathbf{k}}^{2}+m^{2}c^{2}-p_{\mathbf{k}}^{2}\right) \tag{31}$$

$$= m^{2}\frac{c^{2}}{\hbar^{2}}=\mu^{2} \tag{32}$$

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