The main object today is to quantize the Klein-Gordon equ, to obtain a quantum field theory for spinless particles.

It was explained earlier how Schrödinger derived the Klein-Gordon equation, following ideas of Einstein and de Broglie. The KG equ is an encoding of the relativistic energy-momentum relation for a particle of mass m,

$$E^2 = m^2c^4 + c^2p^2,$$

into operators via the Einstein relations (and de Broglie),

$$\left.\begin{aligned} E &\to i\hbar \frac{\partial}{\partial t} \\ \vec{p} &\to -i\hbar\nabla \end{aligned}\right\}.$$

which gives

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = (m^2c^4 - c^2\hbar^2\nabla^2)\psi,$$

or

$$\Box\psi \equiv \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi = -\left(\frac{mc}{\hbar}\right)^2\psi .$$

This is the K-G equ.

We put this into covariant form by writing

$$x^\mu = \begin{pmatrix} ct \\ \vec{x} \end{pmatrix}, \quad x_\mu = \begin{pmatrix} ct \\ -\vec{x} \end{pmatrix}, \quad p^\mu = \begin{pmatrix} E/c \\ \vec{p} \end{pmatrix},$$

$$p_\mu = \begin{pmatrix} E/c \\ -\vec{p} \end{pmatrix},$$ and then writing the Einstein - de Broglie relations,

$$p_\mu = \begin{pmatrix} E/c \\ -\vec{p} \end{pmatrix} \to \begin{pmatrix} i\hbar\, \partial/\partial(ct) \\ i\hbar\nabla \end{pmatrix} = i\hbar \frac{\partial}{\partial x^\mu}.$$

Then the KG eqn can be written

$$p_\mu p^\mu \psi = -\hbar^2 \Box \psi = m^2 c^2 \psi ,$$

obviously an encoding of the classical but relativistic relation $p_\mu p^\mu = m^2 c^2$.

~~this is as far as we got~~.

Let's also write

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \begin{pmatrix} \partial/\partial(ct) \\ \nabla \end{pmatrix},$$

$$\partial^\mu = \frac{\partial}{\partial x_\mu} = \begin{pmatrix} \partial/\partial(ct) \\ -\nabla \end{pmatrix}.$$

Then $p_\mu = i\hbar\partial_\mu$, $p^\mu = i\hbar\partial^\mu$ when interpreted as operators, and $\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 = \partial_\mu\partial^\mu$.

In the following we will choose units such that $\hbar = c = 1$, which simplifies writing. These are called <u>natural units</u>.

Actually, I may be slightly schizophrenic about units, setting $\hbar$ or c or both $= 1$ sometimes, and sometimes putting them back in when it's more clear.

Now let's ask for a Lagrangian formulation of the KG eqn.

Recall that in 3D field theory, the <u>Lagrangian</u> L is the spatial integral of the <u>Lagrangian density</u> $\mathcal{L}$:

$$L = \int d^3x \; \mathcal{L}\left(\psi, \frac{\partial \psi}{\partial t}, \nabla\psi\right),$$

where $\mathcal{L}$ is a function of ψ and its space-time derivatives. Here ψ is a generic field (not necessarily the K-G field).

Then the action is the time integral of the Lagrangian, which becomes a space-time integral of the Lagrangian density:

$$A[\psi(\vec{x},t)] = \int dt \; L = \int dt \, d^3x \; \mathcal{L} = \int d^4x \; \mathcal{L}.$$

Finally, the Euler-Lagrange equations are

$$\frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \psi}{\partial t}\right)}\right) + \nabla\cdot\left(\frac{\partial \mathcal{L}}{\partial(\nabla\psi)}\right) = \frac{\partial \mathcal{L}}{\partial \psi}. \qquad (*)$$

Now in relativity we require equations of motion that are covariant, i.e. have the same form in all Lorentz frames. Since the variational principle involves the action, if the action is a Lorentz scalar then if it's stationary in one frame it will be stationary in all frames, and the form of the Euler-Lagrange equations will be the same in all frames. And since the 4-volume element d^4x is invariant under Lorentz transformations, $A = \int d^4x \; \mathcal{L}$ will be invariant if $\mathcal{L}$ is invariant.

Therefore to get Lorentz covariant equations, we may seek Lagrangian densities $\mathcal{L}$ that are Lorentz invariants.

Consider for example the Klein-Gordon field ψ. This field is a Lorentz scalar, $\psi(x) = \psi(x')$, because it describes a spin-0 particle. So how do we construct a Lorentz scalar out of the scalar ψ and its first space-time derivatives, $\partial_\mu \psi = \frac{\partial \psi}{\partial x^\mu}$? Obviously any function of ψ is a scalar, but if we want linear equations of motion (the KG eqn is linear) then the function must be quadratic, which gives us ψ^2. As for $\partial_\mu\psi$, it transforms as a covariant vector. To construct a scalar we may take the ~~so~~ (Minkowski) scalar product of this vector with itself to get

$$\eta^{\mu\nu}(\partial_\mu\psi)(\partial_\nu\psi) = (\partial_\mu\psi)(\partial^\mu\psi)$$
$$= \left(\frac{\partial\psi}{\partial t}\right)^2 - (\nabla\psi)^2. \qquad (c=1)$$

This is also quadratic in ψ. So the only Lorentz scalar Lagrangian density that is quadratic in ψ and constructed out of ψ and $\partial_\mu\psi$ is a linear combination of ψ^2 and $(\partial_\mu\psi)(\partial^\mu\psi)$. Adjusting the coefficients to make the KG eqn come out, we get

$$\mathcal{L} = \frac{1}{2}\left[(\partial_\mu\psi)(\partial^\mu\psi) - m^2\psi^2\right]$$
$$= \frac{1}{2}\left[\left(\frac{\partial\psi}{\partial t}\right)^2 - (\nabla\psi)^2 - m^2\psi^2\right].$$

One point of this exercise is that Lorentz covariance almost uniquely determines the Lagrangian and hence the equations of motion.

BTW, the EL eqns (*) on p.3, can be put into covariant form. It is

$$\boxed{\frac{\partial}{\partial x^\mu}\left(\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi}{\partial x^\mu}\right)}\right) = \frac{\partial\mathcal{L}}{\partial\psi}}$$

Now I want to say something about Hamiltonians in classical field theory. We need a classical Hamiltonian before we can quantize and go over to a quantum Hamiltonian.

In ordinary particle mechanics we have a Lagrangian $L(q^i, \dot{q}^i)$, where $i = 1, \dots, n$ = the number of degrees of freedom. We define the momentum by

$$p_i = \frac{\partial L}{\partial \dot{q}_i},$$

and then the Hamiltonian by

$$H = \sum_i p_i \dot{q}_i - L.$$

Without justification, I will quote the corresponding formulas in field theory. Given a Lagrangian density, $\mathcal{L}(\psi, \dot{\psi}, \nabla\psi)$, where $\dot{\psi}$ means $\frac{\partial \psi}{\partial t}$, we define the momentum field conjugate to ψ by

$$\pi(\vec{x}) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}},$$

and then the Hamiltonian by

$$H = \int d^3\vec{x}\ \pi(\vec{x})\,\dot{\psi}(\vec{x}) \quad - L$$

The integral replaces the $\sum_i$ in the usual formula in mechanics, because in field theory the degrees of freedom carry a continuous index. But $L = \int d^3\vec{x}\, \mathcal{L}$, so the entire right-hand side is an integral, and we can write,

$$H = \int d^3\vec{x}\ \mathcal{H},$$

where $\mathcal{H}$ is called the Hamiltonian density and is given by

$$\mathcal{H} = \pi \dot{\psi} - \mathcal{L}.$$

For example, in the KG case, we have

$$\mathcal{L} = \frac{1}{2}\left[\dot{\psi}^2 - (\nabla\psi)^2 - m^2\psi^2\right],$$

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \dot{\psi}$$

$$\mathcal{H} = \pi\dot{\psi} - \mathcal{L} = \dot{\psi}^2 - \frac{1}{2}\left[\dot{\psi}^2 - (\nabla\psi)^2 - m^2\psi^2\right]$$

$$= \frac{1}{2}\left[\dot{\psi}^2 + (\nabla\psi)^2 + m^2\psi^2\right].$$

$$= \frac{1}{2}\left[\pi^2 + (\nabla\psi)^2 + m^2\psi^2\right].$$

So,
$$H = \frac{1}{2}\int d^3\vec{x}\left(\pi^2 + (\nabla\psi)^2 + m^2\psi^2\right). \qquad (*)\ \text{(KG Hamiltonian)}$$

Just a note, if you do this for the EM field, you find

$$H = \frac{1}{8\pi}\int d^3\vec{x}\ (E^2 + B^2),$$

the usual expression for the energy (and energy density) in the EM field.

Now to cite some facts about the simple harmonic oscillator. Let's consider a mechanical oscillator (this is all classical at this point) with Hamiltonian

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2.$$

Here m, the mass of the particle in the oscillator, has nothing to do with m, the mass of Klein-Gordon particle (it's just a conflict of notation.) We can check that Hamilton's equations give the correct eqns of motion:

$$\dot{x} = \frac{\partial H}{\partial p} = p/m$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -m\omega^2 x.$$

so, $\ddot{x} = \frac{\dot{p}}{m} = -\omega^2 x$, or $\ddot{x} = -\omega^2 x$, which is correct.

A change of variables puts this Hamiltonian into a more symmetrical form that is useful sometimes. Define Q and P by

$$\left.\begin{aligned} p &= \sqrt{m\omega}\, P, \\ x &= \frac{Q}{\sqrt{m\omega}}, \end{aligned}\right\} \quad \text{or} \quad \left.\begin{aligned} P &= \frac{p}{\sqrt{m\omega}} \\ Q &= \sqrt{m\omega}\, x \end{aligned}\right\}. \qquad (*)$$

These new variables squeeze x and expand p by the same factor, so the xp area is the same as the QP area. Such an area-preserving transformation is called a canonical transformation in classical mechanics, and it has the property that the form of Hamilton's equations is preserved.

it's easy to check this. Transforming H to the new variables (Q, P) we have

$$H = \frac{\omega}{2}\left(Q^2 + P^2\right), \qquad (*)$$

which treats Q and P on a symmetical basis. Now we have

$$\dot{Q} = \frac{\partial H}{\partial P} = \omega P$$

$$\dot{P} = -\frac{\partial H}{\partial Q} = -\omega Q,$$

or $\ddot{Q} = \omega \dot{P} = -\omega^2 Q$. But if $\ddot{Q} = -\omega^2 Q$, then $\ddot{x} = -\omega^2 x$, since $Q = \sqrt{m\omega}\, x$. The symmetrical form $(*)$ of the harmonic oscillator Hamiltonian is sometimes more useful.

To return to the variables x, p, the general solution of the equations of motion is

$$x = B_0 \cos(\omega t + \phi),$$

where B_0, the real amplitude, satisfies $B_0 = \text{real}, \geq 0$, and where ϕ is the initial phase. The general solution of a 2nd order differential equation must have two constants of integration, and here we have B_0 and ϕ. The 0-subscript on B_0 is just a reminder that it is a constant of motion.

Now let's write the solution in a variety of ways.

$$x = \mathrm{Re}\left[B_0\, e^{-i(\omega t + \phi)}\right]$$

$$= \mathrm{Re}\left[A_0\, e^{-i\omega t}\right], \quad \text{where } A_0 = B_0\, e^{-i\phi}.$$

We will call A_0 the <u>complex amplitude</u>; it contains both the real amplitude and the phase ϕ. Finally let's set

$$A(t) = A_0 e^{-i\omega t},$$

so

$$x(t) = \mathrm{Re}\,[A(t)].$$

As for the momentum, we have $\dot{A} = -i\omega A$, $p = m\dot{x}$,

so

$$p(t) = \mathrm{Re}\,[-im\omega A(t)] = m\omega\, \mathrm{Im}\,[A(t)].$$

The position and momentum are related to the real and imaginary parts of the one complex number $A(t)$.

This may remind you of the creation and annihilation operators in the quantum theory of the harmonic oscillator. The annihilation operator is defined by

$$a = \sqrt{\frac{m\omega}{2\hbar}}\, x + \frac{i\, p}{\sqrt{2m\omega\hbar}}$$

(look this up in a QM book).

Although this definition comes from QM, let's borrow it and use it in the classical harmonic oscillator. Then a is not an operator, it's a number like x and p, and, like them, it's a function of time.

Now $a(t)$ is related to $A(t)$ introduced above. From the above we have

$$\mathrm{Re}\,[A(t)] = x(t)$$
$$\mathrm{Im}\,[A(t)] = p(t)/m\omega,$$

so $$A(t) = x(t) + i\,\frac{p(t)}{m\omega}.$$

But from the definition of a, we have

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right) = \sqrt{\frac{m\omega}{2\hbar}}\, A,$$

$$A = \sqrt{\frac{2\hbar}{m\omega}}\, a.$$

BTW it may seem strange to be using formulas that involve $\hbar$ in classical mechanics, but there's no harm in doing so. If we wanted to we could get rid of them by absorbing a factor of $\sqrt{\hbar}$ into the definition of the (classical) a, but I prefer to keep the same dimensions of a as in the quantum H.O.

Let's also note the expressions for a in terms of the more symmetrical variables Q and P (see (*) on p. 7),

$$a = \frac{Q+iP}{\sqrt{2\hbar}}, \qquad A = \frac{Q+iP}{\sqrt{m\omega}}. \qquad (*)$$

Now let's express the Hamiltonian in terms of the complex variable a. See (*) on p. 8, and note,

$$|a|^2 = aa^* = \frac{Q^2+P^2}{2\hbar}.$$

So we get

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 = \frac{\omega}{2}(Q^2+P^2) = \hbar\omega |a|^2, \qquad (**)$$

The last expression is the classical analog of the quantum formula,

$$H = \hbar\omega\,(a^\dagger a + 1/2).$$

The 1/2 in the quantum formula comes from the fact that a and $a^\dagger$ don't commute, whereas classically a and a^* do commute (everything commutes classically).

Now return to the KG eqn.

$$\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi = -m^2\psi \qquad (\hbar = c = 1).$$

Consider a plane wave,

$$\psi(\vec{x},t) = B_0 \cos(\vec{k}\cdot\vec{x} - \omega t - \phi). \qquad (*)$$

[Aside: The K-G wave fn ψ was originally conceived of, by Schrödinger and Klein and Gordon, as a kind of Schrödinger wave fn. ψ, except applying to a relativistic particle. As such, it should be a complex function. However, later when the proper understanding of the KG equation was achieved, in which ψ is interpreted as a quantum field, it was realized that the KG ψ at the classical level could be either real or complex, depending on the physical interpretation. A real ψ corresponds to a spinless boson that is equal to its own antiparticle, such as the π^0 meson, while a complex ψ corresponds to a spinless boson that is not equal to its antiparticle, because it carries a charge. This corresponds to pair π^+, π^-, for example. We will choose the classical KG field to be real, for simplicity, in order to avoid having to talk about antiparticles.]

Since $\psi(\vec{x},t)$ is real in (*) on p. 11, B_0 = real and ≥ 0, and ϕ is the initial phase. Plugging this into the KG eqn, we find that this plane wave for $\psi(\vec{x},t)$ is a solution if

$$\omega^2 = k^2 + m^2 .$$

This is called the dispersion relation for the KG eqn. If we restore factors of c and $\hbar$, using $E = \hbar\omega$ and $\vec{p} = \hbar k$, this becomes

$$E^2 = c^2 p^2 + m^2 c^4 ,$$

which was the starting point for Schrödinger's derivation of the KG eqn.

In the following we will always assume that ω is a function of $\vec{k}$ given by

$$\omega = \sqrt{k^2 + m^2} . \qquad (*)$$

Sometimes we may write $\omega(\vec{k})$ or $\omega_{\vec{k}}$ to emphasize this. This makes $\omega(\vec{k}) > 0$, and $\omega(\vec{k}) = \omega(-\vec{k})$.

You may worry about the solution

$$\omega = -\sqrt{k^2 + m^2} .$$

These give the "negative energy" solutions of the KG eqn that gave so much trouble when ψ is interpreted as the quantum wave function of a single relativistic particle. We will not need to worry about them, for reasons explained below, and we will always take ω to be given by $(*)$ on p. 12, so that $\omega > 0$.

To return to the plane wave,

$$\psi(\vec{x},t) = B_0 \cos(\vec{k}\cdot\vec{x} - \omega t - \phi),$$

where now $\omega = \omega(\vec{k})$, it is obvious that it is a kind of oscillatory motion that should be describable somehow as a harmonic oscillator. Let us rewrite this in various forms,

$$\psi(\vec{x},t) = \mathrm{Re}\left[B_0 e^{i(\vec{k}\cdot\vec{x} - \omega t - \phi)} \right] \qquad (*)$$

$$= \mathrm{Re}\left[A_0 e^{i(\vec{k}\cdot\vec{x} - \omega t)} \right] \qquad \text{where } A_0 = B_0 e^{-i\phi}$$

$$= \mathrm{Re}\left[A(t) e^{i\vec{k}\cdot\vec{x}} \right], \qquad \text{where } A(t) = A_0 e^{-i\omega t}$$

following the same steps we used for the H.O. and using the same notation.

By differentiating we get

$$\frac{\partial\psi}{\partial t} = \dot{\psi}(\vec{x},t) = \mathrm{Re}\left[-i\omega A e^{i\vec{k}\cdot\vec{x}}\right] = \omega\, \mathrm{Im}\left[A e^{i\vec{k}\cdot\vec{x}}\right]$$

$$\nabla\psi = \mathrm{Re}\left[i\vec{k} A e^{i\vec{k}\cdot\vec{x}} \right] = -\vec{k}\, \mathrm{Im}\left[A e^{i\vec{k}\cdot\vec{x}}\right]$$

where we use $\dot{A} = -i\omega A$.

Let's also write these in real form,

$$\left.\begin{aligned} \psi(\vec{x},t) &= B_0 \cos(\vec{k}\cdot\vec{x} - \omega t - \phi) \\ \frac{\partial\psi}{\partial t} &= \omega B_0 \sin(\vec{k}\cdot\vec{x} - \omega t - \phi) \\ \nabla\psi &= -\vec{k} B_0 \sin(\vec{k}\cdot\vec{x} - \omega t - \phi). \end{aligned}\right\} \quad (*)$$

Now the Hamiltonian for the KG field is (x) on p.6,

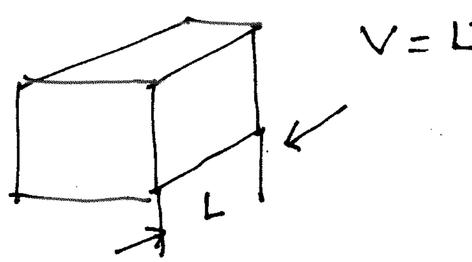
$$H = \frac{1}{2}\int d^3\vec{x}\, \left(\dot{\psi}^2 + (\nabla\psi)^2 + m^2\psi^2 \right),$$

which should give us the energy of our wave if we plug in (*):

$$H\binom{\text{plane}}{\text{wave}} = \frac{1}{2}\int d^3\vec{x} \left[\omega^2 B_0^2 \sin^2\alpha + k^2 B_0^2 \sin^2\alpha + m^2 B_0^2 \cos^2\alpha \right], \quad (**)$$

where $\alpha = \vec{k}\cdot\vec{x} - \omega t - \phi$. But the average of $\sin^2\alpha$ or $\cos^2\alpha$ is $1/2$, so when integrated over all space the result is $H = \infty$. This is not surprising; a plane wave of finite amplitude B_0 fills all space and has a nonzero energy density, so the total energy is infinite. Plane waves are idealizations that are convenient mathematically but which are not very realistic. More realistic is some kind of wave packet, i.e., localized wave function, which can always be represented as linear combinations of plane waves.

To fix this we adopt <u>box normalization</u>. We assume the universe is divided into large boxes of side L and volume $V = L^3$, and that all the physics (waves, particles, etc) is periodic.

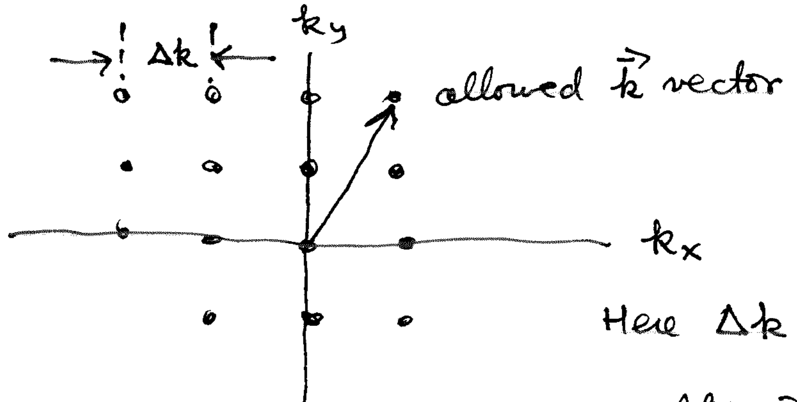


Then we can form localized wave functions in the middle of the box as linear combinations of periodic plane waves. These are repeated in neighboring boxes, but when we take the physical limit $L \to \infty$, $V \to \infty$, we are left with only the box we are in (the whole universe) and the rest disappear.

If the waves are periodic in the box, then the wave vector $\vec{k}$ is restricted to a discrete set of values,

$$\vec{k} = \frac{2\pi}{L} \vec{n},$$

where $\vec{n} = (n_x, n_y, n_z)$ is a vector of integers (positive, negative, or zero). The allowed $\vec{k}$ values form a discrete, cubical lattice in $\vec{k}$-space. Here is a 2-D drawing:



Here $\Delta k = \frac{2\pi}{L}$ = lattice spacing.

The density of lattice points in $\vec{k}$-space (number of points per unit volume in $\vec{k}$-space) is the inverse of the volume of a single cubical cell,

$$\text{density of points} = \frac{\#\text{ points}}{\vec{k}\text{-volume}} = \left(\frac{L}{2\pi}\right)^3 = \frac{V}{(2\pi)^3}.$$

As $L \to \infty$ this density goes to ∞ and the allowed $\vec{k}$-values become a continuum. Box normalization allows us to work with Fourier series, instead of Fourier integrals.

To return to the KG wave, we get a finite energy if we just integrate over the volume of the box:

$$H = \frac{1}{2}\int_{\text{box}} d^3\vec{x}\; B_0^2\left[\omega^2 \sin^2\alpha + k^2 \sin^2\alpha + m^2\cos^2\alpha\right]$$

$$= \frac{V}{4} B_0^2\left(\omega^2 + k^2 + m^2\right) = \frac{V}{2} B_0^2\omega^2,$$

where we use the fact that the average of $\sin^2\alpha$ or $\cos^2\alpha$ is $1/2$, and we use the dispersion relation $\omega^2 = k^2 + m^2$.

This is the energy (within a box) of a single wave. In order to interpret it as a Hamiltonian, we must express it in terms of the variables describing how the wave evolves, and ultimately a set of q's and p's. Because the wave is oscillatory, we expect a harmonic oscillator.

Using (*) on p. 13, $A_0 = B_0 e^{-i\phi}$ and $A(t) = A_0 e^{-i\omega t}$,

we can write H for the wave as

$$H = \frac{V\omega^2}{2} |A|^2 . \qquad (*)$$

If we want to put this into a harmonic oscillator in the symmetric form (*) on p. 8, we have to be able to write this as

$$H = \frac{\omega}{2} (Q^2 + P^2). \qquad (**) .$$

Taking a hint from the ordinary H.O., where A is proportional to $Q + iP$ (see (*) on p. 10), we write (in the case of the wave)

$$A = \sqrt{\frac{1}{\omega V}} (Q + iP),$$

which turns (*) into (**). Then we can borrow (*) from p. 10,

$a = \frac{Q+iP}{\sqrt{2\hbar}}$, to get

$$H = \hbar\omega |a|^2,$$

just like in (**) on p. 10.

In this way we have guessed a Harmonic oscillator Hamiltonian for a single plane wave. To summary, the Hamiltonian is

$$H = \frac{\omega}{2} (Q^2 + P^2) = \hbar |a|^2 \quad \text{where } a = \frac{Q+iP}{\sqrt{2\hbar}},$$

the wave is $\quad \psi(\vec{x}, t) = \mathrm{Re}\left[A(t) e^{i\vec{k}\cdot\vec{x}} \right],$

$$\text{where } A = \frac{1}{\sqrt{\omega V}} (Q + iP).$$

Does this Hamiltonian give the correct equs of evolution for the wave? Well, Hamilton's equs are

$$\dot{Q} = \frac{\partial H}{\partial P} = \omega P$$
$$\dot{P} = -\frac{\partial H}{\partial Q} = -\omega Q$$

so $$\dot{A} = \frac{1}{\sqrt{\omega V}}(\dot{Q} + i\dot{P}) = \frac{1}{\sqrt{\omega V}}\,\omega\,(P - iQ) = -i\omega A.$$

so $$A(t) = A_0 e^{-i\omega t}, \quad \text{and}$$

$$\psi(\vec{x}, t) = \mathrm{Re}\left[A_0 e^{i(\vec{k}\cdot\vec{x} - \omega t)}\right],$$

which is the correct time evolution.

This single harmonic oscillator takes care of a single plane wave with definite $\vec{k}$ (and ~~~~ hence ω since $\omega = \omega(\vec{k})$). It is a particular solution of the KG equ. Of course $\vec{k}$ must lie on one of the lattice points to satisfy periodic boundary conditions.

The general solution is a general linear combination of such solutions,

$$\psi(\vec{x}, t) = \sum_{\vec{k}}' B_{0\vec{k}} \cos(\vec{k}\cdot\vec{x} - \omega t - \phi_{\vec{k}}),$$

where now we allow B_0 and ϕ to depend on $\vec{k}$ (the different waves can have different amplitudes and phases). The sum is taken over all lattice points in $\vec{k}$-space.

We follow the earlier definitions, except now we attach a $\vec{k}$- subscript to indicate which normal mode we are referring to:

$$A_{0\vec{k}} = B_{0\vec{k}}\, e^{-i\phi_{\vec{k}}}$$

$$A_{\vec{k}}(t) = e^{-i\omega_{\vec{k}} t} A_{0\vec{k}}$$

$$\psi(\vec{x},t) = \sum_{\vec{k}} \mathrm{Re}\left\{ B_{0\vec{k}}\, e^{i(\vec{k}\cdot\vec{x}-\omega_{\vec{k}} t - \phi_{\vec{k}})}\right\}$$

$$= \sum_{\vec{k}} \mathrm{Re}\left\{ A_{0\vec{k}}\, e^{i(\vec{k}\cdot\vec{x}-\omega_{\vec{k}} t)}\right\}$$

$$= \sum_{\vec{k}} \mathrm{Re}\left\{ A_{\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{x}}\right\}$$

$$= \frac{1}{2}\sum_{\vec{k}} \left\{ A_{\vec{k}}(t)\, e^{i\vec{k}\cdot\vec{x}} + A^*_{\vec{k}}(t)\, e^{-i\vec{k}\cdot\vec{x}}\right\}.$$

where

$$\dot{A}_{\vec{k}} = -i\omega_{\vec{k}} A_{\vec{k}}.$$

Also we write

$$A_{\vec{k}} = \frac{1}{\sqrt{\omega_{\vec{k}} V}}\left(Q_{\vec{k}} + iP_{\vec{k}}\right)$$

and

$$a_{\vec{k}} = \frac{Q_{\vec{k}} + iP_{\vec{k}}}{\sqrt{2\hbar}}, \quad \text{so} \quad A_{\vec{k}} = \sqrt{\frac{2\hbar}{\omega_{\vec{k}} V}}\, a_{\vec{k}},$$

so the total energy is

$$H = \sum_{\vec{k}} \frac{V\omega_{\vec{k}}^2}{2}|A_{\vec{k}}|^2 = \sum_{\vec{k}} \frac{\omega_{\vec{k}}}{2}\left(Q_{\vec{k}}^2 + P_{\vec{k}}^2\right) = \sum_{\vec{k}} \hbar\omega_{\vec{k}} |a_{\vec{k}}|^2,$$

and the wave itself is

$$\psi(\vec{x}) = \sqrt{\frac{\hbar}{2V}} \sum_{\vec{k}} \frac{1}{\sqrt{\omega_{\vec{k}}}} \left(a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} + a_{\vec{k}}^{*} e^{-i\vec{k}\cdot\vec{x}} \right).$$

This gives us the classical Hamiltonian for the Klein Gordon field as a sum of harmonic oscillators, expressed in terms of Q's and P's that give the right eqns of motion via Hamilton's equations.

To quantize this, we postulate that $Q_{\vec{k}}$ and $P_{\vec{k}}$ become operators that satisfy the commutation relations,

$$[Q_{\vec{k}}, P_{\vec{k}'}] = i\hbar\, \delta_{\vec{k}\vec{k}'}$$

$$[Q_{\vec{k}}, Q_{\vec{k}'}] = [P_{\vec{k}}, P_{\vec{k}'}] = 0.$$

Then with

$$a_{\vec{k}} = \frac{Q_{\vec{k}} + iP_{\vec{k}}}{\sqrt{2\hbar}}, \qquad a_{\vec{k}}^{+} = \frac{Q_{\vec{k}} - iP_{\vec{k}}}{\sqrt{2\hbar}},$$

we have

$$[a_{\vec{k}}, a_{\vec{k}'}^{+}] = \delta_{\vec{k}\vec{k}'}$$

and $[a_{\vec{k}}, a_{\vec{k}'}] = [a_{\vec{k}}^{+}, a_{\vec{k}'}^{+}] = 0.$

Also, the Hamiltonian becomes

$$H = \sum_{\vec{k}} \frac{\omega_{\vec{k}}}{2} \left(Q_{\vec{k}}^2 + P_{\vec{k}}^2 \right) = \sum_{\vec{k}} \hbar\omega_{\vec{k}} \left(a_{\vec{k}}^{+} a_{\vec{k}} + 1/2 \right).$$

Further discussion in class.