Quantization of Klein-Gordon Fields

The real Klein Gordon field is described by the Lagrangian density

$$\mathcal{L}_{RKG} = \frac{1}{2} \partial_\mu \varphi \, \partial^\mu \varphi - \frac{m^2}{2} \varphi^2 \qquad (1)$$

Indeed the Euler-Lagrange equation

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)} - \frac{\partial \mathcal{L}}{\partial \varphi} = 0 \qquad (2)$$

reads, using

$$\frac{\partial \mathcal{L}}{\partial \varphi} = m^2 \varphi \, , \quad \frac{\partial \mathcal{L}}{\partial_\mu \varphi} = \partial^\mu \varphi \, , \qquad (3)$$

$$\partial_\mu \partial^\mu \varphi + m^2 \varphi = 0 \qquad (4)$$

which is the Klein-Gordon equation

The Lagrangian density does not depend explicitly on space and time, i.e., the action integral

$$S = \int dx^\mu \, \mathcal{L}(\varphi, \partial_\mu \varphi) \qquad (5)$$

is invariant under the coordinate transformation (shift in time and position)

$$\Delta X^\mu = A^\mu \quad (\text{constant}) \qquad (6)$$

$$\Delta \Phi = 0 \qquad (7)$$

One can write (6)

$$\Delta X^\mu = X^\mu{}_\nu \, \delta\omega^\nu \qquad (8)$$

where $X^\mu{}_\nu = \delta^\mu{}_\nu$ and $\delta\omega^\nu = A^\nu$

For $\delta\omega^0 \neq 0$, $\delta\vec{\omega} = 0$ holds (9)

according to the Noether theorem

$$\partial_\mu J^\mu{}_0 = 0 \qquad (10)$$

where

$$J^\mu{}_\rho = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)} \Phi_\rho - \Theta^\mu{}_\nu X^\nu{}_\rho \qquad (11)$$

or with (7), (8), (9)

$$J^\mu{}_0 = - \Theta^\mu{}_0 \qquad (12)$$

From (10) follows

$$\partial_t J^0{}_0 = - \nabla \cdot \vec{J}_0 \qquad (13)$$

or after integration, using Gauss theorem and assuming vanishing $\vec{J}$ at ∂V_∞

$$Q_0 = -\int_{V_\infty} d^3x \; J^0{}_0 \quad \text{indep. of time} \qquad (14)$$

It holds

$$J^\mu{}_\nu = -\Theta^\mu{}_\nu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)} \partial_\nu \varphi - \mathcal{L}\, \delta^\mu{}_\nu \qquad (15)$$

and, hence,

$$J^0{}_0 = \frac{\partial \mathcal{L}}{\partial \dot\varphi} \dot\varphi - \mathcal{L} \qquad (16)$$

Altogether, we can state that

$$\int d^3x \left[\frac{\partial \mathcal{L}}{\partial \dot\varphi} \dot\varphi - \mathcal{L} \right] = H \qquad (17)$$

V_α

is conserved. One can interprete H as total energy as it is well known that invariance with respect to time shift $t \to t + \tau$, $\tau = \text{const.}$ is connected with energy conservation.

Momentum Conservation

(H₁)

Likewise, the transformation

$$\vec{x} \to \vec{x} + \vec{a} \qquad \vec{a} \text{ const.} \qquad (18)$$

is connected with momentum conservation.

Prove that the independence of S under (18) implies, according to the Noether theorem, the time-independence (conservation) of

$$\vec{P} = -\int_{V_\infty} d^3x \;\; \dot{\varphi}\, \nabla \varphi \qquad (18)$$

One can further express (17) using (1)

$$H = \int d^3x \left[\dot{\varphi}^2 - \tfrac{1}{2}\dot{\varphi}^2 + \tfrac{1}{2}(\nabla\varphi)^2 + \tfrac{m^2}{2}\varphi^2 \right] \qquad (19)$$

or

$$H = \int d^3x \left[\frac{1}{2}(\partial_t \varphi)^2 + \frac{1}{2}(\nabla\varphi)^2 + \frac{m^2}{2}\varphi^2 \right] \qquad (20)$$

The field energy is positive definite!

The present formulation provides a good starting point for a consistent quantum theory since negative energies, in particular, unbounded negative energies do not arise.

We will now introduce the assumption made to provide a quantum theory of the field $\varphi(x^\mu)$. This will be established by providing a Hamiltonian formulation from the present Lagrangian formulation and the interpreting $\varphi(x)$ as an operator that is specified through certain commutation properties.

Before we proceed with the quantization we recall the solutions of the KGE (see class notes)

$$\psi_0(\vec{k}, \lambda = +1 | x^\mu) = N(\vec{k})\, e^{-i k_\mu x^\mu} \qquad (21)$$

(positive energy solutions, $k_0 = \sqrt{\vec{k}^2 + m^2}$

We simplify the notation

$$\psi_0(\vec{k}, \lambda = + 1 | x^\mu) = f_{\vec{k}}(x^\mu).$$

We define the "scalar product"

$$(\varphi_n | \varphi_m)_{x^0} = i \int\limits_{x^0 \text{ fixed}} d^3x \; \varphi_n^*(x^\mu) \overleftrightarrow{\partial_0} \varphi_m(x^\mu) \qquad (22)$$

where $f \overleftrightarrow{\partial_0} g = f(\partial_0 g) - (\partial_0 f) g \qquad (23)$

This scalar product is independent of time as long as φ_n, φ_m are solutions of the KGE.

Indeed if we consider $\ldots = (\varphi_n | \varphi_m)$

$$\int\limits_{x^0 \text{ fixed}} d^3x \ldots - \int\limits_{x^{0\prime} \text{ fixed}} d^3x \ldots = I \qquad (23)$$

one can write the as

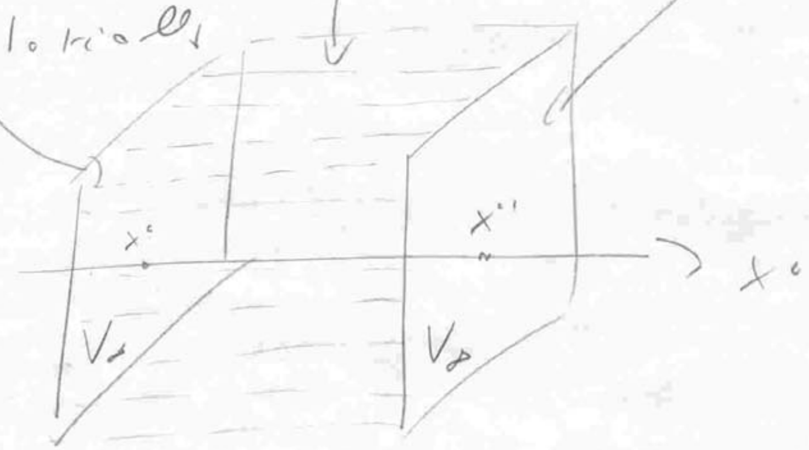
$$\int\limits_{\partial\Omega} d\sigma \ldots = \int\limits_{\Omega} d^4x \underbrace{\partial_\mu \ldots}_{4 \text{ dim. divergence}} \qquad (24)$$

where $\partial\Omega \subset \mathbb{R}^4$ is a surface in $\mathbb{R}^4$

$$\partial\Omega = V_\infty(x^0 \text{ fixed}) \cup V_\infty(x^{0\prime} \text{ fixed}) \qquad (25)$$

$$\cup \{ \text{surface in spatial infinity connecting } x^0 \text{ fixed and } x^{0\prime} \text{ fixed} \}$$

Pictorially



Now we could have written for ... (26)

$\varphi_n^* \overleftrightarrow{\partial^\mu} \varphi_m$ and the surface integral

of $V_\infty(x^0)$ and $V_\infty(x^{0\prime})$ projects out the time component only. Hence, we have shown

$$\langle \varphi_n | \varphi_m \rangle_{x^0} - \langle \varphi_n | \varphi_m \rangle_{x^{0\prime}}$$

$$= \int_\Omega d^4x \; \partial_\mu \left[\varphi_n^* \overleftrightarrow{\partial^\mu} \varphi_m \right]$$

One can readily show $\quad (H_2)$

$$= \int_\Omega d^4x \left\{ \left[(\partial_\mu \partial^\mu + m^2) \varphi_n^* \right] \varphi_m - \varphi_n^* \left[\partial_\mu \partial^\mu + m^2 \right] \varphi_m \right\}$$

which vanishes by assumption

One can show that for H_3

$$f_{\vec{k}} = \frac{1}{\sqrt{(2\pi)^3\, 2E(k)}}\, e^{-i k_\mu x^\mu} \qquad E(k) = k_0 = \sqrt{\vec{k}^2 + m^2}$$
(27)

1) $$\langle f_{\vec{k}} \,|\, f_{\vec{k}'} \rangle = \delta(\vec{k} - \vec{k}') \qquad (28)$$

2) $$\langle f_{\vec{k}} \,|\, f^*_{\vec{k}'} \rangle = 0 \qquad (29)$$

3) $$\langle f^*_{\vec{k}} \,|\, f_{\vec{k}'} \rangle = 0 \qquad (30)$$

The properties derived can be exploited to expand any function $g(x)$, $x \in \mathbb{R}^4$

$$g(x) = \int d^3k \; f_{\vec{k}}(x)\, \alpha(\vec{k})$$
(31)

$$\alpha(\vec{k}| = (f_{\vec{k}} | g)_{t^0} \quad (32)$$

(H_4) Prove (32).

Quantization of the Field

We first illustrate the quantization principle for particle dynamics. In that case we take the steps

1) Define conjugate momentum and Hamiltonian

For $\mathcal{L} = \sum_j \frac{1}{2} m_j \dot{q}_j^2 - V(q_1, \dots, q_N)$ we define

momenta $p_j = \frac{\partial \mathcal{L}}{\partial \dot{q}_j} = m_j \dot{q}_j \quad (33)$

energy $H = \sum_j \frac{\partial \mathcal{L}}{\partial \dot{q}_j} \dot{q}_j - \mathcal{L} = \sum_j \frac{1}{2} m_j \dot{q}_j^2 + V \quad (34)$

$\rightarrow H = \sum_j \frac{p_j^2}{2m_j} + V(q_1, \dots, q_N) \quad (35)$

2) Using Poisson bracket $\{f, g\} = \sum_j \left(\frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q_j} - \frac{\partial f}{\partial q_j} \frac{\partial g}{\partial p_j} \right) \quad (36)$

it holds

$$\{p_j, q_j\} = \delta_{jk} \qquad \dot{F}(q_j, p_j) = \{H, F\} \quad (37)$$

Interpret p_j, q_j, $F(p_j, q_j)$ as operators

$$p_j \to \hat{p}_j \quad q_j \to \hat{q}_j \,, \quad F \to \hat{F} \quad (38)$$

that obey commutation relationships analogous to Poisson bracket properties

$$\{\ ,\ \} \to i[\ ,\ ] \qquad (39)$$

$$i[\hat{p}_j, \hat{q}_j] = \delta_{jk} \qquad (40)$$

$$\dot{\hat{F}} = i[\hat{H}, \hat{F}] \qquad (41)$$

H5 Show that (40) is consistent with $\hat{q}_j$ multiplication, $\hat{p}_j = -i\partial_j$ (42)

Postulate for Field Quantization

Step 1: We define the conjugate momentum (conjugate to $\phi(x)$)

$$\pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi} \qquad (43)$$

and express the Hamiltonian (19)

$$\mathcal{H} = \frac{1}{2}\left\{ \pi^2(x) + (\nabla\phi)^2 + m^2\phi^2 \right\} \qquad (44)$$

Step 2:

We interpret $\hat{\phi}(x^\mu), \hat{\pi}(x^\mu), \hat{H}, \hat{\vec{P}}$ as operators

$$\hat{H} = \int d^3x \left[\frac{1}{2}\left\{ \hat{\pi}^2(x) + (\nabla\hat{\phi})^2 + m^2\hat{\phi}^2 \right\} \right] \qquad (45)$$

$$\hat{\vec{P}} = -\int d^3x \; \hat{\pi}(x) \, \nabla\hat{\phi}(x) \qquad (46)$$

that obey commutation properties

$$i\,[\hat{\pi}(x^\mu),\ \hat{\varphi}(x'^\mu)]_{x^0=x^{0\prime}} = \delta(\vec{x}-\vec{x}') \qquad (47)$$

$$[\hat{\varphi}(x^\mu),\ \hat{\varphi}(x'^\mu)]_{x^0=x^{0\prime}} = 0 \qquad (48)$$

$$[\hat{\pi}(x^\mu),\ \hat{\pi}(x'^\mu)]_{x^0=x^{0\prime}} = 0 \qquad (49)$$

(H_6) Using $P = (\hat{H}, \hat{\vec{P}})$ show (51)

for any $F(x^\mu)$

(a) $$\partial_\mu \hat{F} = i\,[P_\mu, F] \qquad (51)$$

(b) $$F(x'^\mu) = e^{i\hat{P}_\mu (x'^\mu - x^\mu)}\, F(x^\mu)\, e^{-i\hat{P}_\mu (x'^\mu - x^\mu)} \qquad (52)$$

Normal modes

We expand now the field operator $\hat{\varphi}(x^\mu)$ in terms of new operators $\hat{a}(\vec{k})$, $\hat{a}^+(\vec{k})$ using the basis functions $f_{\vec{k}}(x^\mu)$ (27)

$$\hat{\varphi}(x) = \int d^3k \left[f_{\vec{k}}(x)\,\hat{a}(k) + f^*_{\vec{k}}(x)\,a^+(k) \right] \quad (53)$$

Note that $\hat{\varphi}(x)$ is hermitean (self-adjoint) if $\hat{a}^+(\vec{k})$ is the adjoint to $a(\vec{k})$! As an operator $\hat{\varphi}(x)$ should be self-adjoint since it represents a real field (note that a self adjoint operator always real eigenvalues!)

From (28) – (30) follows

$$\hat{a}(k) = i \int d^3x \, f^*_{\vec{k}}(x) \overleftrightarrow{\partial_0} \hat{\varphi}(x) \tag{54}$$

$$\hat{a}^+(k) = -i \int d^3x \, f_{\vec{k}}(x) \overleftrightarrow{\partial_0} \hat{\varphi}(x) \tag{55}$$

$\hat{a}(k)$ and $\hat{a}^+(k)$ thus defined are independent of time. Indeed

$$\partial_0 a(\vec{k}) = i \int d^3x \left[f^*_{\vec{k}}(x) \left(\partial_0^2 \hat{\varphi}(x)\right) - \left(\partial_0^2 f^*_{\vec{k}}(x)\right) \hat{\varphi}(x) \right] \tag{56}$$

Using that $f_{\vec{k}}(x)$ and $\hat{\varphi}(x)$ obey the KGE yields

$$= i \int d^3x \left[f^*_{\vec{k}}(x) \nabla^2 \vec{\varphi}(\vec{x}) - (\nabla^2 f^*_{\vec{k}}(x)) \vec{\varphi} \right] \quad (57)$$

Green's 2nd theorem yields a surface integral that should vanish since the surface is at infinity.

The commutator $[\hat{a}(\vec{k}), \hat{a}^+(\vec{k}')]$

To determine this commutator we employ the expressions (48), (49)

$$[\hat{a}(\vec{k}), \hat{a}^+(\vec{k}')]_- = -i^2 \int d^3x \int d^3y \quad (58)$$

$$f^*_{\vec{k}}(x)\, f^*_{\vec{k}'}(y) \overleftrightarrow{\frac{\partial}{\partial x_0}} \overleftrightarrow{\frac{\partial}{\partial y_0}} [\hat{\varphi}(x), \hat{\varphi}(y)]_-$$

Using (54), (55) and (43) —

$$= i^2 \int d^3x \int d^3y\, f^*_{\vec{k}}(x) \left(\partial_0 f^*_{\vec{k}'}(y)\right) [\hat{\pi}(x), \hat{\varphi}(y)]$$

$$+ i^2 \int d^3x \int d^3y\, \left(\partial_0 f^*_{\vec{k}}(x)\right) f_{\vec{k}'}(y) [\hat{\varphi}(x), \hat{\pi}(y)]$$

Using (47), (28)

$$= i \int d^3x\, f^*_{\vec{k}}(x) \overleftrightarrow{\partial_0} f_{\vec{k}'}(x)$$

$$= \delta(\vec{k} - \vec{k}')$$

Hence,

$$[\hat{a}(\vec{k}), \hat{a}^+(\vec{k}')]_{k^0 = k^{0\prime}} = \delta(\vec{k} - \vec{k}')$$

(H_7) Show similarly,

$$[\hat{a}(\vec{k}), \hat{a}(\vec{k}')]_{k^0 = k^{0\prime}} = [\hat{a}^+(\vec{k}), \hat{a}^+(\vec{k}')]_{k^0 = k^{0\prime}} = 0$$

H_8

Using the expansion (53) in

$$\hat{H} = \int d^3x \; \frac{1}{2}\left[(\partial_0 \hat{\varphi})^2 + (\nabla \hat{\varphi})^2 + m^2 \hat{\varphi}^2\right]$$

show

H_8

$$\hat{H} = \frac{1}{2} \int d^3k \; E(\vec{k}) \left[\hat{a}^+(\vec{k}) \, \hat{a}(\vec{k}) + \hat{a}(\vec{k}) \, \hat{a}^+(\vec{k})\right]$$

and similarly

$H8$

$$\vec{P} = \frac{1}{2} \int d^3k \; \vec{k} \left[\hat{a}^+(\vec{k}) \, \hat{a}(\vec{k}) + \hat{a}(\vec{k}) \, \hat{a}^+(\vec{k})\right]$$

Note: you will find advice on doing these two derivations on the Phys. 483 web site!
