3. Relativistic formulations

3.1. Klein-Gordon equation

In the following we want to construct a formalism for relativistic non-interacting spin-0 bosons
(why non-interacting theories are important - in spite of the fact that quantum objects typically do interact - is motivated in section 2.4. about perturbation theory)

We first recall the formalism to describe non-relativistic many-body systems (without interactions):

equation of motion:

$$i\hbar \frac{\partial}{\partial t} \underbrace{\varphi_{n.r.}}_{\text{"non-relativistic"}}(\vec{r},t) = -\frac{\hbar^2 \Delta_r}{2m} \varphi_{n.r.}(\vec{r},t) \qquad (*)$$

for the annihilation operator $\varphi_{n.r.}$ (i.e. $\varphi_{n.r.}(\vec{r},t)|0\rangle = 0$)

commutation relations:

$$\left[\varphi_{n.r.}(\vec{r},t), \varphi_{n.r.}(\vec{r}\,',t)\right] = 0 = \left[\varphi^{+}_{n.r.}(\vec{r},t), \varphi^{+}_{n.r.}(\vec{r},t)\right]$$

$$\left[\varphi_{n.r.}(\vec{r},t), \varphi^{+}_{n.r.}(\vec{r}\,',t)\right] = \delta(\vec{r}-\vec{r}\,')$$

Note that $\varphi_{n.r.}$ is not hermitian ($\varphi_{n.r.} \neq \varphi^{+}_{n.r.}$) - otherwise already $(*)$ would have no (non-trivial) solution.

General solution of $(*)$: superposition of plane waves

$$\varphi_{n.r.}(\vec{r},t) = \int \frac{d^3p}{(2\pi\hbar)^3}\, a_{n.r.}(\vec{p})\, e^{-i(\tilde{E}_p t - \vec{p}\cdot\vec{r})/\hbar} \quad \text{with } \tilde{E}_p = \frac{\vec{p}^{\,2}}{2m}$$

Note that only with the relation between (kinetic) energy and momentum

$$\tilde{E}_p = \frac{\vec{p}^{\,2}}{2m}$$

one obtains a solution for (*). Formally one can identify

$$i\hbar \frac{\partial}{\partial t} \rightarrow \hat{E} \;, \quad \frac{\hbar}{i}\vec{\nabla} \rightarrow \hat{\vec{p}}$$

$$\Rightarrow (*) \rightsquigarrow \hat{E}\, f_{n.r.} = \frac{\hat{\vec{p}}^{\,2}}{2m} f_{n.r.}$$

Now we look for an equation of motion which yields the <u>relativistic</u> energy-momentum relation

$$E_p^2 = c^2 \vec{p}^{\,2} + c^4 m^2 \quad \text{with (vacuum) speed of light } c$$

In the following we set for convenience $c = 1$ which is possible since c is a constant of nature (always and everywhere the same according to present-day knowledge)

$$\Rightarrow \quad E_p^2 = \vec{p}^{\,2} + m^2$$

If $|\vec{p}| \ll m$ one gets the non-relativistic limit:

$$E_p = \sqrt{m^2 + \vec{p}^{\,2}} = m \underbrace{\sqrt{1 + \frac{\vec{p}^{\,2}}{m^2}}}_{\approx 1 + \frac{\vec{p}^{\,2}}{2m^2}} \approx \underset{\substack{\uparrow \\ \text{rest energy}}}{m} + \underset{\substack{\uparrow \\ \text{kinetic energy}}}{\frac{\vec{p}^{\,2}}{2m}}$$

$|\vec{p}| \ll m$

Note: A relativistic theory is always a many-body theory since mass can be transformed to energy and vice versa (at least in the presence of interactions). Therefore we look for a generalization of (*) and not of the one-body Schrödinger equation (see page 23).

from $E_p^2 = \vec{p}^{\,2} + m^2$ and $E \to i\hbar \frac{\partial}{\partial t}$, $\vec{p} \to \frac{\hbar}{i}\vec{\nabla}$

one gets the Klein-Gordon equation

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \phi(t,\vec{r}) = -\hbar^2 \Delta_r \phi(t,\vec{r}) + m^2 \phi(t,\vec{r})$$

or with $x = (t, \vec{r})$ and $\mu = \frac{m}{\hbar}$

$$\boxed{\frac{\partial^2}{\partial t^2} \phi(x) = \Delta \phi(x) - \mu^2 \phi(x)}$$

(note that $\mu = \frac{m}{\hbar}$ has the dimension of inverse length or time; it is the lowest possible frequency in the dispersion relation

$$\underset{\text{frequency}}{\omega}^2 = \underset{\text{wave number}}{\vec{k}}^2 + \mu^2$$
)

We have generalized the equation of motion from a non-relativistic to a relativistic formulation. In addition, we have to generalize the commutation relations. More generally we have to figure out the meaning of ϕ as an operator in Fock space.

First, we note that $\phi(x)$ can be hermitian (in contrast to $\rho_{n.r.}$). Even if it is not, one can construct

$$\mathrm{Re}\,\phi := \frac{\phi + \phi^+}{2} \text{ and } \mathrm{Im}\,\phi = \frac{\phi - \phi^+}{2i}$$

Both quantities satisfy a Klein-Gordon equation and are not mixed.

$\rightsquigarrow$ study Klein-Gordon equation for a hermitian $\phi = \phi^+$ (simplest case)

$\rightsquigarrow$ solution: $$\phi(t,\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{1}{2E_p} \left[a(\vec{p})\, e^{-i(E_p t - \vec{p}\cdot\vec{r})/\hbar} + a^+(\vec{p})\, e^{i(E_p t - \vec{p}\cdot\vec{r})/\hbar} \right]$$

with $E_p = \sqrt{\vec{p}^2 + m^2}$

Note: instead of $a(\vec{p})$ one could have introduced $\tilde{a}(\vec{p}) := \frac{a(\vec{p})}{2E_p}$ to make the solution looking more similar to the non-relativistic solution $\rho_{n.r.}$ at page $\boxed{1}$ bottom.

However $\frac{d^3p}{2E_p}$ is Lorentz invariant, while d^3p is not.

(In the exercises it will be shown that all appearing structures, i.e. $\frac{d^3p}{2E_p}$ and the phase $(E_p t - \vec{p}\cdot\vec{r})$ are Lorentz invariant.)

To figure out the meaning of ϕ as an operator, we study the limiting case which we understand already, i.e. the non-relativistic limit. It concerns the modes with small $\vec{p}$.

$\rightsquigarrow$ reconstruct $a(\vec{p})$ from ϕ:

$$\int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\phi(t,\vec{r}) = \int d^3r\, e^{-i\vec{p}\cdot\vec{r}}\int \frac{d^3p'}{(2\pi\hbar)^3\, 2E_{p'}}\left[a(\vec{p}')e^{-i(E_{p'}t-\vec{p}'\cdot\vec{r})/\hbar} + a^+(\vec{p}')e^{+i(\dots)}\right]$$

$$= \int \frac{d^3p'}{2E_{p'}}\left[e^{-iE_{p'}t/\hbar}\delta(\vec{p}-\vec{p}')\,a(\vec{p}') + e^{+iE_{p'}t/\hbar}\delta(\vec{p}+\vec{p}')\,a^+(\vec{p}')\right]$$

$$= \frac{1}{2E_p}\left(e^{-iE_pt/\hbar}a(\vec{p}) + e^{iE_pt/\hbar}a^+(-\vec{p})\right)$$

$$\Rightarrow \int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\dot{\phi}(t,\vec{r}) = \frac{-i}{2\hbar}\left(e^{-iE_pt/\hbar}a(\vec{p}) - e^{iE_pt/\hbar}a^+(-\vec{p})\right)$$

$$\Rightarrow E_p e^{+iE_pt/\hbar}\int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\phi(t,\vec{r}) + i\hbar e^{iE_pt/\hbar}\int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\dot{\phi}(t,\vec{r})$$

$$= \frac{1}{2}a(\vec{p}) + \frac{1}{2}e^{2iE_pt/\hbar}a^+(-\vec{p}) + \frac{1}{2}a(\vec{p}) - \frac{1}{2}e^{2iE_pt/\hbar}a^+(-\vec{p})$$

$$= a(\vec{p})$$

$$\Rightarrow a(\vec{p}) = \int d^3r \; e^{+i(E_p t - \vec{p}\cdot\vec{r})/\hbar} \left(E_p \,\phi(t,\vec{r}) + i\hbar\, \dot{\phi}(t,\vec{r}) \right)$$

for small $\vec{p}$ one might approximate $E_p \approx m + \frac{p^2}{2m}$ or even $E_p \approx m$

$$a(\vec{p}) \approx \int d^3r \; e^{i(\tilde{E}_p t - \vec{p}\cdot\vec{r})/\hbar} \; e^{i\mu t} \left(m\,\phi(t,\vec{r}) + i\hbar\,\dot{\phi}(t,\vec{r}) \right)$$

If $a(\vec{p})$ is similar to $a_{n.r.}(\vec{p})$ (up to a proportionality factor), then

$$\tilde{\varphi}(t,\vec{r}) := e^{i\mu t}\left(m\,\phi(t,\vec{r}) + i\hbar\,\dot{\phi}(t,\vec{r}) \right)$$

might be related to $\varphi_{n.r.}(t,\vec{r})$.

A non-relativistic situation concerns a system where large momenta do not play a role, i.e. states with large momenta are not excited. Concerning waves this means that one can ignore high-frequency modes. Indeed $\phi(t,\vec{r})$ only has large frequencies, the lowest one is μ, but in the construction of $\tilde{\varphi}$ this is compensated by the factor $e^{i\mu t}$

$\rightsquigarrow$ equation of motion for $\tilde{\varphi}$:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t}\tilde{\varphi}(t,\vec{r}) &= -m\, e^{i\mu t}\left(m\,\phi(t,\vec{r}) + i\hbar\,\dot{\phi}(t,\vec{r}) \right) \\ &\quad + e^{i\mu t}\left(i m\hbar\,\dot{\phi}(t,\vec{r}) - \hbar^2\,\ddot{\phi}(t,\vec{r}) \right) \\ &= e^{i\mu t}\left(-\hbar^2\ddot{\phi} - m^2\phi \right) \\ &= e^{i\mu t}\left(-\hbar^2 \Delta \phi \right) \end{aligned}$$

$$\left.\begin{aligned} &\text{from } \tilde{\varphi} = e^{i\mu t}\left(m\,\phi + i\hbar\,\dot{\phi} \right) \\ &\Rightarrow \tilde{\varphi}^{+} = e^{-i\mu t}\left(m\,\phi - i\hbar\,\dot{\phi} \right) \end{aligned}\right\} \Rightarrow \phi = \frac{1}{2m}\left(e^{-i\mu t}\,\tilde{\varphi} + e^{i\mu t}\,\tilde{\varphi}^{+} \right)$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \tilde{\varphi} = -\hbar^2 \Delta \left[\frac{1}{2m} \tilde{\varphi} + \frac{1}{2m} e^{2i\mu t} \tilde{\varphi}^+ \right]$$

If only slowly oscillating modes are relevant, one can ignore the fastly oscillating part $e^{2i\mu t} \tilde{\varphi}^+$ and gets the non-relativistic equation of motion

$$i\hbar \frac{\partial}{\partial t} \tilde{\varphi} = -\frac{\hbar^2 \Delta}{2m} \tilde{\varphi} \quad (+ \text{ fastly oscillating part})$$

Therefore we identify $\tilde{\varphi}$ with $\varphi_{n.r.}$ up to a normalization constant and demand

$$[\tilde{\varphi}(t,\vec{r}), \tilde{\varphi}(t,\vec{r}\,')] = 0$$

$$[\tilde{\varphi}(t,\vec{r}), \tilde{\varphi}^+(t,\vec{r}\,')] = N\,\delta(\vec{r}-\vec{r}\,')$$

$$\Rightarrow [\phi(t,\vec{r}), \phi(t,\vec{r}\,')] = \frac{1}{4m^2} \Big(e^{-2i\mu t} [\tilde{\varphi}(t,\vec{r}), \tilde{\varphi}(t,\vec{r}\,')] + e^{2i\mu t} [\tilde{\varphi}^+(t,\vec{r}), \tilde{\varphi}^+(t,\vec{r}\,')] + [\tilde{\varphi}(t,\vec{r}), \tilde{\varphi}^+(t,\vec{r}\,')] + [\varphi^+(t,\vec{r}), \tilde{\varphi}(t,\vec{r}\,')] \Big)$$

$$= \frac{1}{4m^2} \left(N\,\delta(\vec{r}-\vec{r}\,') - N\,\delta(\vec{r}\,'-\vec{r}) \right) = 0$$

whereas

$$[\phi(t,\vec{r}), \dot{\phi}(t,\vec{r}\,')] = \frac{1}{4m} \frac{+i}{\hbar} \Big(e^{-2i\mu t} [\tilde{\varphi}(t,\vec{r}), \tilde{\varphi}(t,\vec{r}\,')] - e^{2i\mu t} [\tilde{\varphi}^+(t,\vec{r}), \tilde{\varphi}^+(t,\vec{r}\,')] - [\tilde{\varphi}(t,\vec{r}), \tilde{\varphi}^+(t,\vec{r}\,')] + [\tilde{\varphi}^+(t,\vec{r}), \tilde{\varphi}(t,\vec{r}\,')] \Big)$$

$$= \frac{+i}{4m\hbar} 2N\,\delta(\vec{r}-\vec{r}\,')$$

without explicit proof: $[\dot{\phi}(t,\vec{r}), \dot{\phi}(t,\vec{r}\,')] = 0$

It is convenient to choose $N = 2\hbar m$

$\Rightarrow$ Klein-Gordon theory:

equation of motion:

$$\hbar^2 \frac{\partial^2}{\partial t^2}\phi - \hbar^2 \triangle \phi = -m^2 \phi$$

commutation relations:

$$[\phi(t,\vec{r}), \phi(t,\vec{r}\,')] = 0 = [\dot\phi(t,\vec{r}), \dot\phi(t,\vec{r}\,')]$$

$$[\phi(t,\vec{r}), \dot\phi(t,\vec{r}\,')] = i\,\delta(\vec{r}-\vec{r}\,')$$

from the mode decomposition

$$\phi(t,\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3\, 2E_p}\left(a(\vec{p})\, e^{-i(E_p t - \vec{p}\cdot\vec{r})/\hbar} + a^+(\vec{p})\, e^{i(E_p t - \vec{p}\cdot\vec{r})/\hbar}\right)$$

we demand in analogy to the non-relativistic theory

$$a(\vec{p})|0\rangle = 0$$

and define the single-particle momentum eigen states

$$|\vec{p}\rangle := a^+(\vec{p})|0\rangle$$

(their energy is $E_p = \sqrt{\vec{p}^{\,2} + m^2}$)

From the commutation relations it follows

$$[a(\vec{p}), a^+(\vec{p}\,')] = 2E_p\,(2\pi\hbar)^3\,\delta(\vec{p}-\vec{p}\,')$$

(a different choice for the normalisation would modify this relation and the next one)

$\Rightarrow$ normalisation of momentum modes:

$$\langle \vec{p}\,' | \vec{p}\rangle = \langle 0 | a(\vec{p}\,')\, a^+(\vec{p}) | 0\rangle \underset{a|0\rangle = 0}{=} \langle 0 | [a(\vec{p}\,'), a^+(\vec{p})] | 0 \rangle = \underbrace{2E_p (2\pi\hbar)^3 \delta(\vec{p}-\vec{p}\,')}_{\text{Lorentz invariant}}$$

Again one can construct observables from ϕ (and $\dot{\phi}$).
For example we define the operator of total momentum. Since we want that the action of such operators on the vacuum should yield zero, it is convenient to use the normal-ordering operation.

Guess: $\vec{P} = : \frac{1}{N}\int d^3r\, \tilde{\rho}^+(\vec{r},t)\, \frac{\hbar}{i}\vec{\nabla}\, \tilde{\rho}(\vec{r},t) :$

$$= \frac{1}{2im}\int d^3r : \tilde{\rho}^+(\vec{r},t)\, \vec{\nabla}\, \tilde{\rho}(\vec{r},t) :$$

$$= \frac{1}{2im}\int d^3r : (m\phi - i\hbar\dot{\phi})\, \vec{\nabla}\, (m\phi + i\hbar\dot{\phi}) :$$

$$= \frac{1}{2im}\int d^3r : m^2 \phi\vec{\nabla}\phi + \hbar^2 \dot{\phi}\vec{\nabla}\dot{\phi} - im\hbar\dot{\phi}\vec{\nabla}\phi + im\hbar\phi\vec{\nabla}\dot{\phi} :$$

since $\vec{\nabla} :\phi^2: = :(\vec{\nabla}\phi)\phi + \phi\vec{\nabla}\phi: = 2 :\phi\vec{\nabla}\phi:$

$$\Rightarrow \int d^3r : \phi\vec{\nabla}\phi : = 0$$

$$\Rightarrow \vec{P} = \frac{1}{2}\int d^3r : -\dot{\phi}\vec{\nabla}\phi + \phi\vec{\nabla}\dot{\phi} :$$

$$= : -\int d^3r\, \dot{\phi}\vec{\nabla}\phi :$$

partial integration in second term