Quantum mechanics II
Sheet 11

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Exercise 11.1 About the one-particle interpretation of the Klein-Gordon equation

a) The dynamics of non-relativistic free particles is described by the Schrödinger equation,

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi,$$

which may be obtained from the classical, non-relativistic energy-momentum relation $E = \mathbf{p}^2/2m$ using the correspondence principle, i.e.,

$$E \to i\hbar\partial_t \quad \text{and} \quad \mathbf{p} \to -i\hbar\nabla.$$

In a similar way, starting from the relativistic energy-momentum relation,

$$E^2 = c^2\mathbf{p}^2 + m^2c^4, \tag{1}$$

derive the Klein-Gordon equation which captures the physics of relativistic massive spin-0 particles. What is the corresponding equation in the presence of an electromagnetic field?

Hint: Recall that in classical mechanics, an electro-magnetic field is taken into account by making the substitutions $E \to E - e\Phi$ and $\mathbf{p} \to \mathbf{p} - e\mathbf{A}/c$, with Φ and $\mathbf{A}$ the scalar and vector potential, respectively.

b) For the Klein-Gordon equation the quantity $\int_V d\mathbf{r}\, \Psi^*(t,\mathbf{r})\Psi(t,\mathbf{r})$ (with system volume V) generally changes in time and it is therefore not possible to interpret $\Psi^*(t,\mathbf{r})\Psi(t,\mathbf{r})$ as being the probability density for finding a particle at point $\mathbf{r}$. Using the Klein-Gordon equation it can be shown that the quantities

$$\rho(t,\mathbf{r}) = \frac{i\hbar}{2mc^2}\big(\Psi^*\partial_t\Psi - \Psi\partial_t\Psi^*\big) \text{ and} \tag{2}$$

$$\mathbf{j}(t,\mathbf{r}) = \frac{\hbar}{2im}\big(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\big) \tag{3}$$

satisfy the continuity equation, $\partial_t\rho + \nabla\cdot\mathbf{j} = 0$. Verify this and use the continuity equation to prove that $\int_V d\mathbf{r}\, \rho(t,\mathbf{r})$ is constant in time. The quantity (2) is not semi-positive definite as expected for a particle probability density. Thus, the Klein-Gordon equation does not receive an interpretation as a one-particle quantum theory.

Exercise 11.2 About the real Klein-Gordon field and its quantization

The last exercise uncovered two serious problems with the one-particle interpretation of the solutions of the Klein-Gordon (KG) equation: First, the occurrence of negative energy solutions and second, the probabilistic interpretation of the continuity equation is not meaningful. The goal of the present exercise is to learn about the field theory perspective on the *real* solutions of the KG equation (the last exercise also considered the complex solutions). To this purpose we first interpret the real solutions

$$\phi(t,\mathbf{x}) = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_\mathbf{k}}}\left(a_k e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_\mathbf{k}t)} + a_k^\dagger e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_\mathbf{k}t)}\right) \tag{4}$$

($\hbar \equiv c \equiv 1$) of the KG equation as *classical fields*[1] with $\omega_\mathbf{k} = \sqrt{\mathbf{k}^2+m^2}$ and not as wave functions. Afterwards we are quantizing this classical field theory to get a *quantum field theory*

[1] In general a function from space-time to $\mathbb{C}^n$ (here: from space-time to $\mathbb{R}$); a known example is the "4-vector potential" from classical electrodynamics.

(in analogy with the quantization of classical mechanics) which describes a quantum mechanical many-body system.

a) (*Dynamics*) The dynamics of classical KG fields is described by the KG equation. As in classical mechanics we can derive the equation of motion from the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} = 0 \tag{5}$$

corresponding to a *Lagrange density* $\mathcal{L}$. Show that the choice

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi) - \frac{1}{2} m^2 \phi^2 \tag{6}$$

leads to the KG equation using (5). Show that the ϕ and $\pi := \dot{\phi}$ are canonically conjugate fields with respect to $\mathcal{L}$ i.e., $(\partial \mathcal{L} / \partial \dot{\phi}) = \dot{\phi}$, $\dot{\phi} \equiv \partial_0 \phi$. As in classical mechanics we can apply a Legendre transformation replacing $\dot{\phi}$ with π in $\mathcal{L}$ to get the so called *Hamilton density* $\mathcal{H}$ (the observable "energy per volume"). Show that

$$\mathcal{H} = \pi \dot{\phi} - \mathcal{L} = \frac{1}{2}\pi^2 + \frac{1}{2}(\nabla \phi)^2 + \frac{1}{2} m^2 \phi^2 \tag{7}$$

in case of KG fields. The *Hamilton operator* H (the observable "energy") associated to $\mathcal{H}$ is given by $H = \int d^3x \, \mathcal{H}$.

b) (*Canonical Quantization*) Canonical quantization means that one replaces the canonically conjugate quantities in the classical field theory by operators acting on a Hilbert space such that the canonical (or Heisenberg) commutation relations are satisfied. In our case we have to demand

$$\begin{aligned} &[\phi(t, \mathbf{x}), \pi(t, \mathbf{x}')] = i\delta(\mathbf{x} - \mathbf{x}'), \\ &[\phi(t, \mathbf{x}), \phi(t, \mathbf{x}')] = [\pi(\mathbf{x}, t), \pi(\mathbf{x}', t)] = 0 \end{aligned} \tag{8}$$

at equal times. The emergence of the delta function instead of the identity can be understood by rewriting the field theory as the continuum limit of a "field" theory on a lattice. Show that the demand (8) is equivalent to the demand

$$\begin{aligned} &[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = \delta(\mathbf{k} - \mathbf{k}'), \\ &[a_{\mathbf{k}}, a_{\mathbf{k}'}] = [a_{\mathbf{k}}^\dagger, a_{\mathbf{k}'}^\dagger] = 0. \end{aligned} \tag{9}$$

c) As in the lecture we are assuming the existence of a state $|0\rangle$ with the property $a_k|0\rangle = 0$. Try to justify

$$\phi^\dagger(t, \mathbf{x})|0\rangle = \phi(t, \mathbf{x})|0\rangle = |x\rangle. \tag{10}$$

d) Prove that the Hamilton operator H is of the form

$$H = \int d^3k \, \omega_k \left[a_k^\dagger a_k + \frac{1}{2}\delta(0) \right] + [\text{time-dependent terms}]. \tag{11}$$

It will be shown in the quantum field theory lecture why the time-dependent terms can be set to zero. Note that the operator H is positive definite. The first problem of the one-particle wave function interpretation of the solutions of the KG equation thus doesn't emerge in the field theory perspective.