VI.3 Klein-Gordon equation and relativistic single-particle quantum mechanics

We noted at the beginning of chapter VI that relativistic wave equations have the potential difficulty that a localization of a wavepacket to length scales of the Compton length can produce particle pairs. This would lead to a violation of particle number conservation and is incompatible with a single-particle quantum mechanics. So we have to discuss in what respect and under what conditions such a picture is valid.

a reminder:

non-relativistic QM	Schrödinger wave mechanics
$\vert\psi\rangle \in \mathcal{H}$	$\psi(\vec{r}) \in \mathcal{L}^{(2)}(\mathbb{R}^3)$
$\hat{O}, \hat{\vec{r}}, \hat{\vec{p}}$	$O_D, r, \frac{\hbar}{i}\vec{\nabla}$
$\langle\psi\vert\psi'\rangle$	$\int d^3r \; \psi^*(\vec{r})\,\psi'(\vec{r})$
$\langle\psi\vert\hat{O}\vert\psi\rangle$	$\int d^3r \; \psi^*(\vec{r})\big(O_D\,\psi(\vec{r})\big)$

$$|\psi(t)\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle$$

with $i\hbar \frac{d\hat{U}(t,t_0)}{dt} = \hat{H}\,\hat{U}(t,t_0)$

i.e.

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle \qquad i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H_D\,\psi(\vec{r},t)$$

$\Rightarrow$ what is the correspondence for a Klein-Gordon field?

(A) Formal relativistic quantum mechanics

guess: use Schrödinger representation

(397) $$i\hbar\frac{\partial}{\partial t}\underline{\Psi} = \hat{H}\,\underline{\Psi} \qquad \underline{\Psi} = \begin{pmatrix}\varphi\\ \chi\end{pmatrix}$$

but:
- $\hat{H}^+ \neq \hat{H}$ i.e. $\hat{H}$ not Hermitian (in the original sense)
- we have seen that the charge density can be represented as

$$\rho = \underline{\Psi}^+ \sigma_z \underline{\Psi}$$

or the charge

(398) $$Q = \int d^3x\; \underline{\Psi}^+ \sigma_z \underline{\Psi}$$

$\Rightarrow$

Def: generalized scalar product

(399) $$\langle \underline{\Psi} | \underline{\Psi}' \rangle_\phi \equiv \int d^3x\; \underline{\Psi}^+ \sigma_z \underline{\Psi}'$$

Def expectation value

(400) $$\langle\psi|\hat{O}|\psi\rangle_\phi \equiv \int d^3x \; \Psi^\dagger \sigma_z \hat{O} \Psi$$

Def.: an operator $\hat{U}$ is called ϕ-unitary or generalized unitary iff

(401) $$\langle \hat{U}\psi|\hat{U}\psi'\rangle_\phi = \int d^3x \; \Psi^\dagger U^\dagger \sigma_z U \Psi' \stackrel{!}{=} \langle\psi|\psi'\rangle_\phi = \int d^3x \; \Psi^\dagger \sigma_z \Psi'$$

i.e. if

(402) $$\boxed{U^\dagger \sigma_z U = \sigma_z}$$

or

$$\boxed{U^\dagger \sigma_z = \sigma_z U^{-1}}$$

or using $\sigma_z^2 = \mathbb{1}$

(403) $$\boxed{\sigma_z U^\dagger \sigma_z = U^{-1}}$$

Def: an operator $\hat{L}$ is called ϕ-hermitian or generalized hermitian

(404) iff $$\boxed{\sigma_z \hat{L}^\dagger \sigma_z = \hat{L}}$$

The Hamiltonian (of the Schrödinger representation) of the K-G field, eq. (352)

$$\hat{H} = (\sigma_z + i\sigma_y)\frac{\hat{\vec{p}}^2}{2m_0} + \sigma_z m_0 c^2$$

fulfills this condition

(405) $$\hat{H}^+ = (\sigma_z - i\sigma_y)\frac{\hat{\vec{p}}^2}{2m_0} + \sigma_z m_0 c^2 = \sigma_z \hat{H} \sigma_z \quad \checkmark$$

$\boxed{\text{expectation values of } \phi\text{-hermitian operators evaluated according to eq. (400) are real}}$

<u>proof:</u> $$\langle \hat{L} \rangle_\phi = \int d^3x \, \underline{\Psi}^+ \sigma_z \hat{L} \underline{\Psi}$$

$$\langle \hat{L} \rangle_\phi^* = \int d^3x \, \underline{\Psi}^+ \hat{L}^+ \sigma_z \underline{\Psi} = \langle \hat{L} \rangle_\phi$$

since $\sigma_z \hat{L} \sigma_z = \hat{L}^+$ or $\sigma_z \hat{L} = \hat{L}^+ \sigma_z$

remark: If $\hat{O}$ is ϕ-hermitian than

(406) $$\boxed{\hat{\bar{O}} \equiv \sigma_z \hat{O}}$$

is hermitian in the usual sense!

$$\hat{\bar{O}}^+ = (\sigma_z \hat{O})^+ = \hat{O}^+ \sigma_z = \sigma_z \hat{O} = \hat{\bar{O}} \quad \square$$

From these consideration we can now formulate the analogy to formal quantum mechanics

(i) observables are ϕ-hermitian operators

(ii) the dynamics is described by a ϕ-unitary transformation

$$\Psi(t) = e^{-i\hat{H}t/\hbar}\,\Psi(0) \tag{407}$$

$$i\hbar\,\partial_t \Psi(t) = \hat{H}\,\Psi(t) \tag{408}$$

(409) and $\hat{S}(t) \equiv e^{-i\hat{H}t/\hbar}$ is ϕ unitary

$$\sigma_z \hat{S}^{+} \sigma_z = \sigma_z \left(e^{-i\hat{H}t/\hbar}\right)^{+} \sigma_z$$

$$= \sigma_z\, e^{+i\hat{H}^{+}t/\hbar}\,\sigma_z$$

$$= \sigma_z \left[1 + \frac{i\hat{H}^{+}t}{\hbar} + \left(\frac{it}{\hbar}\right)^2 \frac{1}{2!}\hat{H}^{+2} + \cdots\right] \sigma_z$$

$$= 1 + \frac{i\hat{H}t}{\hbar} + \left(\frac{it}{\hbar}\right)^2 \frac{1}{2!}\hat{H}^{2} + \cdots$$

$$= \hat{S}^{-1} \qquad \square$$

(B) True single-particle observables

Question: Are all ϕ-hermitian operators observables of a relativistic single-particle quantum mechanics?

reminder: Solutions of KGE with positive frequencies $\longrightarrow$ particle

Solutions of KGE with negative frequencies $\longrightarrow$ anti-particle

To preserve the single-particle picture we are only allowed to consider operators that do not mix positive and negative frequency components!

Def: Let $\mathcal{H}_{(\pm)} \subset \mathcal{H}$ the Hilbert-subspaces of states with positive / negative frequency. ~~An~~ An operator $\hat{O}$ is called true single-particle operator or even if

$$\langle \psi_{(+)} | \hat{O} | \psi'_{(-)} \rangle = 0 \qquad \forall \; \psi_{(+)} \in \mathcal{H}_{(+)}, \; \psi'_{(-)} \in \mathcal{H}_{(-)} \tag{410}$$

example:

- $\hat{H} = (\sigma_z + i\sigma_y)\left(-\frac{\hbar^2}{2m}\Delta\right) + \sigma_z m_0 c^2$
- $\hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}$

are true single particle operators

however $\hat{\vec{X}}$ is not ! $\Rightarrow$ problem session

Def: An operator $\hat{O}$ is called odd iff

(411) $$\langle \psi_{(+)} | \hat{O} | \psi'_{(+)} \rangle = \langle \psi_{(-)} | \hat{O} | \psi'_{(-)} \rangle = 0$$

for all $|\psi^{(\prime)}_{(+)}\rangle \in \mathcal{H}_{(+)}$ and $|\psi^{(\prime)}_{(-)}\rangle \in \mathcal{H}_{(-)}$

Every operator $\hat{O}$ can be decomposed into an even and odd part

(412) $$\hat{O} = [\hat{O}] + \{\hat{O}\}$$

where $[\hat{O}]$ is even and $\{\hat{O}\}$ is odd

- If one constructs $[\hat{\vec{X}}]$ one finds that its eigenstates have the asymptotic form

(413) $$\Psi_{\vec{x}}(\vec{y}) \sim \frac{1}{Z^{7/4}} e^{-Z} \qquad Z = \frac{|\vec{x}-\vec{y}|}{\hbar/m_0 c}$$

and not $\delta^{(3)}(\vec{x}-\vec{y})$. I.e. the eigenstates of $[\hat{\vec{X}}]$ are smeared out over the Compton length

$$|\vec{x}-\vec{y}| \sim \frac{\hbar}{m_0 c} = \lambda_c$$

Relativistically it does not make sense to talk about a localization in space better than λ_c