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tube with

Klein Gordon Particles in a piston

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dedicated to Hans-Jürgen Treder

Probably I met Hans Jürgen Treder the first time in Jena, at a "Spezialtagung über Feldtheorie" organized in April, 1957, by G. Heber and E. Schmutzer. Knowing each other such a long time, I like to contribute something at the occasion of his 65-th birthday. It concerns a rather old story, opened by Tomonaga [1] and Schwinger [3] with the idea to associate to every (Cauchy) space-like hypersurface a quantized Hamitonian. I try to explain the problem using the most simple example I can imagine.

It is my aim to consider a Klein Gordon particle in a 1-dimensional piston. To this end let us consider the strip

$$0 \le x \le 1, \quad -\infty < t < \infty \tag{1}$$

equipped with the metric

$$ds^2 := dt^2 - L(t)^2\, dx^2 \tag{2}$$

This setting describes the geometry of a 1-dimensional piston with variable length $L = L(t)$ in our $(1+1)$-dimensional space time if considering the space-like "hypersurfaces" given by $t =$ const. For these hypersurfaces the time derivative and the normal derivative coincide.

The differential operator

$$\varphi \mapsto -\frac{1}{L^2}\frac{\partial^2 \varphi}{\partial x^2} + \kappa^2 \varphi \tag{3}$$

with Dirichlet boundary conditions on $0 < x < 1$ can be identified with a selfadjoint and positive operator on the Hilbert space

$$\mathcal{H} := \{\psi(x)\,;\ <\psi,\psi> := \int_0^1 |\psi|^2 dx < \infty\,\} \tag{4}$$

This Hilbert space is assumed to consist of the probability amplitudes for the position of the particle in the piston, i.e. of the Schrödinger functions. A complete orthonormal system of $\mathcal{H}$ respecting Dirichlet boundary conditions is given by

$$\psi_j = \sqrt{2}\,\sin(j\pi x), \qquad j = 1, 2, 3, \ldots \tag{5}$$

Let us denote by $\mathcal{D}$ the form domain of the operator (3). This domain is independent of t and it consists of all vectors

$$\psi = \sum \lambda_j \psi_j \quad \text{with} \quad \sum j^2 |\lambda_j|^2 < \infty \tag{6}$$

Being the form domain of (3), $\mathcal{D}$ is the domain of definition of its positive square root

$$H = H_t := \sqrt{-\frac{1}{L^2}\frac{\partial^2}{\partial x^2} + \kappa^2} \tag{7}$$

The latter is identified with an operator representing the (bare) energy of a free particle within the piston at a given instant of time. (5) is a complete orthonormal system of eigenvectors of H_t. The Klein Gordon equation with rest mass κ reads in our case

$$-\frac{1}{L^2}\frac{\partial^2\varphi}{\partial x^2} + \kappa^2\varphi + \frac{1}{L}\frac{\partial}{\partial t}(L\frac{\partial\varphi}{\partial t}) = 0 \tag{8}$$

One has to choose a suitable class of solutions of (8). This is done by requiring φ to be contained in $\mathcal{D}$.

$$\varphi \in \mathcal{L} \quad \text{if and only if} \quad \varphi \in \mathcal{D}, \quad \frac{\partial\varphi}{\partial t} \in \mathcal{D} \quad \text{for all } t \tag{9}$$

Then φ remains in the form domain of (3), and one gets as usual the integrated continuity equation showing that the symplectic sesquilinear form

$$(\varphi_1, \varphi_2) := \frac{L}{2i}(< \frac{\partial\varphi_1}{\partial t}, \varphi_2 > - < \varphi_1, \frac{\partial\varphi_2}{\partial t} >) \tag{10}$$

is time independent. It satisfies further

$$\overline{(\varphi_1, \varphi_2)} = (\varphi_2, \varphi_1) = -(\bar{\varphi}_2, \bar{\varphi}_1) \tag{11}$$

If the length of the piston is changing there is no time independent definition of one-particle states because particle creation and annihilition processes are unavoidable. Therefore one tries to define one-particle states at every instant $t = \tau$ separately. This will be done in two steps. The first is to require an osculating Schrödinger equation, a slight generalization of what one can learn (for instance) from Schweber [6], and the second step is to relate it to the Hilbert space (4) according to Newton and Wigner [2]. The osculating Schrödinger equation is formed with the Hamiltonian (7) so that one falls back to the well established one-particle definition (i.e. to the so-called positive frequency condition) if the piston's length remains constant. Thus

$$\mathcal{L}_\tau^\pm := \{\varphi \in \mathcal{L}, \quad \left(i\frac{\partial\varphi}{\partial t} \mp H_t\varphi\right)_{|t=\tau} = 0\} \tag{12}$$

Because H_t is positive definite, these two linear spaces are disjoint. This means

$$\mathcal{L}_\tau^+ + \mathcal{L}_\tau^- = \mathcal{L}, \qquad \mathcal{L}_\tau^+ \cap \mathcal{L}_\tau^- = 0 \tag{13}$$

Assuming now $\varphi^\pm \in \mathcal{L}_\tau^\pm$ one gets

$$(\varphi^\pm, \varphi^\pm) = \pm L < \varphi^\pm, H_\tau\varphi^\pm >, \qquad (\varphi^+, \varphi^-) = 0 \tag{14}$$

so that (10) defines a positive definite scalar product on every $\mathcal{L}_\tau^+$, as it should be for a (time dependent) one-particle interpretation.
The Newton and Wigner setting [2] can be recalled this way: For every given instant of time, $t = \tau$, and for ever Schrödinger function $\psi \in \mathcal{D}$ there is one and only one $\varphi^+ \in \mathcal{L}_\tau^+$, and one and only one $\varphi^- \in \mathcal{L}_\tau^-$ satisfying

$$\varphi^\pm(\tau) = H_\tau^{-1/2}\psi, \quad \text{and} \quad \frac{\partial\varphi^\pm}{\partial t}(\tau) = \mp iH_\tau^{1/2}\psi. \tag{15}$$

This setting are Cauchy data guarantying at $t = \tau$ osculating Schröder equations (with different signs of the time derivative). An essential effect of (15) is

$$(\varphi^{\pm}, \varphi^{\pm}) = \pm L < \psi, \psi > \tag{16}$$

i.e. the existence of isometrical mappings, scaled by $\pm L$, from $\mathcal{D} \subset \mathcal{H}$ into $\mathcal{L}^{\pm}$ at every instant of time. These mappings shall be called

$$I_\tau^{\pm} : \quad \mathcal{D} \mapsto \mathcal{L}_\tau^{\pm} \tag{17}$$

and they encode the selection of those solutions of the Klein Gordon equation (8) which fullfil at time τ the Cauchy initial conditions (15).

The task of the Bogoljubov transformation [4] is to relate solutions of the Klein Gordon equations which respect the initial conditions (15) for different times. It is the same question to ask for relations of the mappings (17) at different times. As explicite relations for finite time intervalls are scarcely available, one remains with its differential version. Then the problem is to find operators, A, B, such that

$$\lim_{\delta\to 0} \frac{1}{\delta}(I_{\tau+\delta}^{+} - I_\tau^{+}) = \frac{d}{d\tau} I_\tau^{+} = A\, I_\tau^{+} + B\, I_\tau^{-} \tag{18}$$

and similarly with I^-.

This can be solved as following. Define

$$\varphi^{\pm}(\tau, t) = I_\tau^{\pm}\psi \quad \text{with} \quad \psi \in \mathcal{H} \tag{19}$$

which is a solution of the Klein Gordon equation in t. We need

$$\lim_{\delta\to 0} \frac{\varphi^{+}(\tau+\delta, t) - \varphi^{+}(\tau, t)}{\delta}, \qquad \lim_{\delta\to 0} \frac{\dot\varphi^{+}(\tau+\delta, t) - \dot\varphi^{+}(\tau, t)}{\delta} \quad \text{for} \quad t = \tau \tag{20}$$

where the dot indicates t-differentiation. Let us work with the more general Cauchy data

$$\varphi^{\pm}(\tau, \tau) = X^{-1}\psi, \qquad \dot\varphi^{\pm}(\tau, \tau) = \mp i X^{*}\psi \tag{21}$$

with τ-dependent invertible operators $X = X(\tau)$. For the time being they replace the more special initial conditions (15). To calculate the first expression in (20) we use the Taylor expansion

$$\varphi(\tau+\delta, t) = \varphi(\tau+\delta, \tau+\delta) + (t - \tau - \delta)\,\dot\varphi(\tau+\delta, \tau+\delta) + \ldots \tag{22}$$

and take it at $t = \tau$. Inserting into (20), and take account of (21) yields

$$\lim_{\delta\to 0} \frac{\varphi^{+}(\tau+\delta, \tau) - \varphi^{+}(\tau, \tau)}{\delta} == \left(\frac{d(X)^{-1}}{d\tau} + iX^{*}\right)\psi \tag{23}$$

Next we have to calculate similarily

$$\lim_{\delta\to 0} \frac{\dot\varphi^{+}(\tau+\delta, \tau+\delta) - \dot\varphi^{+}(\tau, \tau)}{\delta} - \ddot\varphi^{+}(\tau, \tau) = (H_\tau^2 X^{-1} - i\frac{dX^{*}}{d\tau} - i\frac{\dot L}{L} X^{*})\psi \tag{24}$$

Equation (18) is valid for all t. Sufficient for such an equality is the coincidence of the Cauchy data at one time. Therefore, to get A, B, it suffices to consider (23) and (24). The result is

$$\left(\frac{d(X)^{-1}}{d\tau} + iX^*\right) = (A+B)X^{-1}$$
$$(H_\tau^2 X^{-1} - i\frac{dX^*}{d\tau} - i\frac{\dot{L}}{L}X^*) = \tfrac{1}{i}(A-B)X^* \qquad (25)$$

This looks rather cumbersome. However, returning to the initial values

$$X = X^* = H^{1/2}, \qquad H\dot{H} = \dot{H}H, \qquad (26)$$

(25) reduces itself to

$$A = iH + \frac{1}{2}\frac{\dot{L}}{L}, \qquad B = -\frac{1}{2}(\frac{\dot{H}}{H} + \frac{\dot{L}}{L}) \qquad (27)$$

Now all requisites to play the second quantizations are prepared. It will be done in three steps. The first one is essentially the starting point of Segal's quantization procedure. [5], [7]. It is the generation of an abstract *-algebra $\mathcal{A}$ with unit element, the elements of which may be viewed as a formalized version of Heisenbergs "q-numbers". $\mathcal{A}$ is generated by a unit element, called **1**, and by elements $\mathbf{a}(\varphi)$ with $\varphi \in \mathcal{D}$ subject to the folllowing defining relations:

$$\mathbf{a}(\lambda_1\varphi_1 + \lambda_2\varphi_2) = \lambda_1\mathbf{a}(\varphi_1) + \lambda_2\mathbf{a}(\varphi_2) \qquad (28)$$
$$\mathbf{a}(\varphi)^* = \mathbf{a}(\bar{\varphi}) \qquad (29)$$
$$[\mathbf{a}(\varphi_1), \mathbf{a}(\varphi_2)] = (\bar{\varphi}_1, \varphi_2)\,\mathbf{1} \qquad (30)$$

$\mathcal{A}$ is a CCR-algebra because its defining relations, in particular (30) expresses the canonical commutation relations. This is more transparent in the next step in which one has to identify the creation or annihilation operators among the generators $\mathbf{a}(\varphi)$. This has to be done for every instant of time, $t = \tau$, because they should create or annihilate what is called "particle" just at that instant of time. $\mathbf{a}(\varphi)$ is considered as an creation operator at time τ iff $\varphi \in \mathcal{L}_\tau^+$.
The basic definitions for this purpose are

$$\mathbf{a}_\psi^+(\tau) = L^{-1/2}\,\mathbf{a}(I_\tau^+\,\psi), \quad \mathbf{a}_\psi^-(\tau) = L^{-1/2}\,\mathbf{a}(I_\tau^-\,\bar{\psi}), \qquad \psi \in \mathcal{D} \subset \mathcal{H} \qquad (31)$$

In this way the creation operators depend linearly and the annihilation operators antilinearly on the Schrödinger amplitude, as it should be. Looking at (11), (14), and (16) the defining relations (29) and (30) are transformed into

$$[\mathbf{a}_\psi^+(\tau), \mathbf{a}_{\psi'}^+(\tau)] = [\mathbf{a}_\psi^-(\tau), \mathbf{a}_{\psi'}^-(\tau)] = 0 \qquad (32)$$

$$[\mathbf{a}_\psi^-(\tau), \mathbf{a}_{\psi'}^+(\tau)] = <\psi, \psi'>\,\mathbf{1}, \qquad (\mathbf{a}_\psi^+(\tau))^* = \mathbf{a}_\psi^-(\tau) \qquad (33)$$

We now use the complete orthonormal base (5) of eigenvectors of the one-particle Hamiltonian H_t. To every time $t = \tau$ and to every element of the base belong a creation and an annihilation operator:

$$\psi_j \mapsto \mathbf{a}_j^\pm(\tau) \qquad (34)$$

where the index ψ_j is replaced by j. Then, at every $t = \tau$,

$$[\mathbf{a}_j^-, \mathbf{a}_k^+] = \delta_{jk}, \quad [\mathbf{a}_j^+, \mathbf{a}_k^+] = [\mathbf{a}_j^-, \mathbf{a}_k^-] = 0 \qquad (35)$$

I now return shortly to a general creation operator in order to consider its time dependence. From (31) one concludes

$$\frac{d}{d\tau}\mathbf{a}_\psi^+ = \frac{dL^{-1/2}}{d\tau}L^{1/2}\mathbf{a}_\psi^+ + L^{-1/2}\mathbf{a}(\frac{d}{d\tau}I_\tau^+\psi) \tag{36}$$

By the help of (27) this can be examined further. The resulting relation becomes particulary simple in the case of an eigenvector ψ_j of the one-particle Hamiltonian. One gets, (writing now t instead af τ),

$$\frac{d}{dt}\mathbf{a}_j^\pm = \pm iE_j\,\mathbf{a}_j^\pm - \frac{1}{2}(\frac{\dot{E}_j}{E_j} + \frac{\dot{L}}{L})\mathbf{a}_j^\mp \tag{37}$$

To write this in a more general form let us introduce an auxiliary one-particle operator

$$G := \frac{1}{2}(\frac{\dot{H}_t}{H_t} + \frac{\dot{L}}{L}) \tag{38}$$

For an arbitrary Schrödinger amplitude $\psi \in \mathcal{D}$ it is

$$\frac{d}{dt}\mathbf{a}_\psi^+(t) = i\mathbf{a}_{\psi'}^+(t) - \mathbf{a}_{\psi''}^-(t), \qquad \psi' = H\psi, \quad \psi'' = G\psi \tag{39}$$

and similarily with the annihilition operators. Now it should be clear that the time derivative is defined for every element A of the CCR-algebra $\mathcal{A}$. Indeed, given a time t. Then $\mathcal{A}$ is generated by all the creation and annihilation operators at that instant of time. Then there is a *-derivation (a linear map satisfying Leibniz' rule) which coincides with (39) for creation operators. This derivation can be written

$$t \mapsto \frac{dA}{dt} = i[\mathbf{H}(t), A], \qquad \mathbf{H}^*(t) = \mathbf{H}(t) \tag{40}$$

for all $A \in \mathcal{A}$. In the approach presented here, the time-dependent operator $\mathbf{H}(t)$ is the Hamiltonian of the second quantization. Up to an arbitrary additive constant an explicit expression is given by

$$\mathbf{H} = \sum E_j\mathbf{a}_j^+\mathbf{a}_j^- + \frac{i}{2}\sum G_j[\mathbf{a}_j^-\mathbf{a}_j^- - \mathbf{a}_j^+\mathbf{a}_j^+] \tag{41}$$

where

$$G_j = <\psi_j, G\psi_j> = \frac{1}{2}(\frac{\dot{E}_j}{E_j} + \frac{\dot{L}}{L}) = \frac{1}{2}\frac{\dot{L}}{L}\frac{\kappa^2L^2}{\kappa^2L^2 + j^2\pi^2} \tag{42}$$

By the by I remark that all these equations remain correct in higher spacial dimensions n (and for Robertson Walker metrics) if L is replaced by L^n.
Looking at (41) it becomes evident that this is not the end of the second quantization story. There should be a further Bogoljubov transform

$$\mathbf{b}_j^+ = \mathbf{a}_j^+\cosh\xi_j + i\mathbf{a}_j^-\sinh\xi_j, \quad \mathbf{b}_j^- = \mathbf{a}_j^-\cosh\xi_j - i\mathbf{a}_j^+\sinh\xi_j \tag{43}$$

such that the second quantized Hamiltonian $\mathbf{H}$ may be written

$$\mathbf{H} = \sum E_j^{\text{ren}}\mathbf{b}_j^+\mathbf{b}_j^- + c'\mathbf{1} \tag{44}$$

where the superscript *ren* indicates a renormalization of the energy levels, or a "dressing" of the particles depending on the velocity the volume of the piston is changing. A straightforward calculation yields

$$E_j \tanh(2\xi) = G_j, \qquad E_j = E_j^{\text{ren}} \cosh(2\xi) \tag{45}$$

so that

$$E_j^{\text{ren}} = \sqrt{E_j^2 - G_j^2} \tag{46}$$

Remark that ξ, G_j, and $\dot{L}$ always have the same sign or vanish simultaneously. Of course ξ depends also on the considered energy level, $\xi = \xi_j$. If j goes to infinity, ξ_j and G_j tend to zero.
The time derivative of the b-operators can be seen from

$$\frac{d}{dt} b_j^+ = i[\mathrm{H}, b_j^+] + \frac{\partial}{\partial t} b_j^+ \quad \text{or,} \quad \frac{d}{dt} b_j^+ = i E_j^{\text{ren}} b_j^+ + i\dot{\xi}_j b_j^- \tag{47}$$

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