NONRELATIVISTIC FIELD THEORY - FOURIER EXPANSION

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References: W. Greiner & J. Reinhardt, Field Quantization, Springer-Verlag (1996), Chapter 3, Section 3.2.

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We’ve seen how we can construct a nonrelativistic quantum field theory by taking the wave function \( \psi(x,t) \) and translating it into a field operator \( \hat{\psi}(x,t) \). The properties of \( \hat{\psi} \) are defined by its equal-time commutation relations

\[
\left[ \hat{\psi}(x,t), \hat{\psi}^\dagger(x',t) \right] = \delta^3(x-x')
\]

(1)

with all other commutators being zero.

At this point, \( \hat{\psi} \) is a purely abstract operator and the space of vectors \( |\Phi\rangle \) in which it lives is equally abstract. We can get a bit more of a feel for what \( \hat{\psi} \) is physically if we expand it in a Fourier series over a complete set of functions \( u_i(x) \). These functions are not operators; they are merely complex-valued numerical functions. The Fourier expansion is

\[
\hat{\psi}(x,t) = \sum_i \hat{\alpha}_i(t) u_i(x) \quad (2)
\]

\[
\hat{\psi}^\dagger(x,t) = \sum_i \hat{\alpha}_i^\dagger(t) u_i^\ast(x) \quad (3)
\]

The Fourier coefficients \( \hat{\alpha}_i \) are operators, and include the time dependence. Thus these expansions constitute a snapshot of the field operators \( \hat{\psi} \) at a particular time \( t \). Although we’ve written the expansion as a sum over a discrete set of functions, in practice the sum could also include an integral over some continuum area.

The functions \( u_i \) are assumed to be a complete (in the sense that any other function can be expanded in terms of them) and orthogonal set, so that

\[
\int d^3x \, u_i^\ast(x) u_j(x) = \delta_{ij} \quad (4)
\]

\[
\sum_i u_i(x) u_i^\ast(x') = \delta^3(x-x') \quad (5)
\]
Since the $u_i$s are just numerical functions (not operators), they commute with each other. We can therefore work out the commutators of the coefficients $\hat{a}_i$ by inserting the series back into (1). We get

$$\left[\hat{\psi}(x,t), \hat{\psi}^\dagger(x',t)\right] = \left[\sum_i \hat{a}_i(t) u_i(x), \sum_j \hat{a}_j^\dagger(t) u_j^*(x')\right] = \sum_i \hat{a}_i(t) u_i(x) \sum_j \hat{a}_j^\dagger(t) u_j^*(x') - \sum_j \hat{a}_j^\dagger(t) u_j^*(x') \sum_i \hat{a}_i(t) u_i(x)$$

$$= \sum_i \sum_j \left(\hat{a}_i(t) \hat{a}_j^\dagger(t) - \hat{a}_j^\dagger(t) \hat{a}_i(t)\right) u_i(x) u_j^*(x')$$

$$= \sum_i \sum_j \left[\hat{a}_i(t), \hat{a}_j^\dagger(t)\right] u_i(x) u_j^*(x')$$

We require this to be equal to $\delta^3(x-x')$ from (1) and we can see this will be true if

$$\left[\hat{a}_i(t), \hat{a}_j^\dagger(t)\right] = \delta_{ij}$$

since this gives

$$\sum_i \sum_j \left[\hat{a}_i(t), \hat{a}_j^\dagger(t)\right] u_i(x) u_j^*(x') = \sum_i \sum_j \delta_{ij} u_i(x) u_j^*(x') = \sum_i u_i(x) u_i^*(x') = \delta^3(x-x')$$

From (2) and (3) and because $\left[\hat{\psi}, \hat{\psi}\right] = \left[\hat{\psi}^\dagger, \hat{\psi}^\dagger\right] = 0$, we must also have

$$\left[\hat{a}_i, \hat{a}_j\right] = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0$$

As usual for a Fourier expansion, we can get expressions for the coefficients $\hat{a}_i$ by multiplying (2) by $u_i^*$ (after changing the dummy index of summation to $j$) and integrating, using (4).
\[ \int d^3x \, u_i^*(x) \, \hat{\psi}(x,t) = \sum_j \hat{\alpha}_j(t) \int d^3x \, u_j^*(x) \, u_j(x) \]

\[ = \sum_j \hat{\alpha}_j(t) \delta_{ij} \]

\[ = \hat{\alpha}_i(t) \]  

(16)

Likewise, the adjoint operator is obtained by multiplying by \( u_i(x) \) and integrating:

\[ \hat{\alpha}_i^\dagger(t) = \int d^3x \, u_i(x) \, \hat{\psi}^\dagger(x,t) \]  

(19)

We can use these expressions to verify the commutation relations (since they were derived without using \( \hat{\alpha} \) or \( \hat{\psi} \)). For example

\[ \left[ \hat{\alpha}_i(t), \hat{\alpha}_j^\dagger(t) \right] = \int d^3x \, u_i^*(x) \, \hat{\psi}(x,t) \int d^3x' \, u_j(x') \, \hat{\psi}^\dagger(x',t) - \int d^3x' \, u_j(x') \, \hat{\psi}(x',t) \int d^3x \, u_i^*(x) \, \hat{\psi}(x,t) \]

\[ = \int d^3x \int d^3x' \, u_i^*(x) \, u_j(x') \left[ \hat{\psi}(x,t), \hat{\psi}^\dagger(x',t) \right] \]

\[ = \int d^3x \int d^3x' \, u_i^*(x) \, u_j(x') \, \delta^3(x - x') \]

\[ = \int d^3x \, u_i^*(x) \, u_j(x) \]

\[ = \delta_{ij} \]  

(20)

So far, these results are valid for any set of functions \( u_i(x) \) that satisfy \( \hat{\alpha} \) and \( \hat{\psi} \). Suppose now that we choose a set of functions that form the eigenfunctions of the Schrödinger Hamiltonian in the special case where the potential is time-independent. In that case the functions \( u_i \) satisfy the time-independent Schrödinger equation in the form

\[ -\frac{\hbar^2}{2m} \nabla^2 u_i + V(x) u_i = \epsilon_i u_i \]  

(26)

where \( \epsilon_i \) is the energy eigenvalue. The expectation value of the Hamiltonian in the state \( \hat{\psi} \) is then
\[ \hat{H} = \int d^3 x \hat{\psi}^\dagger(x,t) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \hat{\psi}(x,t) \] (27)

\[ = \int d^3 x \hat{\psi}^\dagger(x,t) \sum_i \hat{a}_i(t) \epsilon_i u_i(x) \] (28)

\[ = \int d^3 x \sum_j \hat{a}_j^\dagger(t) u_j^* (x) \sum_i \hat{a}_i(t) \epsilon_i u_i(x) \] (29)

\[ = \sum_j \sum_i \hat{a}_j^\dagger(t) \hat{a}_i(t) \epsilon_i \int d^3 x u_j^*(x) u_i(x) \] (30)

\[ = \sum_j \sum_i \hat{a}_j^\dagger(t) \hat{a}_i(t) \epsilon_i \delta_{ij} \] (31)

\[ = \sum_i \hat{a}_i^\dagger(t) \hat{a}_i(t) \epsilon_i \] (32)

\[ = \sum_i \hat{a}_i^\dagger(t) \hat{a}_i(t) \epsilon_i \] (33)

The energy value can be interpreted as that of a many-particle state in which the operator \( \hat{a}_i^\dagger(t) \hat{a}_i(t) \) represents the number of particles with energy \( \epsilon_i \). Greiner says this is 'obvious', and although it is certainly a reasonable interpretation, I wouldn't exactly call it obvious.

Finally, we can derive the time dependence of the operators \( \hat{a}_i(t) \) in this case, using the usual prescription for time dependence.

\[ i\hbar \hat{a}_i(t) = [\hat{a}_i(t), \hat{H}] \] (34)

\[ = \sum_j \left[ \hat{a}_i(t), \hat{a}_j^\dagger(t) \right] \hat{a}_j(t) \epsilon_j \] (35)

\[ = \sum_j \delta_{ij} \hat{a}_j(t) \epsilon_j \] (36)

\[ = \epsilon_i \hat{a}_i(t) \] (37)

This has the solution

\[ \hat{a}_i(t) = \hat{a}_i(0) e^{-i\epsilon_i t / \hbar} \] (38)

\[ \equiv \hat{a}_i e^{-i\epsilon_i t / \hbar} \] (39)

where Greiner defines the operator \( \hat{a}_i \) (without any explicit time dependence) as the value
\[ \hat{a}_i \equiv \hat{a}_i (0) \] (40)

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