

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 $\psi(\mathbf{x}, t)$ and translating it into a field operator $\hat{\psi}(\mathbf{x}, t)$. The properties of $\hat{\psi}$ are defined by its equal-time commutation relations

$$\left[\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t) \right] = \delta^3(\mathbf{x} - \mathbf{x}') \quad (1)$$

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 $u_i(\mathbf{x})$. These functions are *not* operators; they are merely complex-valued numerical functions. The Fourier expansion is

$$\hat{\psi}(\mathbf{x}, t) = \sum_i \hat{a}_i(t) u_i(\mathbf{x}) \quad (2)$$

$$\hat{\psi}^\dagger(\mathbf{x}, t) = \sum_i \hat{a}_i^\dagger(t) u_i^*(\mathbf{x}) \quad (3)$$

The Fourier coefficients \hat{a}_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

$$\int d^3x u_i^*(\mathbf{x}) u_j(\mathbf{x}) = \delta_{ij} \quad (4)$$

$$\sum_i u_i(\mathbf{x}) u_i^*(\mathbf{x}') = \delta^3(\mathbf{x} - \mathbf{x}') \quad (5)$$

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

$$\left[\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t) \right] = \left[\sum_i \hat{a}_i(t) u_i(\mathbf{x}), \sum_j \hat{a}_j^\dagger(t) u_j^*(\mathbf{x}') \right] \quad (6)$$

$$= \sum_i \hat{a}_i(t) u_i(\mathbf{x}) \sum_j \hat{a}_j^\dagger(t) u_j^*(\mathbf{x}') - \quad (7)$$

$$\sum_j \hat{a}_j^\dagger(t) u_j^*(\mathbf{x}') \sum_i \hat{a}_i(t) u_i(\mathbf{x}) \quad (8)$$

$$= \sum_i \sum_j \left(\hat{a}_i(t) \hat{a}_j^\dagger(t) - \hat{a}_j^\dagger(t) \hat{a}_i(t) \right) u_i(\mathbf{x}) u_j^*(\mathbf{x}') \quad (9)$$

$$= \sum_i \sum_j \left[\hat{a}_i(t), \hat{a}_j^\dagger(t) \right] u_i(\mathbf{x}) u_j^*(\mathbf{x}') \quad (10)$$

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

$$\left[\hat{a}_i(t), \hat{a}_j^\dagger(t) \right] = \delta_{ij} \quad (11)$$

since this gives

$$\sum_i \sum_j \left[\hat{a}_i(t), \hat{a}_j^\dagger(t) \right] u_i(\mathbf{x}) u_j^*(\mathbf{x}') = \sum_i \sum_j \delta_{ij} u_i(\mathbf{x}) u_j^*(\mathbf{x}') \quad (12)$$

$$= \sum_i u_i(\mathbf{x}) u_i^*(\mathbf{x}') \quad (13)$$

$$= \delta^3(\mathbf{x} - \mathbf{x}') \quad (14)$$

using 5.

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

$$\left[\hat{a}_i, \hat{a}_j \right] = \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger \right] = 0 \quad (15)$$

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:

$$\int d^3x u_i^*(\mathbf{x}) \hat{\psi}(\mathbf{x}, t) = \sum_j \hat{a}_j(t) \int d^3x u_i^*(\mathbf{x}) u_j(\mathbf{x}) \quad (16)$$

$$= \sum_j \hat{a}_j(t) \delta_{ij} \quad (17)$$

$$= \hat{a}_i(t) \quad (18)$$

Likewise, the adjoint operator is obtained by multiplying 3 by $u_i(\mathbf{x})$ and integrating:

$$\hat{a}_i^\dagger(t) = \int d^3x u_i(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}, t) \quad (19)$$

We can use these expressions to verify the commutation relations (since they were derived without using 11 or 15). For example

$$[\hat{a}_i(t), \hat{a}_j^\dagger(t)] = \int d^3x u_i^*(\mathbf{x}) \hat{\psi}(\mathbf{x}, t) \int d^3x' u_j(\mathbf{x}') \hat{\psi}^\dagger(\mathbf{x}', t) - \quad (20)$$

$$\int d^3x' u_j(\mathbf{x}') \hat{\psi}^\dagger(\mathbf{x}', t) \int d^3x u_i^*(\mathbf{x}) \hat{\psi}(\mathbf{x}, t) \quad (21)$$

$$= \int d^3x \int d^3x' u_i^*(\mathbf{x}) u_j(\mathbf{x}') [\hat{\psi}(\mathbf{x}, t), \hat{\psi}^\dagger(\mathbf{x}', t)] \quad (22)$$

$$= \int d^3x \int d^3x' u_i^*(\mathbf{x}) u_j(\mathbf{x}') \delta^3(\mathbf{x} - \mathbf{x}') \quad (23)$$

$$= \int d^3x u_i^*(\mathbf{x}) u_j(\mathbf{x}) \quad (24)$$

$$= \delta_{ij} \quad (25)$$

So far, these results are valid for any set of functions $u_i(\mathbf{x})$ that satisfy 4 and 5. 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

$$-\frac{\hbar^2}{2m} \nabla^2 u_i + V(\mathbf{x}) u_i = \varepsilon_i u_i \quad (26)$$

where ε_i is the energy eigenvalue. The expectation value of the hamiltonian in the state $\hat{\psi}$ is then

$$\hat{H} = \int d^3x \hat{\psi}^\dagger(\mathbf{x}, t) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right] \hat{\psi}(\mathbf{x}, t) \quad (27)$$

$$= \int d^3x \hat{\psi}^\dagger(\mathbf{x}, t) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right] \sum_i \hat{a}_i(t) u_i(\mathbf{x}) \quad (28)$$

$$= \int d^3x \hat{\psi}^\dagger(\mathbf{x}, t) \sum_i \hat{a}_i(t) \varepsilon_i u_i(\mathbf{x}) \quad (29)$$

$$= \int d^3x \sum_j \hat{a}_j^\dagger(t) u_j^*(\mathbf{x}) \sum_i \hat{a}_i(t) \varepsilon_i u_i(\mathbf{x}) \quad (30)$$

$$= \sum_j \sum_i \hat{a}_j^\dagger(t) \hat{a}_i(t) \varepsilon_i \int d^3x u_j^*(\mathbf{x}) u_i(\mathbf{x}) \quad (31)$$

$$= \sum_j \sum_i \hat{a}_j^\dagger(t) \hat{a}_i(t) \varepsilon_i \delta_{ij} \quad (32)$$

$$= \sum_i \hat{a}_i^\dagger(t) \hat{a}_i(t) \varepsilon_i \quad (33)$$

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 ε_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.

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

$$= \sum_j [\hat{a}_i(t), \hat{a}_j^\dagger(t)] \hat{a}_j(t) \varepsilon_j \quad (35)$$

$$= \sum_j \delta_{ij} \hat{a}_j(t) \varepsilon_j \quad (36)$$

$$= \varepsilon_i \hat{a}_i(t) \quad (37)$$

This has the solution

$$\hat{a}_i(t) = \hat{a}_i(0) e^{-i\varepsilon_i t/\hbar} \quad (38)$$

$$\equiv \hat{a}_i e^{-i\varepsilon_i t/\hbar} \quad (39)$$

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

$$\hat{a}_i \equiv \hat{a}_i(0) \quad (40)$$

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