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

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

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 expnasion is

$$\hat{\psi}(\mathbf{x},t)=\sum_{i}\hat{a}_{i}(t)\,u_{i}(\mathbf{x}) \tag{2}$$

$$\hat{\psi}^{\dagger}(\mathbf{x},t)=\sum_{i}\hat{a}_{i}^{\dagger}(t)\,u_{i}^{*}(\mathbf{x}) \tag{3}$$

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

$$\int d^{3}x\,u_{i}^{*}(\mathbf{x})\,u_{j}(\mathbf{x})=\delta_{ij} \tag{4}$$

$$\sum_{i}u_{i}(\mathbf{x})\,u_{i}^{*}\left(\mathbf{x}'\right)=\delta^{3}\left(\mathbf{x}-\mathbf{x}'\right) \tag{5}$$

Since the u_is 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

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

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

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

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

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

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

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

since this gives

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

$$= \sum_i u_i(\mathbf{x})\,u_i^*\left(\mathbf{x}'\right) \tag{13}$$

$$= \delta^3\left(\mathbf{x}-\mathbf{x}'\right) \tag{14}$$

using 5.

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

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

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:

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

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

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

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

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

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

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

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

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

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

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

$$= \delta_{ij} \tag{25}$$

So far, these results are valid for any set of functions $u_i(\mathbf{x})$ that satsify 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

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

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

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

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

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

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

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

$$= \sum_j\sum_i \hat{a}_j^\dagger(t)\,\hat{a}_i(t)\,\epsilon_i\delta_{ij} \tag{32}$$

$$= \sum_i \hat{a}_i^\dagger(t)\,\hat{a}_i(t)\,\epsilon_i \tag{33}$$

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.

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

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

$$= \sum_j \delta_{ij}\hat{a}_j(t)\,\epsilon_j \tag{36}$$

$$= \epsilon_i\hat{a}_i(t) \tag{37}$$

This has the solution

$$\hat{a}_i(t) = \hat{a}_i(0)\,e^{-i\epsilon_i t/\hbar} \tag{38}$$

$$\equiv \hat{a}_i e^{-i\epsilon_i t/\hbar} \tag{39}$$

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

$$\hat{a}_i \equiv \hat{a}_i\left(0\right) \tag{40}$$

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