Lessons in Quantum Field Theory

The Physical Interpretation of States in Number Representation

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§1 Lesson Objectives

We take up two examples to provide motivation for

1. interpretation of $\psi^\dagger(\mathbf{x})\psi(\mathbf{x})$ as number density, *i.e.* the number of particles per unit volume.

2. interpretation of $N_\mathbf{k}$ for the cases of periodic boundary conditions and of delta function normalization.

3. the interpretation of the states $|\nu_1, \nu_2, ..\rangle$ as corresponding to ν_1 particles in $u_1(x)$, ν_2 particles in state ν_2 and so on.

§2 Recall and Discuss

§2.1 Canonical Quantization

The canonical quantization of Schrödinger field is completed by postulating the equal time commutator relation (ETCR)

$$\big[\psi(x,t), \pi(y,t)\big] = i\hbar\delta(x-y) \tag{1}$$

is the first and last step towards quantization.

§2.2 Mathematical properties of $a_k, a_k^\dagger, N_k$

1. The creation operators $a_\mathbf{k}^\dagger$ and annihilation operators $a_\mathbf{k}$ and number operators obey the commutation relations

$$[a_\mathbf{k}, a_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k},\mathbf{k}'}; \tag{2}$$

$$[a_\mathbf{k}, a_{\mathbf{k}'}] = 0 \qquad [a_\mathbf{k}^\dagger, a_{\mathbf{k}'}^\dagger] = 0; \tag{3}$$

2. The operators $N_\mathbf{k} = a_\mathbf{k}^\dagger a_\mathbf{k}$ form a commuting set of hermitian operators and obey commutation relations.

$$[a_\mathbf{k}^\dagger, N_\mathbf{k}] = 1, \qquad [a_\mathbf{k}, N_\mathbf{k}] = -1$$

all other commutators, $N_\mathbf{p}$ with $a_\mathbf{q}$ or $a_\mathbf{q}^\dagger$ are zero for $\mathbf{p} \neq \mathbf{q}$.

We had defined number operators N_k which are hermitian and commute pairwise. Their eigenvalues can be worked out. In fact their algebra is the same as one encounters in the treatment of the harmonic oscillator. The eigenvalues are all non-negative integers.

§2.3 Choosing an o.n. basis

The fact that $N_k, k = 1, 2, 3..$ commute pairwise, their eigenvectors form a complete orthonormal set. This means that the basis vectors are specified by a sequence of corresponding eigenvalues $\nu_1, \nu_2, \ldots$. The details of interpretation of states $|\nu_1, \nu_2, \ldots, \nu_k, \ldots\rangle$ depends on the choice of the orthonormal set $\{u_n(x)|n = 1, 2, \ldots\}$

§3 Physical Interpretation of Particle Number States

§3.1 Example 1

Consider quantum mechanics of a point particle in one dimension in a potential having only bound states.

$$\widehat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})$$

Let $u_n(x)$ denote the eigenfunctions of the Hamiltonian $\widehat{H}$ with eigenvalues E_n.

$$\widehat{H} u_n(x) = E_n u_n(x) \tag{4}$$

The Hamiltonian of the Schrodinger field is

$$\begin{aligned} \mathcal{H} &= \int d\mathbf{x} \mathscr{H}(\pi(\mathbf{x}), \psi(\mathbf{x}), \nabla\psi(\mathbf{x})) &(5)\\ \mathscr{H} &= \pi(\mathbf{x})\frac{d\psi(\mathbf{x})}{dt} - \mathscr{L} &(6)\\ &= \frac{\hbar^2}{2m}\nabla\psi^\dagger(x)\nabla\psi(x) + \psi^\dagger(x)V(x)\psi(x) &(7)\end{aligned}$$

Expressed in terms of operators $a_k, a_k^\dagger$ the Hamiltonian $\mathcal{H}$ takes the form

$$\mathcal{H} = \sum_k N_k E_k \qquad \text{Verify this equation!} \tag{8}$$

The state $|\nu_1, \nu_2, \ldots, \nu_k, \ldots\rangle$ is an eigenstate of $\mathcal{H}$:

$$\mathcal{H}|\nu_1, \nu_2, \ldots, \nu_k, \ldots\rangle = \Big(\sum_m E_m \nu_m)|\nu_1, \nu_2, \ldots, \nu_k, \ldots\rangle \tag{9}$$

Thus we have

$$\begin{aligned} \mathcal{H}|0\rangle &= 0\\ \mathcal{H}|0, 0, ..\nu_k, 0, 0, ..\rangle &= \nu_k E_k|0, 0, ..\nu_k, 0, 0, ..\rangle\\ \mathcal{H}|0, 0, ..\nu_k, 0, \nu_\ell, 0..\rangle &= (\nu_k E_k + \nu_\ell E_\ell)|0, 0, ..\nu_k, 0, \nu_\ell, 0..\rangle.\end{aligned}$$

This shows that the state $|0\rangle$ has no particle, the state $|0, 0, ..\nu_k, 0, 0, ..\rangle$ has ν_k particles with energy E_k, and the state $|0, 0, ..\nu_k, 0, \nu_\ell, 0..\rangle$ has ν_k and ν_ℓ particles in energy levels E_k, E_ℓ respectively.

Continuing the above argument, we can interpret the state $|\nu_1, \nu_2, \ldots, \nu_k, \ldots\rangle$ as a state in which the first level E_1 is occupied by ν_1 particles, the second level E_2 is occupied with ν_2 particles and so on.

The operator a_k destroys one particle in the state E_k. So for example,

$$a_k|\nu_1, \nu_2, \ldots, \nu_k \ldots\rangle = \sqrt{\nu_k}|\nu_1, \nu_2, \ldots, \nu_k - 1 \ldots\rangle \tag{10}$$

and $a_k^\dagger$ creates particle in state

$$a_k^\dagger|\nu_1, \nu_2, \ldots, \nu_k \ldots\rangle = \sqrt{\nu_k + 1}|\nu_1, \nu_2, \ldots, \nu_k + 1 \ldots\rangle \tag{11}$$

§3.2 Example 2

Consider free particle Schrodinger equation in one dimension

$$i\hbar\frac{d\psi(\mathbf{x},t)}{dt} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) \tag{12}$$

§3.2.1 Periodic Boundary Condition

We choose the orthonormal functions $u_{\mathbf{k}}(\mathbf{x}) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(L)^{3/2}}$ as the basis set for expansion of Schrodinger field

$$\psi(\mathbf{x}) = \sum_{\{n_1,n_2,n_3\}} u_{\mathbf{k}}(\mathbf{x})a_{\mathbf{k}} \tag{13}$$

where the periodic boundary conditions on plane waves imply that $\mathbf{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$

Then the Hamiltonian for free Schrodinger field becomes

$$\mathcal{H} = \sum_{\{n_1,n_2,n_3\}} N_{\mathbf{k}}E_{\mathbf{k}}, \quad \text{where} \quad E_{\mathbf{k}} = \frac{h^2}{8mL^2}(n_1^2 + n_2^2 + n_3^2) \tag{14}$$

An expression for momentum of the Schrodinger field, obtained using Noether's theorem, is given by

$$\mathcal{P} = -i\hbar\int \psi^\dagger(\mathbf{x})\nabla\psi(\mathbf{x})\,d\mathbf{x}. \tag{15}$$

When expressed in terms of $a, a^\dagger$ the above expression takes the form

$$\mathcal{P} = \sum_{\{n_1,n_2,n_3\}} \hbar\mathbf{k}\,N_{\mathbf{k}}. \qquad \text{Verify!} \tag{16}$$

So we have the following interpretation

1. $N_{\mathbf{k}}$ is the number of particle having momentum value $\mathbf{k}$ The motivation for this interpretation comes from the following statements already proved.

   (*a*) The eigenvalues of $N_{\mathbf{k}}$ are non-negative integers.

   (*b*) The total energy is equal to sum of number of particles in a level × energy of the level. The summation being overall levels $\{n_1, n_2, n_3\}$, see Eq.(14).

2. $\psi^\dagger(\mathbf{x})\psi(\mathbf{x})$ is the total number of particles per unit volume because we have the total number operator given by **Remember this!**

$$N = \sum_{\{n_1,n_2,n_3\}} N_{\mathbf{k}} = \int d\mathbf{x}\psi^\dagger(\mathbf{x})\psi(\mathbf{x}) \qquad \text{Verify!} \tag{17}$$

§3.2.2 Delta function normalization

We choose the orthonormal functions $u_{\mathbf{k}}(\mathbf{x}) = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}}$ as the basis set for expansion of Schrodinger field

$$\psi(\mathbf{x}) = \int d\mathbf{k}u_{\mathbf{k}}(\mathbf{x})a_{\mathbf{k}} = \int \frac{d\mathbf{k}}{(2\pi)^{3/2}}u_{\mathbf{k}}(\mathbf{x})a_{\mathbf{k}} \tag{18}$$

In case of delta function normalization, all values of$k$ are allowed. We have the total number operator given by

$$\int d\mathbf{x}\psi^\dagger(\mathbf{x})\psi(\mathbf{x}) = \int d\mathbf{k}N_\mathbf{k} = N \tag{19}$$

Then the Hamiltonian for free Schrodinger field becomes

$$\mathcal{H} = \int d\mathbf{k}N_\mathbf{k}E_\mathbf{k}, \quad \text{where} \quad E_\mathbf{k} = \frac{\hbar^2\mathbf{k}^2}{2m} \tag{20}$$

An expression for momentum of the Schrodinger field, obtained using Noether's theorem, is given by

$$\mathcal{P} = -i\hbar \int \psi^\dagger(\mathbf{x})\nabla\psi(\mathbf{x})\, d\mathbf{x}. \tag{21}$$

When expressed in terms of $a, a^\dagger$ the above expression takes the form

$$\mathcal{P} = \int d\mathbf{k}\,(\hbar\mathbf{k})\,N_\mathbf{k} \qquad \text{Verify!}\,. \tag{22}$$

So we have the following interpretations, Remember this

1. $N_\mathbf{k}\, d\mathbf{k}$ is the number of particle in the momentum range $d\mathbf{k}$ and $\mathbf{k} + d\mathbf{k}$ Different from Example 1
2. $\psi^\dagger(\mathbf{x})\psi(\mathbf{x})$ is the number of particles per unit volume. Same as in Example 1

§4 EndNotes

Note carefully, and remember

- ✍ that $\psi^\dagger\psi$ is number of particles per unit volume in both the cases of delta function normalization and of box normalization.
- ✍ how the interpretation of $N_\mathbf{k}$ differs in the case of periodic boundary conditions from that of delta function normalization.
- ✍ In case of box normalization $N_\mathbf{k}$ is the number of particles with momentum $\mathbf{k}$.
- ✍ In case of delta function normalization, $N_\mathbf{k}\, d\mathbf{k}$ is the number of particles having momentum in volume $d\mathbf{k}$ at the momentum value $\mathbf{k}$.