1.2 Many-Particle Quantum Mechanics: Second Quantization 17

$$\exp\left(\frac{\mathrm{i}}{\hbar}\hat{\theta}_n\right)(\hat{N}_n)^m \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{\theta}_n\right) = \left[\exp\left(\frac{\mathrm{i}}{\hbar}\hat{\theta}_n\right)\hat{N}_n \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{\theta}_n\right)\right]^m$$
$$= (\hat{N}_n + 1)^m \qquad (1.2.25)$$

holds. For a general function g(N) we obtain

$$\exp\left(\frac{\mathrm{i}}{\hbar}\hat{\theta}_n\right)g(\hat{N}_n)\,\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{\theta}_n\right) = g(\hat{N}_n+1) \quad . \tag{1.2.26}$$

This means that  $\hat{U} = \exp(\frac{i}{\hbar}\hat{\theta}_n)$  is a linear operator acting on  $\hat{N}_n$ , just like  $\hat{U}(a)$  in (1.1.60). If  $\hat{\theta}_n$  were Hermitian, then  $\hat{U}$  would be a unitary operator with  $\hat{U}^{\dagger}\hat{U} = \hat{U}\hat{U}^{\dagger} = 1$ . However, this identity is not true. This can be seen from (1.2.26):  $\hat{U}^{\dagger}$  increases  $\hat{N}_n$  by one,  $\hat{U}$  decreases  $\hat{N}_n$  by one. Acting with  $\hat{U}$  on the vacuum state with no particles  $|N_n = 0\rangle$  we obtain  $\hat{U}|N_n = 0\rangle = 0$ . Acting on this equation with  $\hat{U}^{\dagger}$  we obtain of course  $\hat{U}^{\dagger}\hat{U}|N_n = 0\rangle = 0$ . However, because of  $\hat{U}\hat{U}^{\dagger}|N_n = 0\rangle = \hat{U}|N_n = 1\rangle = |N_n = 0\rangle \neq 0$  we have just demonstrated that  $\hat{U}^{\dagger}\hat{U} \neq \hat{U}\hat{U}^{\dagger}$ . Therefore, we conclude that because the particle number  $N_n$  is bounded from below,  $\hat{\theta}$  is not Hermitian. However, when only states with  $N_n \gg 1$  are considered, the existence of a lower bound can be neglected, and  $\hat{\theta}$  can be regarded to be Hermitian.

Next, we deduce the Hamiltonian occurring after second quantization. Continuing in a heuristic manner as above, we declare in (1.2.8)  $\langle \hat{H} \rangle$  to be an operator again and write

$$\hat{H} = \sum_{n,m} \hat{A}_n^{\dagger} \langle \phi_n | \hat{H}_1 | \phi_m \rangle \hat{A}_m \quad . \tag{1.2.27}$$

Here,  $\hat{H}_1$  is the single-particle Hamiltonian, being an operator in the sense that it acts on single-particle wave functions  $\phi_n^*(\mathbf{r})$  and  $\phi_m(\mathbf{r})$ .  $\hat{H}$  is an operator because  $\hat{A}_n^{\dagger}$  and  $\hat{A}_m$  are operators; however,  $\langle \phi_n | \hat{H}_1 | \phi_m \rangle$  is a simple complex number.

Equation (1.2.27) can also be expressed in terms of the field operators  $\hat{\psi}^{\dagger}(\mathbf{r})$  and  $\hat{\psi}(\mathbf{r})$ :

$$\hat{H} = \int \mathbf{d}^3 \boldsymbol{r} \, \hat{\psi}^{\dagger}(\boldsymbol{r}) \hat{H}_1 \hat{\psi}(\boldsymbol{r}) \quad . \tag{1.2.28}$$

The Heisenberg equation of motion of  $\hat{\psi}$  is given by

$$i\hbar \frac{\partial \hat{\psi}(\boldsymbol{r},t)}{\partial t} = [\hat{\psi}(\boldsymbol{r},t), \hat{H}] = \hat{H}_1 \hat{\psi}(\boldsymbol{r},t) \quad . \tag{1.2.29}$$

If  $\hat{\psi}(\mathbf{r})$  were a single-particle wave function, then this equation would be the Schrödinger equation (1.1.1); however, again we mention that  $\hat{\psi}(\mathbf{r})$  is an operator, and the above equation describes the time evolution of this operator in the Heisenberg picture, which leads to a totally different meaning.