TITOLO TESI

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ii

Contents

Abstract

Sommario

Acknowledgements

Chapter 1

Introduction

Chapter 2

Second quantization

2.1   Many particle systems

2.1.1   Occupation numbers representation

In condensed matter physics we often have to deal with systems of many particles. We can describe such a system starting from the wavefunctions of the single particles $|\psi_k\rangle$, where the particle is in the eigenstate of eigenvalue k of an operator $\hat{K}$. We suppose this set of vectors to be orthonormal. We could initially write the total state vector as the product of the single ones.

$$|\Psi\rangle = \left|\psi_{P[k_1]}\right\rangle \left|\psi_{P[k_2]}\right\rangle \ldots \left|\psi_{P[k_N]}\right\rangle \tag{2.1}$$

However, the former expression does not take into account the indistinguishability of quantum particles. In fact, the physics of the system must be invariant under the exchange of two particles. This is possible only if $|\Psi\rangle$ is symmetric or antisymmetric for the exchange of two particles. The former case is true for bosons, the latter for fermions.

In order to satisfy this condition, we have to modify eq. (2.1). An appropriate linear combination of the products of the single kets, compatible with the symmetry constraints required by Bose and Fermi statistics is given by

$$|\Psi\rangle = |\psi_{k_1}, \psi_{k_2}, \ldots, \psi_{k_N}\rangle = \sqrt{\frac{1}{N!}} \sum_P \xi^P \left|\psi_{P[k_1]}\right\rangle \left|\psi_{P[k_2]}\right\rangle \ldots \left|\psi_{P[k_N]}\right\rangle \tag{2.2}$$

where the sum is extended to all the $N!$ permutations P of $k_1, k_2, \ldots k_N$. $\xi = 1$ for bosons and $\xi = -1$ for fermions, so that for fermions $\xi^P = 1$ for even permutations and $\xi^P = -1$ for odd permutations. This construction assures that the total wavefunction is symmetric for the exchange of two bosons and antisymmetric for the exchange of two fermions. It is important to notice that eq. (2.2) has an ambiguity in the phase of the final vector. To remove it, we chose the permutation to be even when $k_1 < k_2 < \ldots k_N$.

It is useful to compute the product of a base bra and a base ket of two total state vectors.

$$
\begin{aligned}
\langle \psi_{m_1}, \ldots, \psi_{m_N} | \psi_{k_1}, \ldots, \psi_{k_N} \rangle &= \frac{1}{N!} \\
&= \sum_P \sum_{P'} \xi^{P+P'} \left\langle \psi_{P[m_1]} \right| \left\langle \psi_{P[m_2]} \right| \ldots \left\langle \psi_{P[m_N]} \right| \times \left|\psi_{P'[k_1]}\right\rangle \left|\psi_{P'[k_2]}\right\rangle \ldots \left|\psi_{P'[k_N]}\right\rangle \\
&= \sum_{P''} \xi^{P''} \left\langle \psi_{m_1} | \psi_{P''[k_1]} \right\rangle \ldots \left\langle \psi_{m_N} | \psi_{P''[k_N]} \right\rangle \\
&= \begin{vmatrix}
\langle \psi_{m_1} | \psi_{k_1} \rangle & \langle \psi_{m_1} | \psi_{k_2} \rangle & \ldots & \langle \psi_{m_1} | \psi_{k_N} \rangle \\
\langle \psi_{m_2} | \psi_{k_2} \rangle & \langle \psi_{m_2} | \psi_{k_2} \rangle & \ldots & \langle \psi_{m_2} | \psi_{k_N} \rangle \\
\ldots & \ldots & \ldots & \ldots \\
\langle \psi_{m_N} | \psi_{k_1} \rangle & \langle \psi_{m_N} | \psi_{k_2} \rangle & \ldots & \langle \psi_{m_N} | \psi_{k_N} \rangle
\end{vmatrix}_\xi
\end{aligned} \tag{2.3}
$$

where $|\cdot|_{\xi=1}$ represents a permanent and $|\cdot|_{\xi=-1}$ a determinant. Given the orthonormality of the single state kets, the only terms of the sum that differ from zero are the ones where

$$P''\{k_1, \ldots, k_N\} = \{m_1, \ldots, m_N\} \tag{2.4}$$

If a state ψ_j appears n_j times, the norm of the state vector will be

$$\langle \psi_{k_1}, \ldots, \psi_{k_N} | \psi_{k_1}, \ldots, \psi_{k_N} \rangle = n_1! n_2! \ldots n_N! \tag{2.5}$$

Thus, the normalized state vector is

$$|\psi_{k_1}, \ldots, \psi_{k_N}\rangle_n = \frac{1}{\sqrt{n_1! n_2! \ldots n_N!}} |\psi_{k_1}, \ldots, \psi_{k_N}\rangle \tag{2.6}$$

Given the indisinguishibility of the particles, a simpler way to describe this state vector is using only the number n_j of particles that are in the state ψ_{k_j}.

$$|n_1, n_2, \ldots n_i, \ldots\rangle = |\psi_{k_1}, \ldots, \psi_{k_N}\rangle_n \tag{2.7}$$

where ψ_{k_j} is repeated n_j times. This eliminates the inconvenience of having multiple kets describing the same state as we had before. This representation is called occupation numbers representation, and the kets are said to be elements of the Fock space.

Two special cases of states in the Fock space are the following. The vacuum state

$$|0, 0, \ldots 0\rangle = |\mathbf{0}\rangle \tag{2.8}$$

is a state with no particles in any single-particle states. The second is

$$|0, 0, \ldots, n_i = 1, \ldots\rangle = |\psi_{k_i}\rangle \tag{2.9}$$

where there is exactly one particle in the k_i state.

2.1.2 Creation and annihilation operators

Now that we have defined the base kets, we can introduce two operators that are used to transform the kets. We define a *creation operator* as

$$\hat{a}_i^\dagger |\psi_{k_1}, \psi_{k_2}, \ldots\rangle = |\psi_{k_i}, \psi_{k_1}, \psi_{k_2}, \ldots\rangle \tag{2.10}$$

Below we show several properties that derive from these definition, but its essential role can be understood applying it to the vacuum state.

$$\hat{a}_i^\dagger |\mathbf{0}\rangle = |\psi_{k_i}\rangle \tag{2.11}$$

Its effect is to add a particle in k_i state to the system. It is easy to interpret its adjoint as an *annihilation operator*, in fact

$$1 = \langle \psi_{k_i} | \psi_{k_i} \rangle = \langle \mathbf{0} | \hat{a}_i \hat{a}_i^\dagger | \mathbf{0} \rangle = \langle \mathbf{0} | \hat{a}_i | \psi_{k_i} \rangle \tag{2.12}$$

which implies that

$$\hat{a}_i | \psi_{k_i} \rangle = | \mathbf{0} \rangle \tag{2.13}$$

We now try to prove these properties on a general base ket. We consider the transition matrix element

$$\mathcal{A} = \langle \phi_{m_1}, \dots, \phi_{m_{N-1}} | \hat{a}_i | \psi_{k_1}, \dots, \psi_{k_N} \rangle =$$
$$= \langle \psi_{k_1}, \dots, \psi_{k_N} | \hat{a}_i^\dagger | \phi_{m_1}, \dots, \phi_{m_{N-1}} \rangle^* = \langle \psi_{k_1}, \dots, \psi_{k_N} | \psi_{k_i}, \phi_{m_1}, \dots, \phi_{m_{N-1}} \rangle^* \tag{2.14}$$

using eq. (2.3)

$$\mathcal{A} = \begin{vmatrix} \langle \psi_{k_1} | \psi_{k_i} \rangle & \langle \psi_{k_1} | \phi_{m_1} \rangle & \cdots & \langle \psi_{k_1} | \phi_{m_{N-1}} \rangle \\ \langle \psi_{k_2} | \psi_{k_i} \rangle & \langle \psi_{k_2} | \phi_{m_1} \rangle & \cdots & \langle \psi_{k_2} | \phi_{m_{N-1}} \rangle \\ \cdots & \cdots & \cdots & \cdots \\ \langle \psi_{k_N} | \psi_{k_i} \rangle & \langle \psi_{k_N} | \phi_{m_1} \rangle & \cdots & \langle \psi_{k_N} | \phi_{m_{N-1}} \rangle \end{vmatrix}^*_\xi \tag{2.15}$$

and developing it along the first column

$$\mathcal{A} = \left(\sum_{j=1}^N \xi^{j+1} \langle \psi_{k_j} | \psi_{k_i} \rangle \begin{vmatrix} \langle \psi_{k_1} | \phi_{m_1} \rangle & \cdots & \langle \psi_{k_1} | \phi_{m_{N-1}} \rangle \\ \langle \psi_{k_2} | \phi_{m_1} \rangle & \cdots & \langle \psi_{k_2} | \phi_{m_{N-1}} \rangle \\ \cdots & (\text{no } \psi_{k_j}) & \cdots \\ \langle \psi_{k_N} | \phi_{m_1} \rangle & \cdots & \langle \psi_{k_N} | \phi_{m_{N-1}} \rangle \end{vmatrix}_\xi \right)^*$$

$$= \sum_{j=1}^N \xi^{j+1} \langle \psi_{k_i} | \psi_{k_j} \rangle \langle \psi_{k_1}, \dots (\text{no } \psi_{k_j}), \psi_{k_N} | \phi_{m_1}, \dots, \phi_{m_{N-1}} \rangle^*$$

$$= \sum_{j=1}^N \xi^{j+1} \delta_{k_i k_j} \langle \phi_{m_1}, \dots, \phi_{m_{N-1}} | \psi_{k_1}, \dots (\text{no } \psi_{k_j}), \psi_{k_N} \rangle \tag{2.16}$$

Confronting it with eq. (2.14) we conclude

$$\hat{a}_i | \psi_{k_1}, \dots, \psi_{k_N} \rangle = \sum_{j=1}^N \xi^{j+1} \delta_{k_i k_j} | \psi_{k_1}, \dots (\text{no } \psi_{k_j}), \psi_{k_N} \rangle \tag{2.17}$$

If k_i is not present in $| \psi_{k_1}, \dots, \psi_{k_N} \rangle$, $\delta_{k_i k_j} = 0$ and overall $\hat{a}_i | \psi_{k_1}, \dots, \psi_{k_N} \rangle = 0$. On the other hand, if k_i is included in the ket n times, there will be n_i non-null terms in the sum.

In the case of bosons,

$$\hat{a}_i | \psi_{k_1}, \dots, \psi_{k_N} \rangle = n_i | \psi_{k_1}, \dots (\text{one less } \psi_{k_i}), \psi_{k_N} \rangle \tag{2.18}$$

We can use eq. (2.7) to express the last relation in the occupation numbers representation.

$$\hat{a}_i \left| n_1, n_2, \ldots, n_i, \ldots \right\rangle = \hat{a}_i \left| \psi_{k_1}, \ldots, \psi_{k_N} \right\rangle_n$$

$$= \hat{a}_i \left(\prod_{j=1}^{N} \sqrt{n_j!} \right)^{-1} \left| \psi_{k_1}, \ldots, \psi_{k_N} \right\rangle = n_i \left(\prod_{j=1}^{N} \sqrt{n_j!} \right)^{-1} \left| \psi_{k_1}, \ldots \text{(one less } \psi_{k_i}\text{)}, \psi_{k_N} \right\rangle$$

$$= \sqrt{n_i} \left| \psi_{k_1}, \ldots \text{(one less } \psi_{k_i}\text{)}, \psi_{k_N} \right\rangle_n = \sqrt{n_i} \left| n_1, n_2, \ldots, n_i - 1, \ldots \right\rangle \quad (2.19)$$

The same argument, developed for the creation operator $\hat{a}_i^\dagger$, leads to

$$\hat{a}_i^\dagger \left| n_1, n_2, \ldots, n_i, \ldots \right\rangle = \sqrt{n_i + 1} \left| n_1, n_2, \ldots, n_i + 1, \ldots \right\rangle \quad (2.20)$$

For fermions, the occupation numbers can either be 1 or 0. The creation operator $\hat{a}_i^\dagger$ returns a phase factor of 0 if $n_i = 1$ and 1 or -1 if $n_i = 0$ The annihilation operator $\hat{a}_i$ does the opposite.

It is useful defining a new operator, the number operator $\hat{N}_i = \hat{a}_i^\dagger \hat{a}_i$. If we apply it to base ket of a system made of bosons

$$\hat{N}_i \left| n_1, n_2, \ldots, n_i, \ldots \right\rangle = \hat{a}_i^\dagger \hat{a}_i \left| n_1, n_2, \ldots, n_i, \ldots \right\rangle$$

$$= \hat{a}_i^\dagger \sqrt{n_i} \left| n_1, n_2, \ldots, n_i - 1, \ldots \right\rangle = n_i \left| n_1, n_2, \ldots, n_i, \ldots \right\rangle \quad (2.21)$$

2.1.3 Commutation relations