THE STATISTICS OF SPIN AND POLAR EXCITATIONS IN A CRYSTAL

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The statistics of quasi-particles, the elementary excitations of the spin and electronic system of a crystal, are investigated.

1. Some recent papers[1-3] have asserted, contrary to the general opinion, that spin-waves behave like fermions rather than like bosons. Doubt was also thrown upon the idea that the elementary polar excitations (pairs and holes) in the electronic system of a crystal could behave like bosons.[4] It seems therefore worth while to study once again the statistical properties of spin-waves and polar excitations. In the present paper we point out some defects in the usual treatment of spin and polar excitations in crystals. In particular, these defects give rise to the appearance of fictitious states.[2,5,6] We show that when these defects are removed the spin-waves behave like bosons, and we find the conditions under which polar excitations behave like bosons. We also formulate in this paper a method of second quantization for systems of a finite number of particles described by symmetric wave-functions.

2. The Schrödinger equation with an exchange interaction has the following well-known form:

$$\varepsilon\alpha(f_1,\ldots,f_r)+\sum_{f_1'\ldots f_r'}J_{st}[\alpha(f_1',\ldots,f_r')-\alpha(f_1,\ldots,f_r)]=0, \quad (1)$$

Here $(f_1,\ldots,f_r)$ are the numbers of the vertices at which r reversed spins are situated. $(f_1',\ldots,f_r')$ is a set of numbers differing from $(f_1,\ldots,f_r)$ by the exchange of two oppositely oriented spins, and J_{st} is the exchange integral for the vertices between which the exchange has occurred. We introduce the operators

$$\varphi_f=\sqrt{N_f}\,\Delta_f^-;\quad \varphi_f=\Delta_f^+\sqrt{N_f};$$
$$\psi_f=\sqrt{n_f}\,\delta_f^-;\quad \psi_f^+=\delta_f^+\sqrt{n_f}; \quad (2)$$

$$\Delta_f^{\pm}a(\ldots N_f,\ n_f\ldots)=a(\ldots N_f\pm 1,\ n_f\ldots);$$
$$\delta_f^{\pm}a(\ldots N_f,\ n_f\ldots)=a(\ldots N_f,\ n_f\pm 1,\ldots), \quad (3)$$

Here N_f is the number of reversed (or right) spins, and n_f is the number of left spins, at the vertex f. Bloch[7] proceeded from Eq. (1) to a second-quantized formalism with the Hamiltonian

$$\mathcal{H}=\frac{1}{2}\sum_{s\neq t}J_{st}(\varphi_s\psi_t-\psi_s\varphi_t)(\varphi_s^+\psi_t^+-\psi_s^+\varphi_t^+). \quad (4)$$

According to Eq. (3), the operators (2) obey the Bose commutation rules

$$\varphi_f^+\varphi_{f'}-\varphi_{f'}\varphi_f^+=\delta_{ff'},\quad \psi_f^+\psi_{f'}-\psi_{f'}\psi_f^+=\delta_{ff'}. \quad (5)$$

The operators (2) have the unsatisfactory feature that, according to Eq. (5), they do not place any limit on the occupation numbers of left and right spins at each vertex. Thus they do not obey the Pauli principle. Therefore, instead of Eq. (4), we shall give another representation for the operators $\Delta_f^{\pm}$ and $\delta_f^{\pm}$:

$$\begin{aligned}
\Delta_f^-a(\ldots N_f,\ n_f\ldots)&=\begin{cases}0 & \text{for } N_f=0\\ a(\ldots 0_f,\ n_f\ldots) & \text{for } N_f=1\end{cases}\\
\delta_f^-a(\ldots N_f,\ n_f\ldots)&=\begin{cases}0 & \text{for } n_f=0\\ a(\ldots N_f,\ 0_f\ldots) & \text{for } n_f=1\end{cases}\\
\Delta_f^+a(\ldots N_f,\ n_f\ldots)&=\begin{cases}a(\ldots 1_f,\ n_f\ldots) & \text{for } N_f=0\\ 0 & \text{for } N_f=1\end{cases}\\
\delta_f^+a(\ldots N_f,\ n_f\ldots)&=\begin{cases}a(\ldots N_f,\ 1_f\ldots) & \text{for } n_f=0\\ 0 & \text{for } n_f=1\end{cases}
\end{aligned} \quad (6)$$

By using Eq. (6) instead of (3), we ensure the fulfilment of the Pauli principle, and yet the deduction of Eq. (4) from (1) is still valid. Equations (2) and (6) imply, instead of Eq. (5), the following commutation rules

$$\begin{aligned}
&[\varphi_f^+\varphi_f]_+=[\psi_f^+\psi_f]_+=1,\\
&[\varphi_f^+\varphi_{f'}]_-=[\psi_f^+\psi_{f'}]_-=0 \qquad (f\neq f'),\\
&[\varphi_f\varphi_{f'}]_-=[\varphi_f^+\varphi_{f'}^+]_-=[\psi_f\psi_{f'}]_-=[\psi_f^+\psi_{f'}^+]_-=0.
\end{aligned} \quad (7)$$

The commutation rules for φ_f and ψ_f are therefore different both from the Fermi and the Bose rules. For brevity we call the relations (7) the "plus-minus quantization."

In the homopolar approximation

$$N_f+n_f=1 \quad (8)$$

we need not write the occupation number n_f in the

wave-function, because it is uniquely determined by the occupation number N_f. Thus instead of the four operators φ_f, φ_f^+, ψ_f and ψ_f^+, we may introduce two operators c_f and c_f^+, acting only on the numbers N_f. The connection between the old and new operators is given by

$$\psi_f\varphi_f^+ a(\ldots N_f,\ n_f\ldots) = \begin{cases} a(\ldots 1_f,\ 0_f\ldots) & \text{for } N_f = 0,\ n_f = 1 \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

$$\varphi_f\psi_f^+ a(\ldots N_f,\ n_f\ldots) = \begin{cases} a(\ldots 0_f,\ 1_f\ldots) & \text{for } N_f = 1,\ n_f = 0 \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

Consequently, if we introduce a creation operator c_f and an annihilation operator c_f^+ for a right spin at the vertex f, we find

$$c_f = \psi_f\varphi_f^+, \qquad c_f^+ = \varphi_f\psi_f^+. \tag{11}$$

Equation (11), with (2), (6), (7), and (8), implies the following commutation rules*

$$[c_f c_f^+]_+ = 1, \tag{12_1}$$

$$[c_f c_{f'}^+]_- = 0 \qquad (f \neq f'), \qquad [c_f c_{f'}]_- = [c_f^+ c_{f'}^+]_- = 0. \tag{12_2}$$

The Hamiltonian (4) may be expressed in terms of the new operators:

$$\mathcal{H} = \sum_{s \neq t} J_{st}(c_s^+ c_s - c_s^+ c_t - N_s N_t). \tag{13}$$

This gives for the linear chain in the nearest-neighbor approximation

$$\mathcal{H} = J \sum_s \sum_{t=s\pm d} (c_s^+ c_s - c_s^+ c_t - N_s N_t), \tag{14}$$

which is identical with the Hamiltonian of Frank.[1] But we differ from Frank in requiring the operators (11) to satisfy not the Fermi commutation rules but the rules (12) of the plus-minus quantization.

To diagonalize (14), we neglect terms of fourth order in the operators[1] c_f, which means that we are neglecting the interaction between spin-waves. We use the Fourier transform

$$c_f = N^{-1/2} \sum_k e^{ikf} c_k, \qquad c_f^+ = N^{-1/2} \sum_k e^{-ikf} c_k^+. \tag{15}$$

Then Eq. (14) gives

$$\mathcal{H} = \sum_k E(k)\, n_k. \tag{16}$$

Here $E(k)$ is the usual energy of a spin-wave with quasi-momentum $\mathbf{k}$, and $n_k = c_k^+ c_k$ is the corresponding occupation number.

To study the statistics of the quasi-particles, we consider the commutation rules for c_k, c_k^+. Equations (12) and (15) imply

$$c_k c_k^+ - c_k^+ c_k = 1 - 2r/N; \tag{17}$$

$$c_k c_{k'}^+ - c_{k'}^+ c_k = -\frac{2}{N} \sum_f e^{i(k'-k)f} N_f \qquad (\text{for } k \neq k'); \tag{18}$$

$$[c_k c_{k'}]_- = [c_k^+ c_{k'}^+]_- = 0. \tag{19}$$

The commutation rules (19) have strictly Bose character, while Eqs. (17) and (18) do not. However, so long as $r/N \ll 1$ (a weakly excited system), Eqs. (17) and (18) approach arbitrarily close to the ordinary Bose relations. In the limit we obtain

$$[c_k c_{k'}^+]_- \approx \delta_{kk'}, \quad [c_k c_{k'}]_- = [c_k^+ c_{k'}^+,]_- = 0. \tag{20}$$

Thus we reach the conclusion that the spin-wave operators obey approximately the ordinary Bose relations, the conditions for these relations to hold being that the number of spin-excitations be small. This condition is satisfied in the region of low temperatures, well below the Curie point.

In spite of the formal similarity of some of our equations to the equations used by Frank[1] and Meyer,[2] our argument differs from theirs in the following respects. Frank introduces the spin-wave creation and annihilation operators c_f and c_f^+, considering them from the beginning as Fermi operators, in view of the fact that N_f can only take the values 0 and 1. He naturally obtains Fermi commutation rules also for the Fourier transformed operators c_k, c_k^+, and deduces from this that spin-waves obey Fermi statistics. Our argument shows that the condition $N_f = 0,\ 1$ implies that only one (namely the first of the relations (12)) of the commutation rules is of Fermi character. The rest of the commutation rules are of Bose type, as is seen from Eqs. (17) to (19). Also the result of applying these operators twice can be found from Eq. (15):

$$c_k c_k = \frac{1}{N} \sum_f e^{-i2kf} c_f c_f + \frac{1}{N} \sum_{f \neq f'} e^{-ik(f+f')} [c_f c_{f'}]_+. \tag{21}$$

The first sum on the right side of Eq. (21) vanishes by Eqs. (11) and (9). The second sum would vanish if the last of the relations (12) had Fermi character. But we have seen that this relation has Bose character, and therefore

$$c_k c_k = \frac{2}{N} \sum_{f<f'} e^{-ik(f+f')} c_f c_{f'}. \tag{22}$$

This expression is in general different from zero,*

*Equation (12_2) was also used by Meyer,[2] who wrote p_ν for c_f, and q_ν for c_f^+. Instead of Eq. (12_1) Meyer used $[p_\nu q_\nu]_- = u_\nu = 2p_\nu q_\nu - 1$. But it is easy to verify that $[p_\nu q_\nu]_+ = 1$, which implies Eq. (12_1).

*However, $(c_k)^{N+m} = 0$ for $m > 0$, since it is impossible in the homopolar approximation to have more than N spins in the same direction.

and therefore it is possible for more than one spin-wave to exist in the state with quasi-momentum **k**, as must be the case if they obey Bose statistics. This example illustrates the importance of the departure of part of the relations (12) from the Fermi type. Fermi commutation rules fail to hold for the majority of the relations (12), because the sign functions of Wigner are absent in the operators (2) and (6). The reason for this is that the antisymmetric character of the wave function of a many-electron system was already taken into account in deriving the Schrödinger equation (1). The exchange of left and right spins represented in Eq. (1) is not accompanied by a change in sign of the wave function. Frank introduced the Wigner sign functions into the fermion operators $b_{f\sigma}$ which he used to construct a Hamiltonian in the Heitler-London model. This procedure would not change anything in our work, since the operators occur in the Hamiltonian in such a way that the sign functions cancel each other out. One can see this, for example, by looking at the expression (A6) for the Hamiltonian of the exchange interaction in reference 3. The same remark applies to the work of Meyer,[2] whose Hamiltonian (12) reduces to Frank's Hamiltonian when the external magnetic field is set equal to zero.

Frank attempted to deduce the Fermi statistics from a direct solution of the Schrödinger equation. We have criticized this work in a paper with Ishmukhametov.[8] Here we only remark that it is unsafe to argue about the statistics of spin-waves on the basis of supplementary conditions in which functions of the type a_{nn}, which ought to vanish by virtue of the Pauli principle, are set equal to non-vanishing quantities. In this connection we may observe that the functions $u_2(R_i, R_i)$, which correspond to the a_{nn}, do vanish in the work of Van Kranendonk.[5]

3. We deduced the Bose statistics for spin-waves from two arguments. First, we showed that more than one spin-wave can exist in a state with a given wave-vector **k**. Second, we showed that when $r/N \ll 1$ the relations (17) to (19) coincide approximately with the usual Bose commutation rules. When we pass from the approximate relations (20) to the exact Bose commutation rules

$$[c_k c_{k'}^+]_- = \delta_{kk'}, \qquad [c_k c_{k'}]_- = [c_k^+ c_{k'}^+]_- = 0 \tag{23}$$

the occupation number n_k becomes unbounded above, although the actual number of spin waves[9] cannot exceed $N/2$. But in the low-temperature region, in which only states with a number of spin-waves small compared to N are measurably excited, the occupation numbers $n_k > N/2$ have no practical effect in calculations of thermodynamic quantities. The contributions from large n_k decrease exponentially. One can verify this by calculating the partition function Z, taking account of the boundedness of the occupation numbers* n_f, as was done in the paper of Tolmachev and Tiablikov.[10] If one uses the operators c_f defined above, one does not need any projection operator P to project the wave function onto the subspace of occupation numbers zero and one. The limitation of the occupation numbers is already included in the definition of the operators c_f. In the zero-order approximation the partition function becomes

$$Z_0 = \sum_{\{n_k\}} \sum_{\{n_f, n_f'\}} S(\ldots n_k \ldots | \ldots n_f \ldots)\, (a_{\ldots n_f \ldots} a_{\ldots n_f' \ldots}) \times S^*(\ldots n_k \ldots | \ldots n_f' \ldots) \exp\{-\sum_k E(k)\, n_k / \varkappa T\}, \tag{24}$$

Here T is the temperature, $\varkappa$ is Boltzmann's constant,

$$a_{\ldots n_f \ldots} = \prod_f (c_f)^{n_f} a_0 \tag{25}$$

are a system of orthonormal functions in the space of occupation numbers $n_f = 0$ or 1, a_0 is the vacuum state, and

$$S(\ldots n_f \ldots | \ldots n_k \ldots) = n^{-r/2} \left(\prod_k n_k!\right)^{-1/2} \sum_{\mathcal{P}_{f_h}} \prod_k \frac{1}{n_k!} \exp\{-ik(f_{h_1} + \ldots)\}, \tag{26}$$

where $\mathcal{P}_{f_h}$ is a permutation of all the right vertices f_h.

Equations (24) to (26) imply the result (15) of reference 10. This means that at low temperatures, for which $\exp(-E(k)/\varkappa T) \ll 1$, the Bloch theory is valid. Compare also the paper of Dyson,[11] where the kinematical interaction, the boundedness of n_f, also produces an exponentially small effect.

So we see that in the low-temperature region it is actually possible to proceed from the approximate Bose relations (20) to the ordinary Bose commutation rules (23).

On the other hand it appears that the requirement that the ordinary Bose commutation rules be strictly valid is not consistent for a system of a finite number of particles, even when the system can be described by a wave-function which is symmetrical with respect to the interchange of particles. The fact is that Eq. (23) can only be satisfied by operators which are represented by infinite matrices. Thus the occupation numbers for particles or quasi-particles in the various states must be unbounded.

*The occupation number of right spins, which was denoted by N_f in Sec. 2, is denoted by n_f in Sec. 3. This is to bring the notations into agreement with those of reference 10.

Nevertheless, for a system to obey Bose statistics it is not necessary that the number of particles be unbounded.*

It seems helpful, when second quantizing a system with a finite number N_1 of particles obeying Bose statistics, to use finite-dimensional operators, which satisfy commutation rules different from (23), but keep the occupation numbers bounded. Repeating the usual derivation of the expression for the Hamiltonian of a system which obeys Bose statistics,[15]

$$\mathcal{H} = \sum_p n_p \varepsilon^{(p)} + \frac{1}{2} \sum_{p_1, p_2, p_3, p_4} b^+_{p_1} b^+_{p_2} (p_1, p_2 | G | p_3, p_4)\, b_{p_4} b_{p_3}, \tag{27}$$

one can verify that the same expression remains valid when one uses the operators

$$b_p = \beta_p \sqrt{n_p}\,, \qquad b^+_p = \sqrt{n_p}\, \beta^+_p\,, \tag{28}$$

Here β_p and β^+_p are defined by

$$\beta_p a(\ldots n_p \ldots) = [1 - \delta(n_p - N_1)]\, a(\ldots, n_p + 1, \ldots), \tag{29}$$

$$\beta^+_d a(\ldots n_p \ldots) = [1 - \delta(n_p)]\, a(\ldots, n_p - 1, \ldots) \tag{30}$$

and can be represented by $(N_1 + 1)$-dimensional matrices of the form

$$\beta_p = \begin{vmatrix} 010\ldots0 \\ 001\ldots0 \\ \cdots\cdots \\ \cdots\cdots \\ 000\ldots1 \\ 000\ldots0 \end{vmatrix} \qquad \beta^+ = \begin{vmatrix} 00\ldots000 \\ 10\ldots000 \\ \cdots\cdots \\ \cdots\cdots \\ 00\ldots100 \\ 00\ldots010 \end{vmatrix} \tag{31}$$

Equations (28) to (31) imply the following relations between the operators b_p and b^+_p:

$$b^+_p b_p = n_p\,, \qquad b_p b^+_p = (n_p + 1)\,[1 - \delta(n_p - N_1)]\,, \tag{32}$$

$$[b_p b^+_p]_- = 1 - (n_p + 1)\,\delta(n_p - N_1), \tag{33$_1$}$$

$$[b_p b^+_{p'}]_- = 0 \qquad (\text{for } p \neq p'), \tag{33$_2$}$$

$$[b_p b_{p'}]_- = [b^+_p b^+_{p'}]_- = 0\,. \tag{33$_3$}$$

The commutation rules arising from the second quantization of a Bose system of a fixed finite number of particles thus differ from the usual commutation rules by the extra term $(n_p + 1)\,\delta(n_p - N_1)$ on the right side of Eq. (33$_1$). This term makes it impossible for any occupation number to exceed the value $(n_p)_{max} = N_1$. To prove this, one can calculate the matrix element of the expression

$$n_p b_p - b_p n_p = -[1 - (n_p + 1)\,\delta(n_p - N_1)]\, b_p\,, \tag{34}$$

by using Eq. (33). In the representation in which n_p is diagonal, the matrix element of b_p can differ from zero only when

$$n'_p - n''_p = -[1 - (n'_p + 1)\,\delta(n'_p - N_1)]\,, \tag{35}$$

which implies

$$n''_p = \begin{cases} n'_p + 1 & \text{for } n'_p < N_1 \\ 0 & \text{for } n'_p = N_1 \end{cases}, \tag{36}$$

Thus n_p can actually never exceed N_1.

We now apply the above arguments in the limiting cases $(n_p)_{max} = \infty$ and $(n_p)_{max} = 1$. In the first case Eq. (33) reduce to the usual Bose relations, since for any value of n_p the δ-function on the right of Eq. (33$_1$) vanishes when $(n_p)_{max} = \infty$. In the second case we may use Eq. (32) to transform (33$_1$) into

$$[b_p b^+_p]_+ = 2n_p + 1 - (n_p + 1)\,\delta(n_p - 1) = 1\,, \tag{37}$$

Together with Eq. (33$_2$) and (33$_3$), this gives the plus-minus quantization rules (12), so that the latter may be considered to be a special case of the quantization of a system with bounded occupation numbers. If the index f had referred to a cell in phase-space instead of to a vertex of a lattice, the boundedness of the occupation numbers n_f would have led in general to intermediate statistics.[13] But in the case considered in section (2), after transforming to momentum-space, the occupation numbers n_k were bounded only by the total number of spin-waves which could exist in the given system. This justifies the use of Bose statistics at low temperatures.

4. We now consider the problem of polar excitations. The Hamiltonian for a many-electron system with polar states may be written in the following form, in the notation of second quantization:[16,17]

$$\mathcal{H} = \sum g(f, f')\, a^+_{f\sigma} a_{f'\sigma} + \frac{1}{2} \sum F(f_1, f_2;\ f'_1,\ f'_2)\, a^+_{f_1\sigma_1} a^+_{f_2\sigma_2} a_{f'_2\sigma_2} a_{f'_1\sigma_1} \tag{38}$$

Here all the indices are to be summed. The σ are spin indices. The $a^+_{f\sigma}$ and $a_{f\sigma}$ are Fermi operators which operate on the occupation numbers $n_{f\sigma}$ of states (f, σ) whose wave-functions θ_f form an orthonormal system. The $g(f, f')$ and $F(f_1, f_2; f'_1, f'_2)$ are matrix elements:

$$g(f, f') = \int \theta_f(r) \left[-\frac{\hbar^2}{2m} \nabla^2 + \sum_{f''} u_{f''}(r) \right] \theta_{f'}(r)\, dr, \tag{39}$$

$$F(f_1, f_2;\ f'_1,\ f'_2) = \int \Phi(r, r')\, \theta_{f_1}(r)\, \theta_{f'_1}(r)\, \theta_{f_2}(r')\, \theta_{f'_2}(r')\, dr\, dr' \tag{40}$$

*Sommerfeld[12] showed that one can use, instead of the usual Bose-Einstein distribution function, the distribution function of Gentile,[13] putting $(n_p)_{max} = N_1$. However, in the approximation in which we use the Stirling formula, the improvement so obtained is inconsequential.[14]

Here $u_f(r)$ is the potential energy of an electron in the field of the atomic core at vertex f, while $\Phi(r, r')$ is the potential energy of the Coulomb repulsion between two electrons. Keeping in Eq. (38) those matrix elements which contain not more than two distinct functions θ_f in the integrand, and using the Fermi commutation rules

$$[a_{f\sigma}a^+_{f'\sigma'}]_+ = \delta_{f\sigma,f'\sigma'},\quad [a_{f\sigma}a_{f'\sigma'}]_+ = [a^+_{f\sigma}a^+_{f'\sigma'}]_+ = 0, \quad (41)$$

we derive from Eq. (38)

$$\begin{aligned}\mathcal{H} &= \sum_f g(f, f)\, n_f + \frac{1}{2} A \sum_f n_f(n_f - 1)\\ &+ \frac{1}{2}\sum_{f\neq f'} B_{ff'} n_f n_{f'} - \frac{1}{2}\sum_{f\neq f'} J_{ff'} \sum_\sigma n_{f\sigma} n_{f'\sigma}\\ &+ \sum_{f\neq f'} L_{ff'} \sum_\sigma a^+_{f\sigma}a_{f'\sigma} + \frac{1}{2}\sum_{f\neq f'} J_{ff'} \sum_{\sigma_1,\,\sigma_2} a^+_{f\sigma_1}a^+_{f\sigma_2}a_{f'\sigma_2}a_{f'\sigma_1}\\ &+ \frac{1}{2}\sum_{f\neq f'} J_{ff'} \sum_{\sigma_1\neq\sigma_2} a^+_{f\sigma_1}a^+_{f'\sigma_2}a_{f\sigma_2}a_{f'\sigma_1}.\end{aligned} \quad (42)$$

Here

$$A = F(f, f; f, f) = \int \Phi(r, r')\,\theta_f^2(r)\,\theta_f^2(r')\,dr\,dr' \quad (43)$$

is the interaction energy between two electrons in the same state θ_f (the self-energy of a pair).

$$B_{ff'} = F(f, f'; f, f') = \int \Phi(r, r')\,\theta_f^2(r)\,\theta_{f'}^2(r')\,dr\,dr' \quad (44)$$

is the energy of Coulomb repulsion of two electrons, one in the state θ_f and the other in the state $\theta_{f'}$.

$$L_{ff'} = g(f, f') + \sum_{f_1}(n_{f_1} - \delta_{ff_1})\,F(f_1, f; f_1, f') \quad (45)$$

is a displacement integral, and

$$\begin{aligned}J_{ff'} &= F(f, f'; f', f) =\\ &\int \Phi(r, r')\,\theta_f(r)\,\theta_{f'}(r)\,\theta_{f'}(r')\,\theta_f(r')\,dr\,dr'\end{aligned} \quad (46)$$

is an exchange integral. In addition we have used the notation $n_f = \sum_\sigma n_{f\sigma}$.

We now define a set of Fermi operators[15]

$$a_{f\sigma} = \alpha_{f\sigma}\nu_{f\sigma},\quad a^+_{f\sigma} = \nu_{f\sigma}\alpha^+_{f\sigma}, \quad (47)$$

where $\nu_{f\sigma}$ are the sign functions of Wigner, and the operators $\alpha_{f\sigma}$ and $\alpha^+_{f\sigma}$ act according to the rules

$$\alpha_{f\sigma}a(\ldots n_{f\sigma}\ldots) = \begin{cases} a(\ldots, n_{f\sigma}+1, \ldots) & \text{for } n_{f\sigma} = 0\\ 0 & \text{for } n_{f\sigma} = 1\end{cases}. \quad (48_1)$$

$$\alpha^+_{f\sigma}a(\ldots n_{f\sigma}\ldots) = \begin{cases} 0 & \text{for } n_{f\sigma} = 0\\ a(\ldots, n_{f\sigma}-1, \ldots) & \text{for } n_{f\sigma} = 1.\end{cases} \quad (48_2)$$

It is easy to verify that the sign functions compensate each other in the diagonal terms and in those of the nondiagonal terms (42) which contain the exchange integrals $J_{ff'}$. But in the terms containing $L_{ff'}$ the functions do not compensate. It is convenient to consider two limiting cases: (a) $|L| \gg |J|$ and (b) $|L| \ll |J|$. Here L and J are the values of $L_{ff'}$ and $J_{ff'}$ for nearest neighbors.

In case (a) the nondiagonal terms are dominated by the term $\sum L_{ff'} \sum a^+_{f\sigma}a_{f'\sigma}$ which contains a double product of operators $a^+_{f\sigma}a_{f'\sigma}$ and describes one-electron transitions. The effect of such transitions upon an electron with left spin will be one of the following: exchange of places between a hole and a left spin, creation of a hole in place of a left spin, creation of a pair in place of a right spin, creation of two single spins in place of a pair and a hole, and finally exchange of places between a pair and a right spin. Analogous processes exist for the transitions of an electron with right spin. We now make a Fourier transformation of the operators $a_{f\sigma}$ and $a^+_{f\sigma}$ according to Eq. (15). The resulting operators $a_{k\sigma}$ and $a^+_{k\sigma}$ obey Fermi commutation rules of the type of Eq. (41). This shows that the quasi-particles in case (a) obey Fermi statistics.

In case (b) the nondiagonal terms are dominated by the last two sums in Eq. (42), which contain a product of four operators $a_{f\sigma}$ and describe two-electron transitions. Of these sums, the sixth term in Eq. (42) represents an exchange between a pair and a hole, while the last term represents an exchange between a left and a right spin. In this case we are neglecting the processes of creation and annihilation of pairs in one-electron transitions. It is therefore convenient to introduce operators acting upon the occupation numbers of pairs, holes and simple right and left spins. We change slightly the notations used in reference 16 in order to be consistent with Eq. (6). The new operators Φ_f, Ψ_f, φ_f and ψ_f are defined as follows:

$$\begin{aligned}&\Phi_f a(\ldots P_f, Q_f, R_f, S_f \ldots)\\ &= \delta(1 - P_f)\,a(\ldots P_f - 1, Q_f, R_f, S_f \ldots),\end{aligned} \quad (49)$$

$$\begin{aligned}&\Phi^+_f a(\ldots P_f, Q_f, R_f, S_f \ldots)\\ &= \delta(P_f)\,a(\ldots P_f + 1, Q_f, R_f, S_f \ldots).\end{aligned} \quad (50)$$

Analogously we define Ψ_f, Ψ^+_f, ψ_f, ψ^+_f, φ_f and φ^+_f. Here P_f, Q_f, R_f and S_f take the following values:

P_f	Q_f	R_f	S_f	
1	0	0	0	if the vertex f is a pair,
0	1	0	0	if the vertex f is a hole,
0	0	1	0	if the vertex f is a right-spin,
0	0	0	1	if the vertex f is a left-spin.

(51)

The same argument which led to Eq. (7) now shows that the operators Ψ_f, Φ_f, φ_f and ψ_f satisfy the following relations:

$$\begin{aligned}
&[\Phi_f\Phi_f^+]_+ = [\Psi_f\Psi_f^+]_+ = [\varphi_f\varphi_f^+]_+ = [\psi_f\psi_f^+]_+ = 1,\\
&[\Phi_{f'}\Phi_f^+]_- = [\Psi_{f'}\Psi_f^+]_- = [\varphi_f\varphi_{f'}^+]_- = [\psi_f\psi_{f'}^+]_- = 0 \quad (\text{for } f \neq f'),\\
&[\Phi_f\Phi_{f'}]_- = [\Psi_f\Psi_{f'}]_- = [\varphi_f\varphi_{f'}]_- = [\psi_f\psi_{f'}]_- = 0,\\
&[\Phi_f^+\Phi_{f'}^+]_- = [\Psi_f^+\Psi_{f'}^+]_- = [\varphi_f^+\varphi_{f'}^+]_- = [\psi_f^+\psi_{f'}^+]_- = 0.
\end{aligned} \tag{52}$$

We thus find a plus-minus quantization similar to Eq. (7). For the reasons discussed in Sec. 2, the quasi-particles in momentum-space now obey Bose statistics.

The choice between the limiting cases (a) and (b) depends on the ratio between the positive and negative terms in the displacement integral $L_{ff'}$. If these terms are approximately equal then $|L_{ff'}| \ll |J_{ff'}|$. But if terms of one sign predominate in $L_{ff'}$, then $|L_{ff'}| \gg |J_{ff'}|$, for $J_{ff'}$ contains one overlap factor more than $L_{ff'}$. The latter state of affairs will exist, for example, among the terms g(f, f'), which are proportional to the effective charge of the atomic core and are negative at least for S-states.

5. We have reached the conclusion that the quasi-particles arising in a many-electron system in a crystal obey Fermi statistics when one-electron transitions are predominant, and obey Bose statistics when two-electron transitions are predominant in the dynamics of the system.* The well-known connection between spin and statistics, according to which particles with half-integer spin obey Fermi statistics and particles with integer spin Bose statistics, is thus preserved. In a single-electron transition in a crystal a half-integer spin moves, while in a two-electron transition an integer spin moves. Our results here confirm the statement of I. M. Lifshitz[4] at the Kiev conference on semiconductors in 1956, concerning the statistics of pairs and holes.*

*The term "transition" is to be understood to refer to the particular model chosen.

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