THE COMPENSATION PRINCIPLE AND THE SELF-CONSISTENT FIELD METHOD

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1. THE COMPENSATION PRINCIPLE

IN the present paper we consider a possible generalization of the principle of compensation of dangerous diagrams to the case of a state which is non-uniform in space, and we shall also establish the connection between it and the self-consistent field method.

The main example used here will be the problem of the electrodynamics of the superconducting state, when we must investigate the reaction of a dynamical system to the application of a non-uniform external field.

Let $\mathbf{A}(\mathbf{r})$ be the vector potential, a function of \mathbf{r} . There will then be in the Hamiltonian of each electron an additional term

$$-\frac{e}{2m}\{(pA)+(Ap)\}+\frac{e^2}{2m}A^2,$$

which violates spatial uniformity.

We note that the presence of terms of this kind makes the compensation of diagrams corresponding to momenta k, -k insufficient. Indeed, if we define A(r) as the superposition of Fourier components

$$A(q)e^{-i(q,r)}$$

we see that diagrams with arbitrary momenta k_1 , k_2 will be dangerous in the same sense, at any rate those for which $q - k_1 + k_2$ is sufficiently small. It is clear that it is impossible to eliminate them by

our usual canonical transformation which mixes the creation and annihilation amplitudes of the momenta $\pm k$, since it contains only one arbitrary function u_k (or v_k).

To compensate diagrams with an arbitrary pair of momenta p_1 , p_2 we must use the more general canonical transformation formulated in reference 1,

$$a_{j} = \sum_{(\mathbf{v})} (u_{j\mathbf{v}}a_{\mathbf{v}} + v_{j\mathbf{v}}a_{\mathbf{v}}), \qquad (1)$$

where $f = (p, \sigma)$, σ is the spin index, while $u_{f\nu}$ and $v_{f\nu}$ are arbitrary functions connected through the peculiar orthonormality relations:

$$\sum_{(\mathbf{v})} \{ u_{f\mathbf{v}} u_{f\mathbf{v}}^{*} + v_{f\mathbf{v}} v_{f'\mathbf{v}}^{*} \} = \delta(f - f'),$$

$$\sum_{(\mathbf{v})} \{ u_{f\mathbf{v}} v_{f'\mathbf{v}} + u_{f'\mathbf{v}} v_{f\mathbf{v}} \} = 0.$$
(2)

These relations assure, indeed, the canonical character of the transformation (1) under consideration.

To simplify our discussion we study here the generalized compensation principle in relation to a Hamiltonian with direct interactions between the particles, since the first approximation will in that case already lead to a nontrivial result. As was already noted earlier,² if we take, for instance, the electron-phonon interaction into account, it is necessary to go to the second approximation.

Having different applications in mind, we shall use a sufficiently general expression for the total Hamiltonian

$$H = \sum_{(f, f')} T(f, f') a_{f}a_{f'} + \frac{1}{2} \sum_{(f_1, f_2, f'_2, f'_1)} U(f_1, f_2; f'_2, f'_1) a_{f_1}a_{f_2}a_{f'_2}a_{f'_1},$$

$$T(f, f') = I(f, f') - \lambda \delta(f - f'),$$
(3)

where λ is the chemical potential, I the Hamiltonian of the individual particles, and U the energy of the interaction between a pair of particles. We shall, of course, assume here that I and U satisfy the usual requirements about symmetry, Hermitian character, and so on.

The principle of compensation of dangerous diagrams in the first approximation under consideration will be

$$\langle \boldsymbol{x}_{\boldsymbol{\gamma}_1} \boldsymbol{x}_{\boldsymbol{\gamma}_2} \boldsymbol{\mu} \rangle_0 = 0. \tag{4}$$

The averaging is taken over the state C_0 , corresponding to the vacuum for the new amplitudes α :

$$\mathbf{x}_{\nu}C_{0} = 0, \quad C_{0}^{*}\mathbf{x}_{\nu} = 0.$$
 (5)

We can write Eq. (4) more explicitly by substituting there Eq. (1) and simply evaluating the vacuum averages. In this way we obtain explicit expressions for the unknowns u, v; these must be solved in conjunction with the conditions (2).

In a number of cases it is more convenient to put these equations in a somewhat different form.

We show thereto that it follows from (4) that

$$\mathfrak{A} \equiv \langle [a_{j_1}a_{j_2}; H] \rangle_{\mathbf{0}} = 0, \\ \mathfrak{B} \equiv \langle [a_{j_1}a_{j_2}; H] \rangle_{\mathbf{0}} = 0. \end{cases}$$

$$(6)$$

We have, indeed,

$$\begin{split} \mathfrak{A} &\equiv \sum_{(\mathbf{v}_{1}, \mathbf{v}_{2})} \langle [(u_{f_{1}\mathbf{v}_{1}}\mathbf{x}_{\mathbf{v}_{1}} + v_{f_{1}\mathbf{v}_{1}}\mathbf{x}_{\mathbf{v}_{1}})(u_{f_{2}\mathbf{v}_{2}}\mathbf{x}_{\mathbf{v}_{2}} + v_{f_{2}\mathbf{v}_{2}}\mathbf{x}_{\mathbf{v}_{2}}); \ H] \rangle_{t} \\ &= \sum_{(\mathbf{v}_{1}, \mathbf{v}_{2})} u_{f_{1}\mathbf{v}_{1}}u_{f_{2}\mathbf{v}_{2}} \langle \mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}}H - H\mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}} \rangle_{0} \\ &+ \sum_{(\mathbf{v}_{1}, \mathbf{v}_{2})} u_{f_{1}\mathbf{v}_{1}}v_{f_{2}\mathbf{v}_{2}} \langle \mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}}H - H\mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}} \rangle_{0} \\ &+ \sum_{(\mathbf{v}_{1}, \mathbf{v}_{2})} v_{f_{1}\mathbf{v}_{1}}u_{f_{2}\mathbf{v}_{2}} \langle \mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}}H - H\mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}} \rangle_{0} \\ &+ \sum_{(\mathbf{v}_{1}, \mathbf{v}_{2})} v_{f_{1}\mathbf{v}_{1}}u_{f_{2}\mathbf{v}_{2}} \langle \mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}}H - H\mathbf{a}_{\mathbf{v}_{1}}\mathbf{a}_{\mathbf{v}_{2}} \rangle_{0} . \end{split}$$

In view of (5), however,

$$\langle H\mathfrak{a}_{\nu_1}\mathfrak{a}_{\nu_2}\rangle_0 = \langle \overset{\circ}{\mathfrak{a}_{\nu_1}}\overset{\circ}{\mathfrak{a}_{\nu_2}}H\rangle_0 = \langle \overset{\circ}{\mathfrak{a}_{\nu_1}}\mathfrak{a}_{\nu_2}H\rangle_0 = \langle H\overset{\circ}{\mathfrak{a}_{\nu_1}}\mathfrak{a}_{\nu_2}\rangle_0 = 0$$

and also

$$\langle \mathfrak{a}_{\nu_1} \overset{*}{\mathfrak{a}_{\nu_2}} H - H \mathfrak{a}_{\nu_1} \overset{*}{\mathfrak{a}_{\nu_2}} \rangle_0 = \langle - \overset{*}{\mathfrak{a}_{\nu_2}} \mathfrak{a}_{\nu_1} H + H \overset{*}{\mathfrak{a}_{\nu_2}} \mathfrak{a}_{\nu_1} \rangle_0 = 0.$$

Using (4) it follows therefore also that

$$\begin{aligned} \mathfrak{A} &= \sum_{(\mathbf{v}_1, \mathbf{v}_2)} u_{f_1 \mathbf{v}_1} u_{f_2 \mathbf{v}_2} \langle \mathfrak{a}_{\mathbf{v}_1} \mathfrak{a}_{\mathbf{v}_2} H \rangle_0 \\ &- \sum_{(\mathbf{v}_1, \mathbf{v}_2)} v_{f_1 \mathbf{v}_1} v_{f_2 \mathbf{v}_2} \langle \mathfrak{a}_{\mathbf{v}_2} \mathfrak{a}_{\mathbf{v}_1} H \rangle_0^* = 0. \end{aligned}$$

The second equation of (6) is proved in a similar way.

We can also easily verify that Eq. (4) follows from Eq. (6). These two sets (4) and (6) are thus completely equivalent.

We shall show now that the expressions \mathfrak{A} and \mathfrak{B} themselves are not independent.

We start with a transformation of the orthonormalization relations (2). We shall introduce the combined indices:

$$g = (f, \rho), \quad \rho = 0.1 \\ \omega = (\nu, \tau), \quad \tau = 0.1$$
(7)

and put

$$\begin{aligned} \varphi_{\mathbf{v},0}(f,0) &= v_{f\mathbf{v}}^{*}, \quad \varphi_{\mathbf{v},0}(f,1) = u_{f\mathbf{v}}, \\ \varphi_{\mathbf{v},1}(f,0) &= u_{f\mathbf{v}}^{*}, \quad \varphi_{\mathbf{v},1}(f,1) = v_{f\mathbf{v}}. \end{aligned}$$

$$(8)$$

In this notation the relations under consideration take the usual form

$$\sum_{(m)} \varphi_m^*(g) \varphi_m(g') = \delta(g - g'), \tag{9}$$

from which it follows that

$$\sum_{(g)} \varphi_{\omega}^{*}(g) \varphi_{\omega'}(g) = \delta(\omega - \omega'),$$

or, in the old notation

$$\sum_{(f)} \left\{ u_{j\gamma_{1}}^{*} u_{j\gamma_{2}} + v_{j\gamma_{2}} v_{j\gamma_{1}} \right\} = \delta(\gamma_{1} - \gamma_{2}),$$

$$\sum_{(f)} \left\{ v_{j\gamma_{1}}^{*} u_{j\gamma_{2}} + v_{j\gamma_{2}}^{*} u_{j\gamma_{1}} \right\} = 0.$$
(10)

With the aid of these relations we can easily express the amplitudes α , $\dot{\alpha}$ in terms of a, \dot{a} :

$$a_{\gamma} = \sum_{(f)} \{ u_{j\gamma}^* a_j + v_{j\gamma} a_j \}.$$
(11)

We now turn our attention to the identity

$$\langle [\mathbf{a}_{\mathbf{v}_1}\mathbf{a}_{\mathbf{v}_2}; H] \rangle_0 = 0, \tag{12}$$

which is a direct consequence of the properties (5). Substituting into this Eq. (11) we find

$$\sum_{(f_1, f_2)} \langle [(u_{f_1 \vee i} a_{f_1} + v_{f_1 \vee i}^* a_{f_1}) (u_{f_2 \vee i}^* a_{f_2} + v_{f_2 \vee i} a_{f_2}); H] \rangle_0 = 0$$

or, explicitly:

$$\sum_{(f_{1}, f_{2})} u_{f_{1} \vee_{i}} u_{f_{2} \vee_{2}}^{*} \langle [a_{f_{1}} a_{f_{2}} ; H] \rangle_{0} + \sum_{(f_{1}, f_{2})} u_{f_{1} \vee_{i}} \cup_{f_{2} \vee_{2}} \langle [a_{f_{1}} a_{f_{2}} ; H] \rangle_{0} \\ + \sum_{(f_{1}, f_{2})} v_{f_{1} \vee_{i}} u_{f_{2} \vee_{2}}^{*} \langle [a_{f_{1}} a_{f_{2}} ; H] \rangle_{0} \\ + \sum_{(f_{1}, f_{2})} v_{f_{1} \vee_{i}} v_{f_{2} \vee_{2}} \langle [a_{f_{1}} a_{f_{2}} ; H] \rangle_{0} = 0.$$

In this way we verify that \mathfrak{N} and \mathfrak{B} are related by the following identity:*

$$\sum_{(f_1, f_2)} \{ u_{f_1 \vee_1} u_{f_2 \vee_2}^* \mathfrak{B}(f_1, f_2) + u_{f_1 \vee_1} v_{f_2 \vee_2} \mathfrak{A}^*(f_1, f_2) + v_{f_1 \vee_1} v_{f_2 \vee_2} \mathfrak{A}^*(f_1, f_2) + v_{f_1 \vee_1} v_{f_2 \vee_2} \mathfrak{B}^*(f_1, f_2) \} = 0.$$
(13)

We shall now turn to the problem of finding explicit expressions for \mathfrak{A} and \mathfrak{B} . We have

$$\mathfrak{A}(f_{1}, f_{2}) = \sum_{\langle f \rangle} \{T(f_{1}, f) \langle a_{f}a_{f_{2}} \rangle_{0} + T(f_{2}, f) \langle a_{f_{1}}a_{f_{2}} \rangle_{0} \}$$

$$+ \sum_{\langle f_{1}', f_{2}' \rangle} U(f_{1}, f_{2}; f_{2}', f_{1}') \langle a_{f_{1}}'a_{f_{2}'} \rangle_{0} + \sum_{\langle f, f_{1}', f_{2}' \rangle} U(f_{1}, f; f_{2}', f_{1}')$$

$$\times \langle a_{f}a_{f_{2}}a_{f_{2}}'a_{f_{1}'} \rangle_{0} + \sum_{\langle f, f_{1}', f_{2}' \rangle} U(f, f_{2}; f_{2}', f_{1}') \langle a_{f}a_{f_{1}}a_{f_{2}}a_{f_{1}'} \rangle_{0}$$

$$(14)$$

and also

$$\mathfrak{B}(f_{1}, f_{2}) = \sum_{(f)} \{T(f_{2}, f) \dot{a}_{f_{1}} a_{f} \rangle_{0} - T(f, f_{1}) \dot{a}_{f} a_{f_{2}} \rangle_{0} \}$$

$$- \sum_{(f, f_{1}', f_{2}')} \{U(f_{1}', f_{2}'; f, f_{1}) \dot{a}_{f_{1}} \dot{a}_{f_{2}} a_{f} a_{f_{2}} \rangle_{0}$$

$$- U(f_{2}, f; f_{2}', f_{1}') \dot{a}_{f_{1}} \dot{a}_{f} a_{f_{2}} a_{f_{1}}' \rangle_{0} \}.$$
(15)

*We note that if we had replaced the averages over the vacuum state C_o in Eqs. (6), which define ${\mathfrak A}$ and ${\mathfrak B}$, by the average

$$\frac{S_p(\ldots D)}{S_p D}$$

over some distribution D which is diagonal in the ... n_{ν} ... $(n_{\nu} = \alpha_{\nu}^{+} \alpha_{\nu})$ representation, then the identity (13) would all the same be true for $\nu_1 = \nu_2$. Indeed, since D is diagonal, $Tr(\alpha_{\nu}^{+}\alpha_{\nu} HD) = Tr(HD\alpha_{\nu}^{+}\alpha_{\nu}) = Tr(H\alpha_{\nu}^{+}\alpha_{\nu} D)$ and, hence,

$$\begin{bmatrix} a_{\nu} \alpha_{\nu}; H \end{bmatrix} = 0$$

We shall determine the vacuum expectation values

$$F(f, f') = \langle a_f a_{f'} \rangle_0, \quad \Phi(f_1, f_2) = \langle a_{f_1} a_{f_2} \rangle_0, \quad (16)$$

$$\begin{cases} F_{2}(f_{1}, f_{2}; f_{2}', f_{1}') = \langle a_{f_{1}}a_{f_{2}}a_{f_{2}}'a_{f_{1}}'\rangle_{0}, \\ \Phi_{2}(f_{1}; f_{2}, f_{3}, f_{4}) = \langle a_{f_{1}}a_{f_{3}}a_{f_{3}}a_{f_{3}}a_{f_{4}}\rangle_{0} \end{cases}$$

$$(17)$$

which occur here by expressing a, a in terms of α , $\dot{\alpha}$ using Eq. (1). We find in that way

$$F(f, f') = \sum_{(v)} v_{fv}^* v_{f'v}, \quad \Phi(f_1, f_2) = \sum_{(v)} u_{f_1v} v_{f_2v}, \quad (18)$$

$$F_{2}(f_{1}, f_{2}; f_{2}', f_{1}') = F(f_{1}, f_{1}')F(f_{2}, f_{2}') - F(f_{1}, f_{2}')F(f_{2}, f_{1}') + \Phi^{*}(f_{1}, f_{2})\Phi(f_{1}', f_{2}'),$$
(19)

$$\Phi_{2}(f_{1}; f_{2}, f_{3}, f_{4}) = F(f_{1}, f_{2}) \Phi(f_{3}, f_{4}) - F(f_{1}, f_{3}) \Phi(f_{2}, f_{4}) + F(f_{1}, f_{4}) \Phi(f_{2}, f_{3}).$$
(20)

Substituting the expressions obtained into (14) and (15) we obtain the required explicit expressions for \mathfrak{A} and \mathfrak{B} :

$$\begin{split} \mathfrak{A} & (f_1, f_2) = \mathfrak{A} & (f_1, f_2/F, \Phi), \\ \mathfrak{B} & (f_1, f_2) = \mathfrak{B} & (f_1, f_2/F, \Phi). \end{split}$$

We have, for instance,

$$\mathfrak{A}(f_{1}, f_{2}/F, \Phi) = \sum_{(f)} \{ E(f_{1}, f) \Phi(f, f_{2}) + E(f_{2}, f) \Phi(f_{1}, f) \}$$

+ $S(f_{1}, f_{2}) - \sum_{(f)} \{ F(f, f_{1}) S(f, f_{2})$
+ $F(f, f_{2}) S(f_{1}, f) \},$ (21)
where

where

$$E(f_{1}, f) = T(f_{1}, f) + \sum_{(f', f')} \{U(f_{1}, f''; f', f) - U(f_{1}, f''; f, f')\} F(f'', f'),$$

$$S(f_{1}, f_{2}) = \sum_{(f'_{1}, f'_{2})} U(f_{1}, f_{2}; f'_{2}, f_{1}) \Phi(f'_{1}, f'_{2}).$$

$$(22)$$

Our generalized compensation principle leads thus in the first approximation to the equations

$$\begin{array}{l} \mathfrak{A}(f_1, f_2/F, \Phi) = 0, \\ \mathfrak{B}(f_1, f_2/F, \Phi) = 0, \end{array}$$
 (23)

which had already been obtained earlier^{3,4} using a generalization of the well-known Hartree-Fock self-consistent field method.

Apart from these equations we have yet an additional condition, namely, that the functions F and Φ must be of the form (18).

It would, clearly, be very advisable to formulate such an additional condition in the form of a number of relations which are directly imposed upon F and Φ .

We note first of all that from (18) it follows at once that

$$F^*(f, f') = F(f', f), \quad \Phi(f_2, f_1) = -\Phi(f_1, f_2).$$
 (24)

We introduce again combined indices g and ω

and consider the matrix

$$K(g, g') = \sum_{\omega} \varphi_{\omega}^{*}(g) \varphi_{\omega}(g') n_{\omega}, \qquad (25)$$

in which

$$n_{\nu,0} = 1, \quad n_{\nu,1} = 0.$$

We have then

$$\begin{split} K(f, 0; f', 0) &= \sum_{(\nu)} v_{f\nu} v_{f'\nu}^*, \quad K(f, 0; f', 1) = \sum_{(\nu)} v_{f\nu} u_{f'\nu}, \\ K(f, 1; f', 0) &= \sum_{(\nu)} u_{f\nu}^* v_{f'\nu}^*, \quad K(f, 1; f', 1) = \sum_{(\nu)} u_{f\nu}^* u_{f'\nu}. \end{split}$$

By virtue of the orthonormalization condition (2) we get then

$$K(g, g') = \begin{vmatrix} F(f', f); & -\Phi(f, f') \\ \Phi^*(f, f'); & \delta(f - f') - F(f, f') \end{vmatrix} .$$
(26)

On the other hand, we see directly from the definition (25) that $\varphi_{\omega}(g)$ and n_{ω} are the eigenvectors and eigenvalues, respectively, of the operator K. Since these eigenvalues are equal to zero or unity, K must be a projection operator and hence

$$K = K^2. \tag{27}$$

If we write this relation out in detail we find the additional conditions which the functions F and Φ must satisfy:

We shall now show that conditions (24) and (28) are completely equivalent to the condition that F and Φ can be written in the form (18). To do this we must still prove that arbitrary F and Φ satisfying the conditions (24) and (28) can, indeed, be written in the form (18).

First we use the trivial conditions (24) and introduce the matrix K(g, g') by Eq. (26). By virtue of (24), K(g, g') is clearly Hermitian and can thus be represented in the form (25), where the $\varphi_{\omega}(g)$ will represent an orthonormal set of eigenvectors of K.

We shall introduce in the point set $\{g\}$ a point transformation T which changes (f, 0) into (f, 1), and vice versa. We have

$$TK = K(Tg; Tg')$$

= $\begin{vmatrix} \dot{a}(f-f') - F(f, f'); & \Phi^*(f, f') \\ -\Phi(f, f'); & F(f', f) \end{vmatrix}$
= $\hat{a}(g-g') - K^*(g, g').$

We can easily show because of this relation that if $\varphi(g)$ is some eigenvector of the operator K, and n is the corresponding eigenvalue, $\varphi^*(Tg)$

and 1-n will also be an eigenvector and eigenvalue for K.

We can thus use a numbering $\{\omega\}$ of the eigenvectors and eigenvalues of the operator K by a system of two indices { ν, τ } ($\tau = 0, 1$), putting

$$\begin{array}{ccc} n_{\nu, 0} = n_{\nu}, & n_{\nu, 1} = 1 - n_{\nu}, \\ \varphi_{\nu, 0}(g) = \varphi_{\nu}(g), & \varphi_{\nu, 1}(g) = \varphi_{\nu}^{*}(Tg). \end{array} \right)$$
(29)

We now use the conditions (28) from which it follows that

$$K = K^2$$

and thus that $n_{\omega} = 0$, 1. We shall write down only the value of n_{ν} and not that of $1-n_{\nu}$, avoiding thereby any arbitrariness contained in splitting the index ω into $(\nu, 0)$ and $(\nu, 1)$.

Having determined $\varphi_{\nu,\theta}(g)$ and $\varphi_{\nu,1}(g)$ we can now determine the functions $u_{f\nu}$ and $v_{f\nu}$ by inverting Eqs. (8). As the $\varphi_{\omega}(g)$ form a normal orthonormal set, we see that the functions u, v which we have found will satisfy Eq. (2).

To conclude our proof we must only still write out Eq. (25) in detail and note that the representations* (18) follow directly from it.

Our problem has thus been reduced to the solving of Eqs. (23) together with the additional conditions (24) and (28). The functions u and v do no longer explicitly occur here. Having found expressions for F and Φ we can then determine also the set of functions u, v using the method stated above.

We emphasize here that the definition of the set u, v contains a large amount of arbitrariness.

Indeed, let $\varphi_{\nu,0}(g)$ be an orthonormal set of eigenvectors for the operator K corresponding to a single eigenvalue. If we subject it to an arbitrary unitary transformation we obtain again an orthonormal set of eigenvectors of the operator K corresponding to a single eigenvalue. The same observation applies, of course, also to the $\varphi_{\nu,1}(g)$. We see, thus that the set $\{\varphi_{\nu,0}(g)\}$ ×

*It is interesting to note that if we were dealing with functions F and Φ which only satisfied conditions (24), we would, by repeating the discussion just given, obtain instead of (18) a representation of the form

$$F(f, f') = \sum_{(v)} \{ v_{fv}^* v_{f'v} (1 - n_v) + u_{fv}^* u_{f'v} n_v \},$$

$$\Phi(f, f') = \sum_{(v)} \{ u_{fv} v_{f'v} (1 - n_v) + v_{fv}^* u_{f'v} n_v \}.$$

We notice also that if F and Φ are determined by the averaging $F(f, f') = Tr\{a_{f}^{+}a_{f'}D\}(Tr D)^{-1}; \Phi(f, f') = Tr\{a_{f}a_{f'}D\}$ $(Tr D)^{-1}$ with an arbitrary positive statistical operator D, the operators K and 1-K must both be non-negative, and we have thus in the representation obtained here $0 \leqslant n_{\nu} \leqslant 1$.

 $\{\varphi_{\nu,1}(g)\}$ is determined only apart from arbitrary unitary transformations acting on the index ν . There is thus the same degree of arbitrariness also in the functions u, v.

We have already said that Eqs. (23) are not independent, since \mathfrak{A} and \mathfrak{B} are connected through the identity (13). It is therefore expedient in many cases to consider one of them:*

$$\mathfrak{A}\left(f_{1}, f_{2} \mid F, \Phi\right) = 0$$

together with the additional conditions (24) and (28). The other equation of (23) will then be satisfied automatically.

We consider as an example the problem of determining the superconducting ground state in superconductivity theory.

We put in our formulae $f = (p, \sigma)$, where p is the momentum and σ the spin index, the two values of which we shall indicate by the signs + and -. We shall, as usual, take[†]

$$I(p, p') = E(p)\delta(p-p'),$$

$$U(f_1, f_2; f'_2, f'_1) = \frac{1}{V}\delta(p_1 + p_2 - p'_1 - p'_2)\delta(\sigma_1 - \sigma'_1)\delta(\sigma_2 - \sigma'_2)$$

$$\times J(p_1, p_2; p'_2, p'_1),$$
(30)

where V is the volume of the system. For J we shall consider a real function which is invariant under reflection of the momenta $p \rightarrow -p$.

We can then easily check that we can satisfy all our equations and the additional conditions, if we put:

$$F(f, f') = \delta(f - f') F(p), \quad \Phi(f, f') = \delta(f + f') \Phi(f), \quad \beta = \Phi(p, -) = \Phi(p), \quad \Phi(p, +) = -\Phi(p), \quad \beta = \Phi(p), \quad \beta$$

where F(p) and $\Phi(p)$ are real functions of p, which are invariant under a reflection of the momenta and which are determined by the equations:

$$\left. \begin{array}{c} 2\xi\left(p\right)\Phi\left(p\right) + \left(1 - 2F\left(p\right)\right) \\ \times \frac{4}{V}\sum_{\left(p'\right)} J\left(p, -p, -p', p'\right)\Phi\left(p'\right) = 0, \\ F\left(p\right) = F^{2}\left(p\right) + \Phi^{2}\left(p\right), \end{array} \right\}$$

$$\left. \begin{array}{c} (32) \end{array}$$

in which

.

$$\xi(p) = E(p) - \lambda + \frac{1}{V} \sum_{(p')} \{2J(p', p; p, p') - J(p, p'; p, p')\}F(p').$$
(33)

*The case can also occur where $\Phi = 0$. The equation $\mathfrak{A} = 0$ is then, on the other hand, satisfied in a trivial manner and we must restrict our considerations to the equation $\mathfrak{B} = 0$.

[†]We call attention to the fact that in our presentation we use a discrete delta-function, i.e., the Kronecker symbol:

$$\delta(p) = 1, \quad p = 0; \quad \delta(p) = 0, \quad p \neq 0.$$

We put here

$$-\frac{1}{V}\sum_{(\mathbf{p}')}J(p, -p; -p', p')\Phi(\mathbf{p}') = C(p).$$

We get then from (32)

$$\Phi(p) = \frac{C(p)}{2\Omega(p)},
\Omega(p) = \sqrt{\xi^{2}(p) + C^{2}(p)},
F(p) = \frac{1}{2} \left\{ 1 - \frac{\xi(p)}{\Omega(p)} \right\}$$
(34)

and we verify that C(p) satisfies the equation

$$C(p) + \frac{1}{V} \sum_{(p')} J(p, -p; -p', p') \frac{C(p')}{2Q(p')} = 0.$$
 (35)

It is clear that we have here gone over to the usual equations of the theory of superconductivity.

The corresponding functions u, v can be determined by putting

 $\begin{array}{l} u_{f\nu} = u\left(p\right)\delta\left(\nu - f\right), & \upsilon_{f\nu} = \upsilon\left(f\right)\delta\left(\nu + f\right), \\ + \right) = \upsilon\left(p\right), & \upsilon\left(p, -\right) = -\upsilon\left(p\right), \end{array} \right\}$ (36) v(p, +) = v(p),where $v^2(p) = F(p),$ $u^{2}(p) = 1 - F(p).$

2. THE SELF-CONSISTENT FIELD METHOD

We considered up to now only the problem of determining a time-independent ground state. One can, however, easily generalize the self-consistent field method to study also processes which depend explicitly on the time.

To do this we introduce the time-dependent functions

$$\begin{cases} F_t(f_1, f_2) = a_{f_1}a_{f_2}, \\ \Phi_t(f_1, f_2) = \overline{a_{f_1}a_{f_2}} \end{cases}$$
(37)

and consider the amplitudes a in the Heisenberg representation. The average that is taken here must then be considered as the average

$$\overline{A} = \frac{S_p (AD)}{S_p D}$$

over some statistical operator D which does not depend on t.

We note now that the following exact relations follow from the equations of motion:

$$\begin{split} i \frac{\partial F\left(f_{1}, f_{2}\right)}{\partial t} &= \left[\overline{a_{f_{1}}a_{f_{2}}}; H\right],\\ i \frac{\partial \Phi\left(f_{1}, f_{2}\right)}{\partial t} &= \left[\overline{a_{f_{1}}a_{f_{2}}; H}\right], \end{split}$$

or, in more explicit form

$$i \frac{\partial F(f_1, f_2)}{\partial t} = \sum_{(f)} \{ T(f_2, f) F(f_1, f) - T(f, f_1) F(f, f_2) \}$$

$$-\sum_{(f_{1},f_{1}',f_{2}')} \{U(f',f_{2}';f_{1},f_{1})F_{2}(f_{1}',f_{2}';f_{1},f_{2}') \\ -U(f_{2},f_{1}',f_{2}')F_{2}(f_{1},f_{1}',f_{2}',f_{1}')\}, \qquad (38)$$

$$i\frac{\partial\Phi(f_{1},f_{2})}{\partial t} = \sum_{(f)} \{T(f_{1},f)\Phi(f,f_{2}) + T(f_{2},f)\Phi(f_{1},f)\}, \\ +\sum_{(f_{1}',f_{2}')} U(f_{1},f_{2};f_{2}',f_{1}')\Phi(f_{1}',f_{2}') \\ +\sum_{(f,f_{1}',f_{2}')} \{U(f_{1},f_{1}',f_{2}',f_{1}')\Phi_{2}(f_{1}',f_{2}',f_{1}'), \\ +U(f_{1},f_{2}',f_{2}',f_{1}')\Phi_{3}(f_{1}',f_{2}',f_{1}')\}, \qquad (39)$$

where again

$$\begin{array}{c} F_{2}(f_{1}, f_{2}; f_{2}', f_{1}') = a_{f_{1}}^{\dagger} a_{f_{2}} a_{f_{2}} a_{f_{1}'}, \\ \Phi_{2}(f_{1}; f_{2}, f_{3}, f_{4}) = a_{f_{1}} a_{f_{2}} a_{f_{3}} a_{f_{4}} \\ \end{array} \right)$$

$$(40)$$

According to the principles of the theory of chains of distribution functions, we should express $\frac{\partial F_2}{\partial t}$ and $\frac{\partial \Phi_2}{\partial t}$ again in terms of distribution func-∂t

tions of higher order, and so on.

The transition to a closed set of approximate equations can be accomplished by "disentangling" one of these equations, for instance, using some appropriate approximation which expresses the higher correlation functions that enter into the equation in terms of the lower ones.

In the self-consistent field method we are satisfied with a simpler and less accurate approach; we restrict ourselves, namely, to the first equations (38) and (39), which we have already obtained and we make in them an approximate substitution of F_2 and Φ_2 in terms of F and Φ .

We take these functions*

$$F(f_{1}, f_{2}) = \frac{\operatorname{Tr} \{a_{f_{1}}(t) a_{f_{2}}(t) D\}}{\operatorname{Tr} D},$$

$$\Phi(f_{1}, f_{2}) = \frac{\operatorname{Tr} \{a_{f_{1}}(t) a_{f_{2}}(t) D\}}{\operatorname{Tr} D},$$

$$F_{2}(f_{1}, f_{2}; f_{2}', f_{1}') = \frac{\operatorname{Tr} \{a_{f_{1}}(t) a_{f_{2}}(t) a_{f_{2}'}(t) a_{f_{1}'}(t) D\}}{\operatorname{Tr} D},$$

$$\Phi_{2}(f_{1}; f_{2}, f_{3}, f_{4}) = \frac{\operatorname{Tr} \{a_{f_{1}}(t) a_{f_{2}}(t) a_{f_{3}}(3) a_{f_{4}}(t) D\}}{\operatorname{Tr} D}$$
(41)

and we assume that the statistical operator D is diagonal in the $\ldots n_{\nu} \ldots$ representation, where $n_{\nu} = \dot{\alpha}_{\nu}(t) \alpha_{\nu}(t)$. Strictly speaking we can make such an assumption only at one fixed moment, since D remains constant while $\alpha(t)$ and $\dot{\alpha}(t)$ change, generally speaking, with time.

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^{*}From this definition it follows at once that F and Φ always satisfy the conditions (24).

Nonetheless, our approximation can be considered to be valid for the first approximation in those cases where the main part of the Hamiltonian H in the amplitudes α is of the form

$$\sum_{(\nu)} Q(\nu) \overset{+}{\alpha}_{\nu} \alpha_{\nu},$$

since then in the "zeroth approximation" the equations of motion will be

$$i \frac{\partial a_{\nu}}{\partial t} = \Omega(\nu) a_{\nu},$$

and for them

$$\dot{a}_{\nu}(t)a_{\nu}(t) = \text{const}$$

The main part of the time dependence of $a_f(t)$ and $\dot{a}_f(t)$ is, so to speak, compensated by the time dependence of the functions u and v.

Using the above-mentioned approximation, we substitute Eq. (1) into (41) and perform the averaging, taking into account the fact that D is diagonal in the $\ldots n_{\nu} \ldots$ representation.

We get

$$\Phi(f_{1}, f_{2}) = \sum_{(v)} \{ u_{f_{1}v} v_{f_{2}v} (1 - \bar{n}_{v}) + v_{f_{1}v} u_{f_{2}v} \bar{n}_{v} \}, \\ F(f_{1}, f_{2}) = \sum_{(v)} \{ v_{f_{1}v}^{*} v_{f_{2}v} (1 - \bar{n}_{v}) + u_{f_{1}v}^{*} u_{f_{2}v} \bar{n}_{v} \},$$
(42)

where \overline{n}_{ν} is the average of $\dot{\alpha}_{\nu}(t) \alpha_{\nu}(t)$. We find also

$$F_{2}(f_{1}, f_{2}; f_{2}', f_{1}') = F(f_{1}, f_{1}') F(f_{2}, f_{2}') - F(f_{1}, f_{2}') F(f_{2}, f_{1}') + \Phi^{*}(f_{1}, f_{2}) \Phi(f_{1}', f_{2}');$$
(43)

$$\Phi_{2}(f_{1}, f_{2}, f_{3}, f_{4}) = F(f_{1}, f_{2}) \Phi(f_{3}, f_{4}) + F(f_{1}, f_{4}) \Phi(f_{2}, f_{3})$$

$$-F(f_1, f_3) \Phi(f_2, f_4).$$
(44)

Substituting these expressions (43) and (44) into Eqs. (38) and (39) we also get the equations of motion of the self-consistent field in the form

$$i \frac{\partial \Phi(f_1, f_2)}{\partial t} = \mathfrak{N}(f_1, f_2/F, \Phi),$$

$$i \frac{\partial F(f_1, f_2)}{\partial t} = \mathfrak{B}(f_1, f_2/F, \Phi).$$
(45)

We see easily that the expressions \mathfrak{A} and \mathfrak{B} which occur here are the same expressions as the earlier ones. This is caused by the fact that the right hand sides of Eqs. (38) and (39) are the same as the corresponding expressions in (14) and (15) and that Eqs. (43) and (44) are the same as Eqs. (19) and (20).

We can thus use the previously-established properties of \mathfrak{A} and \mathfrak{B} .

We now turn our attention to the identity (13) which is correct in the case under consideration* if $\nu_1 = \nu_2$.

On the basis of this we establish the important property of the solutions of Eq. (45), namely, that for any solution

$$\frac{d\tilde{n}_{\gamma}}{dt} = 0. \tag{46}$$

In other words, we shall show that the eigenvalues of the operator K stay constant when the time changes.

Indeed, in accordance with (25)

 $\varphi_{\omega}K=\overline{n}_{\omega}\varphi_{\omega}.$

The statement made will thus be proven when we only verify that for any ω

$$\sum_{(g,g')}\varphi_{\omega}(g)\frac{dK(g,g')}{dt}\varphi_{\omega}(g')=0.$$
(47)

Since, however, always

$$n_{v1} = 1 - n_{v0},$$

we see that we need prove Eq. (47) only for $\omega = (\nu, 0)$.

Using the definition (26) of the operator K and Eqs. (8) we find

$$\sum_{(g,g')} \varphi_{\nu,0}(g) \frac{dK(g,g')}{dt} \varphi_{\nu,0}^*(g')$$

$$= -\sum_{(j,j')} v_{\nu f}^* v_{\nu f'} \frac{dF^*(j,f')}{dt} + \sum_{(f,f')} v_{\nu f}^* u_{\nu f'}^* \frac{d\Phi(f,f')}{dt}$$

$$- \sum_{(f,f')} u_{\nu f} v_{\nu f'} \frac{d\Phi^*(f,f')}{dt} + \sum_{(f,f')} u_{\nu f} u_{\nu f'}^* \frac{dF(f,f')}{dt} = 0,$$

and hence, using (45) and (13)

$$i \sum_{(g,g')} \varphi_{\forall 0}(g) \frac{dK(g,g')}{dt} \varphi_{\forall,0}^*(g')$$

$$= \sum_{(f,f')} \{ v_{\forall f}^* v_{\forall f'} \mathfrak{B}^*(f,f') + v_{\forall f}^* u_{\forall f'}^* \mathfrak{A}(f,f') + u_{\forall f} v_{\forall f'} \mathfrak{A}^*(f,f') + u_{\forall f'} v_{\forall f'} \mathfrak{A}^*(f,f') \} = 0,$$

which proves the statement (46).

We have here a typical property of the selfconsistent field method: the fact that relaxation effects are not taken into account.

Once any set $\ldots n_{\nu} \ldots$ is conserved, the system

$$n_{\mathbf{v}}=0$$

which corresponds to the previously considered ground state will, in particular, also be conserved. Equations (45) are thus compatible with the additional conditions (28).

We now write these equations and the additional conditions in the r -representation for the case where

$$l = \frac{(p - eA)^2}{m}$$

^{*}As was already noticed earlier, the identity (13) will be correct for arbitrary ν_1 , ν_2 if in Eqs. (42) all $\bar{n}_{\nu} = 0$.

and where the interaction is characterized by a potential function $U(r_1, r_2)$ which does not de-

pend on the velocities or the spins. We have*

$$i\frac{\partial\Phi_{\sigma_{1},\sigma_{2}}(r_{1},r_{2})}{dt} = \left\{ \frac{\left(i\frac{\partial}{\partial\mathbf{r}_{1}} + e\mathbf{A}\left(r_{1}\right)\right)^{2}}{2m} + \frac{\left(i\frac{\partial}{\partial\mathbf{r}_{2}} + e\mathbf{A}\left(r_{2}\right)\right)^{2}}{2m} - 2\lambda + \int U\left(r_{1},r'\right)\sum_{(\sigma)}F_{\sigma\sigma}\left(r',r'\right)dr' \\ + \int U\left(r_{2},r'\right)\sum_{(\sigma)}F_{\sigma\sigma}\left(r',r'\right)dr'\right]\Phi_{\sigma_{1},\sigma_{2}}(r_{1},r_{2}) - \sum_{(\sigma)}\int dr'\left\{U\left(r_{1},r'\right)F_{\sigma,\sigma_{1}}\left(r',r_{1}\right)\Phi_{\sigma,\sigma_{2}}\left(r',r_{2}\right)\right. \\ + U\left(r_{2},r'\right)F_{\sigma,\sigma_{2}}\left(r',r_{2}\right)\Phi_{\sigma_{1},\sigma}\left(r_{1},r'\right)\right\} + U\left(r_{1},r_{2}\right)\Phi_{\sigma_{1},\sigma_{2}}\left(r_{1},r_{2}\right) - \sum_{(\sigma)}\int dr'\left\{F_{\sigma,\sigma_{1}}\left(r',r_{1}\right)U\left(r',r_{2}\right)\Phi_{\sigma,\sigma_{2}}\left(r',r_{2}\right)\right. \\ + F_{\sigma,\sigma_{2}}\left(r',r_{2}\right)U\left(r_{1},r'\right)\Phi_{\sigma_{1},\sigma}\left(r_{1},r'\right)\right\},$$

$$(48)$$

$$i \frac{\partial F_{\sigma_{1},\sigma_{2}}(r_{1},r_{2})}{\partial t} = \left\{ \frac{\left(i \frac{\partial}{\partial r_{2}} + eA(r_{2})\right)^{2}}{2m} - \frac{\left(i \frac{\partial}{\partial r_{1}} - eA(r_{1})\right)^{2}}{2m} \right\} F_{\sigma_{1},\sigma_{2}}(r_{1},r_{2}) + \sum_{(\sigma)} \int dr \left\{ \Phi(r_{2},r) - \Phi(r_{1},r) \right\} \left\{ F_{\sigma_{1},\sigma_{2}}(r,r) F_{\sigma_{1},\sigma_{2}}(r_{1},r_{2}) - F_{\sigma_{1},\sigma_{1}}(r_{1},r) F_{\sigma_{1},\sigma_{2}}(r,r_{2}) + \Phi_{\sigma_{1},\sigma_{2}}^{*}(r_{1},r) \Phi_{\sigma_{1},\sigma_{2}}(r,r_{2}) \right\},$$
(49)

$$F_{\sigma_{1},\sigma_{2}}(r_{1}, r_{2}) = \sum_{(\sigma)} \int dr \{F_{\sigma_{1},\sigma}(r_{1}, r) F_{\sigma_{1},\sigma_{2}}(r, r_{2}) + \Phi^{*}_{\sigma_{1},\sigma_{1}}(r, r_{1}) \Phi_{\sigma_{1},\sigma_{2}}(r, r_{2})\},$$

$$\sum_{(\sigma)} \int dr \{F_{\sigma_{1},\sigma}(r_{1}, r) \Phi^{*}_{\sigma_{1},\sigma_{2}}(r, r_{2}) + F_{\sigma_{2},\sigma}(r_{2}, r) \Phi^{*}_{\sigma_{1},\sigma_{1}}(r, r_{1})\} = 0.$$

It is clear that this whole system is gauge invariant. The gauge transformation

$$e\mathbf{A}(r) \rightarrow e\mathbf{A}(r) + \frac{\partial}{\partial r} \varphi(r)$$
 (51)

is compensated by the transformation of the functions F and Φ :

$$\Phi_{\sigma_{1}, \sigma_{2}}(r_{1}, r_{2}) \rightarrow \Phi_{\sigma_{1}, \sigma_{2}}(r_{1}, r_{2}) e^{i\{\varphi(r_{1}) + \varphi(r_{2})\}}, F_{\sigma_{1}, \sigma_{2}}(r_{1}, r_{2}) \rightarrow F_{\sigma_{1}, \sigma_{2}}(r_{1}, r_{2}) e^{i\{-\varphi(r_{i}) + \varphi(r_{z})\}}.$$
(52)

The gauge invariance is here caused by the gauge invariance of the Hamiltonian.

When one considers the problem of the theory of superconductivity in the model where the electron-phonon interaction is replaced by a direct velocity-dependent interaction between the electrons (it is only effective at the Fermi surface), the corresponding Hamiltonian is no longer rigorously gauge invariant. This property holds only approximately and the equations of the self-consistent field method will thus only be gauge invariant with the same degree of accuracy.

It is important to remark here that the approximations used to derive our equations do not by themselves violate the gauge invariance. We shall return to this problem in Sec. 4.

3. THE REPRESENTATION WITH A FIXED NUMBER OF PARTICLES

We shall now consider the correlation function

 $F_2(f_1, f_2; f'_2, f'_1),$

in the r-representation, completely independently from what we have said earlier. We put here $f = (r, \sigma)$, where σ is some discrete index, for instance, the spin index.

Let it be possible to write this function in the form

$$F_{2} = \sum_{n} \Psi_{n}^{*}(f_{1}, f_{2}) \Psi_{n}(f_{1}', f_{2}') + \widetilde{F}_{2} .$$
 (53)

in such a way that:

1) when the distance between the pairs (f_1, f_2) and (f'_1, f'_2) tends to infinity the extra term \widetilde{F}_2 vanishes sufficiently fast;

2) when the distance between the points f_1 and f_2 increases without limit the function $\Psi_n(f_1, f_2)$ will also tend to zero, and the integral

$$\int |\Psi_n(f_1, f_2)|^2 df_2 = \int |\Psi_n(f_2, f_1)|^2 df_2$$
 (54)

will converge.

It is then clear that we can interpret $\Psi_n(f_1, f_2)$ as the wave function of a pair of particles which

*Here, r denotes the vector r and dr a three-dimensional volume element.

(50)

are in one of the bound states, and the integral (54) as being proportional to the number density of those particles at the point f_1 which are bound in a pair which is in the state Ψ_n .

We consider our Eq. (43) from this point of view and, to be specific, take the case of superconductivity theory. We have for the ground state:

$$\Phi_{-+}(r_1, r_2) = \left(\frac{1}{2\pi}\right)^3 \int e^{ih(r_1 - r_2)} \Phi(k) \, dk,$$

$$\Phi(k) = \frac{C(k)}{2\sqrt{\xi^2(k) + C^2(k)}}$$

and

$$F_{\sigma\sigma}(r_1, r_2) = \left(\frac{1}{2\pi}\right)^3 \int e^{ih(r_1 - r_2)} F(k) \, dk,$$
$$F(k) = \frac{1}{2} \left\{ 1 - \frac{\xi(k)}{\sqrt{\xi^2(k) + C^2(k)}} \right\}.$$

It is clear that the above-mentioned conditions (1) and (2) are satisfied here and $\Phi(f_1, f_2) =$ $\Phi_{-+}(r_1, r_2)$ can thus be considered to be the wave function of a bound pair of particles (with opposite spins). In the given case there is only one state $\Phi(f_1, f_2)$ and we can say that all bound quasimolecules are in a condensate. Bound pairs leaving the condensate are not taken into account in the method given here as a matter of principle, because of Eq. (43).*

We now turn our attention to the fact that in our discussions we essentially used the canonical transformation (1). Consequently, the total number of particles $N = \sum \dot{a}_{f} a_{f}$ is not a quantum number either for the state C_0 or for the statistical operator D, nor does it have a rigorously fixed value. On the other hand, N is always an integral of motion for the Hamiltonian (3) considered by us. It is therefore completely natural to demand that we obtain the same results if we work in a representation where N is a quantum number.

Let us see, however, what would be obtained in actual fact were we to attempt our analysis in such a representation.

First, we could no longer mix up the creation and annihilation amplitudes, and should therefore put $v \equiv 0$ in Eqs. (1). But we get then instead of (43) the approximation

$$F(f_1, f_2; f'_2, f'_1) = F(f_1, f'_1) F(f_2, f'_2) - F(f_1, f'_2) F(f_2, f'_1)$$
(55)

of the usual Hartree-Fock method which, in general, does not take into account the possibility of bound states of particle pairs.

The situation can be shown to be even worse,

since independently of any approximation the equation

$$\overline{a_{f_1}a_{f_2}} = 0$$

is valid for any averaging where N is rigorously fixed. A way out of this paradox is, however, not difficult. Simply, if we want to work with fixed N, it is necessary to go further in the chain of equations which connect the correlation functions with one another, and to turn to correlation functions of higher order.

In order not to land into complicated calculations we use now an intuitive, somewhat simplified approach. Starting from the idea that in the dynamical system under consideration there are bound pairs which are all in the same state $\Phi(f_1, f_2)$ we add to Eq. (55) of the usual Hartree-Fock method a term

$$\Phi^*(f_1, f_2) \Phi(f_1', f_2'),$$

which describes the contribution from such pairs. Substituting the expression so obtained into the exact relation (38) we get at once the second of Eqs. (45).

To derive the first of Eqs. (45), which determines Φ , we consider a two-time correlation function of the form

$$\overline{a_{f_1}(t) \, a_{f_2}(t) \, a_{f_2''}(\tau) \, a_{f_1''}(\tau)}$$

and differentiate it with respect to the time t. Using the exact equations of motion we get*

$$i \frac{\partial \langle a_{f_{1}}(t) a_{f_{2}}(t) a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle}{\partial t}$$

$$= \langle [a_{f_{1}}(t) a_{f_{2}}(t); H] a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle$$

$$= \sum_{\langle f \rangle} \{ I(f_{1}, f) \langle a_{f}(t) a_{f}(t) a_{f_{2}}(t) a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle$$

$$+ I(f_{2}, f) \langle a_{f_{1}}(t) a_{f}(t) a_{f_{2}'}(\tau) a_{f_{1}''}(\tau) \rangle \}$$

$$+ \sum_{\langle f_{1}'f_{2}'\rangle} U(f_{1}, f_{2}; f_{2}', f_{1}') \langle a_{f_{1}'}(t) a_{f_{2}'}(t) a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle$$

$$+ \sum_{\langle i_{f}(t) i_{f_{2}}(t) a_{f_{2}}(t) a_{f_{2}'}(t) a_{f_{1}'}(t) a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle$$

$$+ \sum_{\langle i_{f}(t) i_{f_{2}}(t) a_{f_{2}}(t) a_{f_{2}'}(t) a_{f_{1}'}(t) a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle$$

$$+ \sum_{\langle i_{f}(t) i_{f_{2}}(t) a_{f_{2}'}(t) a_{f_{1}'}(t) a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle$$

$$+ \sum_{\langle i_{f}(t) i_{f_{2}}(t) a_{f_{2}'}(t) a_{f_{1}'}(t) a_{f_{2}''}(\tau) a_{f_{1}''}(\tau) \rangle.$$
(56)

We note, by the way, that this relation differs from (39) only in that now there are on the right two operators a which compensate the change in

^{*}They can be taken into account by generalizing the approximation (43) along the lines of Eq. (53).

^{*}The averaging is here not indicated by a bar above, but by brackets <...>, since that is more convenient for long expressions.

the number of particles.

We go now over to an approximate equation by approximately expressing functions of the kind

$$\langle a_{f_1}(t) a_{f_2}(t) a_{f'_2}(t) a_{f'_1}(t) a_{f''_2}(\tau) a_{f''_1}(\tau) \rangle$$

in terms of products of four and two operators. We note that when we make this splitting up we must now take into account that the number N is rigorously kept constant. After that we shall let the pair (f'_2, f'_1) move to infinity in the equation obtained from (56).

We therefore use the following approximation

$$\dot{a_{f_1}}(t) a_{f_2}(t) a_{f'_2}(t) a_{f'_1}(t) a'_{f''_2}(\tau) a_{f'_1}(\tau) \rangle$$

$$= \langle a_{f_1}(t) a_{f_2}(t) \rangle \langle a_{f'_2}(t) a_{f'_1}(t) a'_{f''_2}(\tau) a'_{f'_1}(\tau) \rangle$$

$$- \langle a_{f_1}(t) a_{f'_2}(t) \rangle \langle a_{f_2}(t) a_{f'_1}(t) a'_{f''_2}(\tau) a'_{f'_1}(\tau) \rangle$$

$$+ \langle a_{f_1}(t) a_{f'_1}(t) \rangle \langle a_{f_2}(t) a_{f'_2}(t) a'_{f''_2}(\tau) a'_{f'_1}(\tau) \rangle + S, \quad (57)$$

where S denotes the sum of terms which contain a factor $\langle \dot{a}_{f_1''}(\tau) a_f(t) \rangle$ or $\langle a_{f_2''}(\tau) a_f(t) \rangle$. We shall not write down an explicit expression for S since these terms will vanish when the point pair (f_2'', f_1'') is moved off to infinity.

We substitute (57) into (56) and let these point pairs move off to infinity. Expressions of the form

$$\langle a_{f_1}(t) a_{f_2}(t) a_{f'_2}(\tau) a_{f'_1}(\tau) \rangle$$

will then break up into products

$$\Psi_t(f_1, f_2) \Psi^*_{\tau}(f'_1, f'_2),$$

where $\Psi_t(f_1, f_2)$ denotes the wave function of a bound pair, and we shall get, splitting off the common factor $\Psi_{\tau}^*(f'_1, f'_2)$:

$$\frac{\partial \Psi_{t}(f_{1}, f_{2})}{\partial t} = \sum_{j} \{ I(f_{1}, f) \Psi_{t}(f_{1}f_{2}) + I(f_{2}, f) \Psi_{t}(f_{1}, f) \}.$$

$$+ \sum_{(f_{1}', f_{2}')} U(f_{1}, f_{2}; f_{2}', f_{1}') \Psi_{t}(f_{1}, f_{2}')$$

$$+ \sum_{(f, f_{2}', f_{2}')} U(f_{1}, f; f_{2}', f_{1}') \{ F_{t}(f_{1}, f_{2}) \Psi_{t}(f_{2}', f_{1}')$$

$$- F_{t}(f, f_{2}') \Psi_{t}(f_{2}, f_{1}') + F_{t}(f, f_{1}') \Psi_{t}(f_{2}, f_{2}') \}$$

$$+ \sum_{(f, f_{1}', f_{2}')} U(f_{1}, f_{2}; f_{2}', f_{1}') \{ F_{t}(f_{1}, f_{1}) \Psi_{t}(f_{2}', f_{1}')$$

$$- F_{t}(f, f_{2}') \Psi_{t}(f, f_{1}') + F_{t}(f_{1}, f_{1}') \Psi_{t}(f_{1}, f_{2}') \}.$$
(58)

We note that in the ground state Ψ_t must be proportional to e^{-iEt} where E is the corresponding energy. We introduce the quantity*

*The meaning of such a quantity λ as being the chemical potential can be made clear by the following considerations. On the one hand, the factor e^{-iEt} must express the time-dependence of the pair wave function:

$$\langle C_N^* a_{f_1}(t) a_{f_2}(t) C_{N+2} \rangle$$

$$\lambda = \frac{E}{2}$$

and we put in the general, non-equilibrium, case

$$\Psi_t(f_1, f_2) = e^{-2i\lambda t} \Phi_t(f_1, f_2),$$

so that

$$i \frac{\partial \Psi_t}{\partial t} = e^{-2i\lambda t} \left\{ i \frac{\partial \Phi_t}{\partial t} + 2\lambda \Phi_t \right\} \,.$$

It is thus clear that Eq. (58) obtained in this way becomes the first of Eqs. (45) which we lacked.

We can cast the discussions presented here in a more perfect form and use them to arrive at more rigorous equations, but we shall not consider them. It is now important for us to stress that we can obtain the equations of the generalized selfconsistent field method in a framework with a fixed total number of particles. The meaning of the transformation (1) is then clarified. Namely, by using it we obtain in a lower approximation results that are usually obtained in a higher approximation.

This property is based on the fact that in the variables α the bound states drop out. In the first approximation, used by us, we have thus, for instance,

$$\langle a_{\nu_1}a_{\nu_2}a_{\nu_2'}a_{\nu_1'}\rangle = (1 - \overline{n}_{\nu_1})(1 - \overline{n}_{\nu_2})\{\delta(\nu_1 - \nu_1')\delta(\nu_2 - \nu_2') \\ -\delta(\nu_1 - \nu_2')\delta(\nu_2 - \nu_1')\} = \langle a_{\nu_1}a_{\nu_1'}\rangle \langle a_{\nu_2}a_{\nu_2'}\rangle - \langle a_{\nu_1}a_{\nu_2'}\rangle \langle a_{\nu_2}a_{\nu_1'}\rangle.$$

The same situation can also be achieved for the higher approximations. The principle of compensating dangerous diagrams is also just the proper method for that case. All the diagrams that are compensated according to this principle are exactly those which determine the bound states.

In those cases where the possibility of the occurrence of bound particle pair states (Bosecondensate) makes it impossible to use perturbation theory, the compensation principle, which introduces new variables $\dot{\alpha}$, α in terms of which such states drop out, liquidates thereby this impediment to an application of perturbation theory.

where C_N denotes the lowest state of the system in the case where the number of particles is equal to N.

On the other hand, let the total energy of the system in the state C_N be E(N). The time dependence of the given expression is then determined by the factor

$$e^{-i\{E(N+2)-E(N)\}t}$$

or

We have thus

$$\lambda = \frac{\partial E(N)}{\partial N} \, .$$

 $2\lambda \equiv E = E(N+2) - E(N)$

4. COLLECTIVE OSCILLATIONS

We now turn to the problem of determining the spectrum of the elementary excitations of the ground state.

From the point of view of the self-consistent field method this problem can be solved as follows.

As we have noted already, the numbers \overline{n}_{ν} stay constant and all of them are equal to zero in the ground state. If we wish to study small vibrations around this state, we shall put $\overline{n}_{\nu} = 0$. In other words, we impose the additional conditions (28).

Let F_0 and Φ_0 be the expressions F and Φ

in the ground state. Let us consider infinitesimal changes

$$F = F_0 + \delta F, \qquad \Phi = \Phi_0 + \delta \Phi$$

and let us write down for them the equations, linear in the variations

$$i \frac{\partial^{\delta} \Phi(f_1, f_2)}{\partial t} = \delta \mathfrak{A}(f_1, f_2/F, \Phi),$$

$$i \frac{\partial^{\delta} F(f_1, f_2)}{\partial t} = \delta \mathfrak{B}(f_1, f_2/F, \Phi).$$
(59)

Apart from that, we shall take into account the fact that δF and $\delta \Phi$ must be connected through the additional conditions (28) which lead to

$$\left\{ F\left(f_{1}, f_{2}\right) - \sum_{f} F\left(f_{1}, f\right) F\left(f, f_{2}\right) - \sum_{f} \Phi^{*}\left(f, f_{1}\right) \Phi\left(f, f_{2}\right) \right\} = 0, \\ \left\{ \sum_{f} F\left(f_{1}, f\right) \Phi^{*}\left(f, f_{2}\right) + \sum_{f} F\left(f_{2}, f\right) \Phi^{*}\left(f, f_{1}\right) \right\} = 0.$$

$$\left\{ \left\{ \sum_{f} F\left(f_{1}, f\right) \Phi^{*}\left(f, f_{2}\right) + \sum_{f} F\left(f_{2}, f\right) \Phi^{*}\left(f, f_{1}\right) \right\} = 0. \right\}$$

$$\left\{ \left\{ \sum_{f} F\left(f_{1}, f\right) \Phi^{*}\left(f, f_{2}\right) + \sum_{f} F\left(f_{2}, f\right) \Phi^{*}\left(f, f_{1}\right) \right\} = 0. \right\}$$

$$\left\{ \left\{ \sum_{f} F\left(f_{1}, f\right) \Phi^{*}\left(f, f_{2}\right) + \sum_{f} F\left(f_{2}, f\right) \Phi^{*}\left(f, f_{1}\right) \right\} = 0. \right\}$$

We note also that because of (24) $\delta \Phi$ must be antisymmetric and δF Hermitian.

We shall solve the homogeneous equations obtained here by a superposition of elementary solutions which are proportional to e^{-iEt} . We find in that way* the secular equations to determine the spectrum of the vibrations.

Because of the presence of conditions (60) δF and $\delta \Phi$ are not independent and it is thus technically convenient to express them in terms of new independent unknowns that satisfy (60) automatically. We can immediately obtain such expressions, if we note that because of (60) the infinitesimal transformation is undergone not by $n_{\nu} \equiv 0$, but by $u_{f\nu}$ and $v_{f\nu}$. These transformations must be compatible with the orthonormalization conditions (2).

Instead of varying u, v we can perform an infinitesimal transformation on the α themselves:

$$a_{\nu} \rightarrow a_{\nu} + \sum_{(\nu')} \mu(\nu', \nu) a_{\nu'} + \sum_{(\nu')} \lambda(\nu', \nu) a_{\nu'}, \qquad (61)$$

and it follows then from the fact that the given infinitesimal transformation is canonical that

$$\begin{aligned} \lambda(\nu_1, \nu_2) + \lambda(\nu_2, \nu_1) &= 0, \\ \mu^*(\nu_1, \nu_2) + \mu(\nu_2, \nu_1) &= 0. \end{aligned}$$
 (62)

We have then

$$\langle \alpha_{\nu} \alpha_{\mu} \rangle_{0} \longrightarrow \lambda (\nu, \mu);$$

 $\stackrel{*}{\langle \alpha_{\nu} \alpha_{\mu} \rangle_{0}}$ remain equal to zero

and hence

$$\begin{split} F_{0}(f_{1}, f_{2}) + \delta F(f_{1}, f_{2}) \\ &= \sum_{(\nu_{1}, \nu_{2})} \langle (u_{j_{1}\nu_{1}}^{*} \alpha_{\nu_{1}} + v_{j_{1}\nu_{1}}^{*} \alpha_{\nu_{1}}) (u_{j_{2}\nu_{2}} \alpha_{\nu_{2}} + v_{j_{2}\nu_{2}}^{*} \alpha_{\nu_{2}}) \rangle_{0} \\ &= F_{0}(f_{1}, f_{2}) + \sum_{(\nu_{1}, \nu_{2})} \{ v_{j_{1}\nu_{1}}^{*} u_{j_{2}\nu_{2}} \lambda(\nu_{1}, \nu_{2}) + u_{j_{1}\nu_{1}}^{*} v_{j_{2}\nu_{2}} \lambda^{*}(\nu_{2}, \nu_{1}) \}, \\ \Phi_{0}(f_{1}, f_{2}) + \delta \Phi(f_{1}, f_{2}) \\ &= \sum_{(\nu_{1}, \nu_{2})} \langle (u_{j_{1}\nu_{1}} \alpha_{\nu_{1}} + v_{j_{1}\nu_{1}} \alpha_{\nu_{1}}) (u_{j_{2}\nu_{2}} \alpha_{\nu_{2}} + v_{j_{2}\nu_{2}} \alpha_{\nu_{2}}) \rangle_{0} \\ &= \Phi_{0}(f_{1}, f_{2}) + \sum_{(\nu_{1}, \nu_{2})} \{ u_{j_{1}\nu_{1}} u_{j_{2}\nu_{2}} \lambda(\nu_{1}, \nu_{2}) + v_{j_{1}\nu_{1}} v_{j_{2}\nu_{2}} \lambda^{*}(\nu_{2}, \nu_{1}) \}. \end{split}$$

It is clear that the coefficients μ do not enter into our formulae. This is because in the case under consideration $\overline{n}_{\mu} \equiv 0$. We note also that independently of the considerations given here one can easily verify that the expressions

$$\delta F(f_1, f_2) = \sum_{(\mathbf{v}_1, \mathbf{v}_2)} \{ v_{f_1 \mathbf{v}_1}^* u_{f_2 \mathbf{v}_2} \lambda(\mathbf{v}_1, \mathbf{v}_2) + u_{f_1 \mathbf{v}_1}^* v_{f_2 \mathbf{v}_2} \lambda^*(\mathbf{v}_2, \mathbf{v}_1) \}, \qquad (64)$$

$$\delta \Phi (f_1, f_2) = \sum_{(\mathbf{v}_1, \mathbf{v}_2)} \{ u_{f_1 \mathbf{v}_1} u_{f_2 \mathbf{v}_2} \lambda (\mathbf{v}_1, \mathbf{v}_2) + v_{f_1 \mathbf{v}_1} v_{f_2 \mathbf{v}_2} \lambda^* (\mathbf{v}_2, \mathbf{v}_1) \}$$
(65)

are the general solutions of the additional conditions (60) and (24) for any arbitrary antisymmetric $\lambda (\nu_1, \nu_2)$.

To obtain the equation for $\frac{\partial \lambda}{\partial t}$ it is expedient to express λ also in terms of δF and $\delta \Phi$. To do this we multiply (64) by $v_{f_1\mu_1}^*$ and (65) by $u_{f_1\mu_1}^*$ and sum. In virtue of the orthonormalization condition in the form (10), we find then

^{*}We stress that such a problem of determining the spectrum of the elementary recitations by means of linearizing nonlinear equations goes back in principle to the well-known investigations by A. A. Vlasov.⁵

We must also remark, by the way, that these very investigations exerted a large influence on the development of the concept of collective oscillations.

$$\sum_{(f_1)} \{ v_{f_1\mu_1} \,\delta F(f_1, f_2) + u_{f_1\mu_1}^* \,\delta \Phi(f_1, f_2) \} = \sum_{(\nu_2)} u_{f_2\nu_2} \,\lambda(\mu_1, \nu_2).$$
(66)

We then multiply (64) by $u_{f_1\mu_1}$ and (65) by $v_{f_1\mu_1}^*$ and sum again. We get

$$\sum_{(f_1)} \{ u_{f_1\mu_1} \,\delta F(f_1, f_2) + v_{f_1\mu_1}^* \,\delta \Phi(f_1, f_2) \} = \sum_{(\nu_2)} v_{f_2\nu_2} \,\lambda^*(\nu_2, \mu_1)$$
or
$$\sum_{(f_1)} \{ u_{f_1\mu_2}^* \,\delta F^*(f_1, f_2) + v_{f_1\mu_1} \,\delta \Phi^*(f_1, f_2) \} = -\sum_{(\nu_2)} v_{f_2\nu_2}^* \,\lambda(\mu_1, \nu_2)$$
(67)

From (66) and (67) we find by the same method the required expression for λ :

$$\lambda (\mu_{1}, \mu_{2}) = \sum_{(f_{1}, f_{2})} \{ u_{f_{2}\mu_{2}}^{*} v_{f_{1}\mu_{1}} \delta F(f_{1}, f_{2}) + u_{f_{2}\mu_{2}}^{*} u_{f_{1}\mu_{1}}^{*} \delta \Phi(f_{1}, f_{2}) - v_{f_{2}\mu_{2}} u_{f_{1}\mu_{1}}^{*} \delta \Phi^{*}(f_{1}, f_{2}) \}$$

$$- v_{f_{2}\mu_{2}} u_{f_{1}\mu_{1}}^{*} \delta F^{*}(f_{1}, f_{2}) - v_{f_{2}\mu_{2}} v_{f_{1}\mu_{1}} \delta \Phi^{*}(f_{1}, f_{2}) \}.$$
(68)

Differentiating this expression with respect to t and using (59) we get an equation for λ :

$$i \frac{\partial \lambda (v_{1}, v_{2})}{\partial t} = \sum_{(f_{1}, f_{2})} \{ u_{f_{2}v_{2}}^{*} v_{f_{1}v_{1}} \delta \mathfrak{B} (f_{1}, f_{2}) + u_{f_{2}v_{2}}^{*} u_{f_{1}v_{1}}^{*} \delta \mathfrak{A} (f_{1}, f_{2}) + v_{f_{2}v_{2}} u_{f_{1}v_{1}}^{*} \delta \mathfrak{A}^{*} (f_{1}, f_{2}) + v_{f_{2}v_{2}} v_{f_{1}v_{1}} \delta \mathfrak{A}^{*} (f_{1}, f_{2}) \}.$$
(69)

To write out this equation in full detail we must vary the expressions \mathfrak{A} and \mathfrak{B} , and express δF and $\delta \Phi$ in terms of λ , using Eqs. (64) and (65).

After long, but essentially simple calculations we get*

$$i \frac{\partial \lambda (\mathbf{v}_{1}, \mathbf{v}_{2})}{\partial t} = \sum_{(\omega)} \{ \mathcal{Q} (\mathbf{v}_{2}, \omega) \lambda (\mathbf{v}_{1}, \omega) - \mathcal{Q} (\mathbf{v}_{1}, \omega) \lambda (\mathbf{v}_{2}, \omega) \}$$

+
$$\sum_{(\omega_{1}, \omega_{2})} \{ X (\mathbf{v}_{1}, \mathbf{v}_{2}; \omega_{1}, \omega_{2}) \lambda (\omega_{1}, \omega_{2})$$

+
$$Y (\mathbf{v}_{1}, \mathbf{v}_{2}; \omega_{1}, \omega_{2}) \lambda^{*} (\omega_{2}, \omega_{1}) \},$$
(70)

where

$$\begin{split} & \Omega\left(\mathbf{v},\,\omega\right) = \sum_{(I_{1},\,I_{1}')} \xi\left(f,\,f'\right) \left(u_{fv}^{*}\,u_{f'\omega} - v_{fw}^{*}\,v_{f'v}\right) \\ & + \sum_{(I_{1},\,I_{2},\,I_{1}',\,I_{2}')} U\left(f_{1},\,f_{2};\,f_{2}',\,f_{1}'\right) \Phi_{0}\left(f_{2}',\,f_{1}'\right) u_{f_{1}v}^{*}\,v_{f_{2}v}^{*} \\ & + \sum_{(I_{1}I_{2},\,I_{1}'I_{2}')} U\left(f_{1},\,f_{2};\,f_{2}',\,f_{1}'\right) \Phi_{0}^{*}\left(f_{2},\,f_{1}\right) v_{I_{2}'v}^{*}\,u_{I_{1}'\omega}, \\ \xi\left(f,\,f'\right) = T\left(f,\,f'\right) \\ & + \sum_{(I_{1},I_{1}')} \left\{U\left(f_{1},\,f;\,f',\,f_{1}'\right) - U\left(f_{1},\,f;\,f_{1}',\,f'\right)\right\} F_{0}\left(f_{1},\,f_{1}'\right), \\ X\left(v_{1},\,v_{2};\,\omega_{1},\,\omega_{2}\right) = \frac{1}{2} \sum U\left(f_{1},\,f_{2};\,f_{2}',\,f_{1}'\right) \left(u_{f_{2}v_{1}}^{*}\,u_{f_{1}v_{2}}^{*} - u_{f_{1}v_{1}}^{*}\,u_{f_{2}v_{2}}^{*}\right) \\ & \times u_{I_{1}'\omega_{2}}^{*}\,u_{I_{2}'\omega_{1}}^{*} + \frac{1}{2} \sum U\left(f_{1},\,f_{2};\,f_{2}',\,f_{1}'\right) \left(v_{f_{1}'v_{1}}^{*}\,v_{I_{2}'v_{2}} - v_{f_{2}'v_{1}}^{*}\,v_{I_{1}'v_{2}}\right) \\ & \times v_{f_{1}\omega_{1}}^{*}\,v_{f_{2}\omega_{2}}^{*} + \frac{1}{2} \sum \left\{U\left(f_{1},\,f_{2};\,f_{2}',\,f_{1}'\right) - U\left(f_{1},\,f_{2};\,f_{1}',\,f_{2}'\right)\right\} \\ & \times \left(v_{f_{1}'v_{1}}\,u_{f_{2}v_{2}}^{*} - u_{f_{1}v_{1}}^{*}\,v_{I_{1}'v_{2}}\right) \left(v_{f_{2}\omega_{1}}\,u_{I_{2}'\omega_{2}} - v_{f_{2}\omega_{2}}^{*}\,u_{I_{1}'v_{2}}\right), \end{split}$$

*The index ω is here simply a summation index over ν in contradistinction to the notation of Sec. 1.

$$Y(\mathbf{v}_{1}, \mathbf{v}_{2}; \omega_{1}, \omega_{2}) = \frac{1}{2} \sum U(f_{1}f_{2}; f_{2}'f_{1}')(u_{f_{2}\mathbf{v}_{1}}^{*}u_{f_{1}\mathbf{v}_{2}}^{*} - u_{f_{1}\mathbf{v}_{1}}^{*}u_{f_{2}\mathbf{v}_{2}}^{*})$$

$$\times v_{f_{2}'\omega_{1}}v_{f_{1}'\omega_{2}} + \frac{1}{2} \sum U(f_{1}, f_{2}; f_{2}', f_{1}')$$

$$\times (v_{f_{1}'\mathbf{v}_{1}}v_{f_{2}'\mathbf{v}_{2}} - v_{f_{2}'\mathbf{v}_{1}}v_{f_{1}'\mathbf{v}_{2}})u_{f_{2}\omega_{2}}^{*}u_{f_{1}\omega_{1}}$$

$$+ \frac{1}{2} \sum \{U(f_{1}, f_{2}; f_{2}', f_{1}') - U(f_{1}, f_{2}; f_{1}', f_{2}')\}$$

$$\times (v_{f_{1}'\mathbf{v}_{1}}u_{f_{1}\mathbf{v}_{2}}^{*} - v_{f_{1}'\mathbf{v}_{2}}u_{f_{1}\mathbf{v}_{1}}^{*})(u_{f_{2}\omega_{1}}^{*}v_{f_{2}'\omega_{2}} - u_{f_{2}\omega_{2}}^{*}v_{f_{2}'''}). \quad (71)$$

From (70) we get also

$$-\frac{i\partial\lambda^{*}(\nu_{1}, \nu_{2})}{\partial t} = \sum_{(\omega)} \{ \Omega^{*}(\nu_{2}, \omega) \lambda^{*}(\nu_{1}, \omega) - \Omega^{*}(\nu_{1}, \omega) \lambda^{*}(\nu_{2}, \omega) \}$$
$$+ \sum_{(\omega_{1}, \omega_{2})} \{ X^{*}(\nu_{1}, \nu_{2}; \omega_{1}, \omega_{2}) \lambda^{*}(\omega_{1}, \omega_{2})$$
$$+ Y^{*}(\nu_{1}, \nu_{2}; \omega_{1}, \omega_{2}) \lambda(\omega_{2}, \omega_{1}) \}.$$
(72)

We shall solve the set of linear homogeneous equations (70) and (72) by a superposition of normal vibrations:

$$\lambda (v_1, v_2) = \sum_{(E)} e^{-iEt} \xi_E (v_1, v_2), \lambda^* (v_1, v_2) = \sum_{(E)} e^{-iEt} \eta_E (v_1, v_2), \ \xi^*_{-E} = \eta_E.$$
(73)

Substituting (73) into (70) and (72) we get the secular equations to determine the spectrum in the form

$$E \xi (v_{1}, v_{2}) = \sum \{ \Omega (v_{2}, \omega) \xi (v_{1}, \omega) - \Omega (v_{1}, \omega) \xi (v_{2}, \omega) \} + \sum \{ X (v_{1}, v_{2}; \omega_{1}, \omega_{2}) \xi (\omega_{1}, \omega_{2}) + Y (v_{1}v_{2}; \omega_{1}\omega_{2}) \eta (\omega_{2}, \omega_{1}) \}, - E \eta (v_{1}, v_{2}) = \sum \{ \Omega^{*} (v_{2}, \omega) \eta (v_{1}, \omega) - \Omega^{*} (v_{1}, \omega) \eta (v_{2}, \omega) \} + \sum \{ X^{*} (v_{1}, v_{2}; \omega_{1}, \omega_{2}) \times \eta (\omega_{1}, \omega_{2}) + Y^{*} (v_{1}, v_{2}; \omega_{1}, \omega_{2}) \xi (\omega_{2}, \omega_{1}) \}.$$
(74)

We stress that we would have obtained the same equations if we had used the method of approximate second quantization instead of the self-consistent field method.

In this method we should have introduced Bose amplitudes $\beta_{\nu\gamma}$ ($\beta_{\gamma\nu} = -\beta_{\nu\gamma}$), replacing products of Fermi amplitudes $\alpha_{\nu}\alpha_{\gamma}$ by them. We should then have diagonalized the corresponding Hamiltonian which is a quadratic form in the operators β , $\dot{\beta}$ by means of the canonical transformation

$$\beta_{\nu_{1}\nu_{2}} = \sum_{(n)} \{\xi_{n}(\nu_{1}, \nu_{2})\zeta_{n} + \eta_{n}(\nu_{1}, \nu_{2})\dot{\zeta}_{n}\}$$
(75)

with the normalization law

$$\sum_{n} \{ |\xi_{n}|^{2} - |\eta_{n}|^{2} \} = 1.$$
 (76)

The ζ_n are here the new Bose-amplitudes with a time-dependence determined by the factor e^{-iE_nt} .

It would then be shown that ξ and η must satisfy exactly our Eqs. (74).

$$E \rightarrow -E, \ \xi \rightarrow \eta^* \quad \eta \rightarrow \xi^*$$

leads again to a solution of the same system.

We note, by the way, that the derivation of these equations through the method of approximate second quantization has some advantage over the one which we gave above, since it leads naturally to the normalization condition (76) which determines the sign of E.

In the self-consistent field method this sign is not fixed: we see easily that if E, ξ , η is a solution of the system of secular equations (74), the transformation

We have just constructed the equations for the eigenvibrations. We shall now consider the prob-
lem of forced oscillations excited by small exter-
nal fields causing a variation of
$$I(f, f')$$
 (we as-
sume that the interaction law is independent of the
external fields).

Repeating the previous considerations we then obtain instead of the homogeneous Eqs. (70) and (72) inhomogeneous equations of the form

$$i \frac{\partial \lambda (v_{1}, v_{2})}{\partial t} = \sum_{(\omega)} \{ Q(v_{2}, \omega) \lambda(v_{1}, \omega) - Q(v_{1}, \omega) \lambda(v_{2}, \omega) \} + \sum_{(\omega_{1}, \omega_{2})} \{ X(v_{1}, v_{2}; \omega_{1}, \omega_{2}) \lambda(\omega_{1}, \omega_{2}) + Y(v_{1}, v_{2}; \omega_{1}, \omega_{2}) \lambda^{*}(\omega_{2}, \omega_{1}) \}$$

$$+ \sum_{(ff')} \{ v_{f'v_{1}} u_{fv_{2}}^{*} - u_{fv_{1}}^{*} v_{f'v_{2}} \} \delta I(f_{1}, f'),$$

$$- i \frac{\partial \lambda^{*}(v_{1}v_{2})}{\partial t} = \sum_{(\omega)} \{ Q^{*}(v_{2}\omega) \lambda^{*}(v_{1}, \omega) - Q^{*}(v_{1}, \omega) \lambda^{*}(v_{2}\omega) \} - \sum_{(\omega_{1}, \omega_{2})} \{ X^{*}(v_{1}, v_{2}; \omega_{1}, \omega_{2}) \lambda^{*}(\omega_{1}\omega_{2}) + Y^{*}(v_{1}v_{2}; \omega_{1}\omega_{2}) \lambda(\omega_{2}\omega_{1}) \}$$

$$+ \sum_{(f_{1}f')} \{ v_{f'v_{1}}^{*} u_{fv_{2}} - u_{fv_{1}} v_{f'v_{2}}^{*} \} \delta I^{*}(f, f_{2}).$$

$$(77)$$

We now apply the general equations just derived to the specific case of the dynamical system considered in Sec. 1 in connection with superconductivity theory.

We substitute Eqs. (30), (31), and (36) of Sec. 1 into Eq. (71) and thus expand Eqs. (74).

We note then that the spectrum divides into two branches; for one of these

 $\lambda_{00} = 0$

and the vibrations occur in particle pairs with opposite spins. For the other branch, on the other hand,

 $\lambda_{\perp} = \lambda_{\perp} = 0$

and the vibrations occur in pairs of the same spin. We consider here the first branch and put:

 $\lambda_{-+}(p_1, p_2) = \lambda(p_1, p_2),$ $\xi_{-+}(p_1, p_2) = \xi(p_1, p_2),$ $\eta_{-+}(p_1, p_2) = \eta(p_1, p_2).$

The set of Eqs. (74) then takes on the form

$$E\xi(p_{1}, p_{2}) = \{\Omega(p_{1}) + \Omega(p_{2})\}\xi(p_{1}, p_{2}) + \frac{1}{V}\sum_{(p_{1}', p_{2}')} \delta(p_{1} + p_{2} - p_{1}' - p_{2}')\{X(p_{1}p_{2}; p_{1}'p_{2}') \times \xi(p_{1}'p_{2}')' + Y(p_{1}, p_{2}; p_{1}', p_{2}')\eta(-p_{2}', -p_{1}')\}, - E\eta(-p_{2}, -p_{1}) = \{\Omega(p_{1}) + \Omega(p_{2})\}\eta(-p_{2}, -p_{1}) + \frac{1}{V}\sum_{(p_{1}', p_{2}')} \delta(p_{1} + p_{2} - p_{1}' - p_{2}')\{X(p_{1}, p_{2}; p_{1}', p_{2}') \times \eta(-p_{2}', -p_{1}') + Y(p_{1}p_{2}; p_{1}', p_{2}')\xi(p_{1}', p_{2}')\},$$

$$(78)$$

where $\Omega(p)$ has the same form as in Sec. 1, and where

$$X(p_{1}, p_{2}; p'_{1}, p'_{2}) = J(p_{1}, p_{2}; p'_{2}, p'_{1}) \{u(p_{1}) u(p_{2}) u(p'_{1}) u(p'_{2}) + v(p_{1}) v(p_{2}) v(p'_{1}) v(p'_{2})\} + [J(-p_{1}, p'_{2}; -p'_{1}, p_{2}) - J(p'_{2}, -p_{1}; -p'_{1}, p_{2})] \{v(p_{1}) u(p_{2}) v(p'_{1}) u(p'_{2}) + u(p_{1}) v(p_{2}) u(p'_{1}) v(p'_{2})\} + J(p_{1}, -p'_{1}; p'_{2}, -p_{2}) \\ \times \{u(p_{1}) v(p_{2}) v(p'_{1}) u(p'_{2}) + v(p_{1}) u(p_{2}) u(p'_{1}) v(p'_{2})\}, \\ Y(p_{1}, p_{2}; p'_{1}, p'_{2}) = -J(p_{1}, p_{2}; p'_{2}, p'_{1}) \{u(p_{1}) u(p_{2}) v(p'_{1}) v(p'_{2}) + v(p_{1}) v(p_{2}) u(p'_{1}) u(p'_{2})\} + [J(-p_{1}, p'_{2}; -p'_{1}, p_{2}) \\ -J(p'_{2}, -p_{1}; -p'_{1}, p_{2})] \{u(p_{1}) v(p_{2}) v(p'_{1}) u(p'_{2}) \\ + v(p_{1}) u(p_{2}) u(p'_{1}) v(p'_{2})\} + J(p_{1}, -p'_{1}; p'_{2}, -p_{2}) \\ \times \{v(p_{1}) u(p_{2}) v(p'_{1}) u(p'_{2}) + u(p_{1}) v(p_{2}) u(p'_{1}) v(p'_{2})\}.$$
(79)

It is clear that the equations obtained connect together the functions

$$\xi(p_1, p_2), \quad \eta(-p_2, -p_1)$$

only for a fixed value of $p_1 + p_2$. We note also that the coefficients of X and Y are the same in both Eqs. (78). It is thus convenient to put

 $p_1 = p, \quad p_2 = -p + q,$ $\xi(p_1, p_2) - \eta(-p_2, -p_1) = \theta_q(p),$ $\xi(p_1, p_2) + \eta(-p_2, -p_1) = \vartheta_q(p).$

We transform then Eqs. (78) to the simpler form:

(80)

$$L_{q}(\theta) = E\theta, \quad M_{q}(\theta) = E\theta, \quad (80)$$
where
$$L_{q}(\theta) = \{ \mathfrak{Q}(p) + \mathfrak{Q}(p-q) \} \theta(p) + \frac{1}{V} \sum_{(p')} Q_{q}(p, p') \theta(p'), \\
M_{q}(\theta) = \{ \mathfrak{Q}(p) + \mathfrak{Q}(p-q) \} \vartheta(p) + \frac{1}{V} \sum_{(p')} R_{q}(p, p') \vartheta(p') \} \quad (81)$$

and where

$$\begin{split} Q(p, p') &= J_q(p, p') \{ u(p) u(p-q) + v(p) v(p-q) \} \\ &\times \{ u(p') u(p'-q) + v(p') v(p'-q) \} \\ &+ I_q(p, p') \{ v(p) u(p-q) - u(p) v(p-q) \} \{ v(p') u(p'-q) \} \\ &- u(p') v(p'-q) \}, \end{split}$$

$$R_q(p, p') &= J_q(p, p') \{ u(p) u(p-q) - v(p) v(p-q) \} \\ &\times \{ u(p') u(p'-q) - v(p') v(p'-q) \} \\ &+ G_q(p, p') \{ v(p) u(p-q) + u(p) v(p-q) \} \end{split}$$

 $\times \{v(p') u(p'-q) + u(p') v(p'-q)\},\$

while

$$\begin{cases}
J_{q}(p, p') = J(p, -p+q; -p'+q, p'), \\
I_{q}(p, p') = J(p, p'-q; p', p-q) \\
-J(p, p'-q, p-q, p') \\
-J(p, -p'; -p'+q, p-q), \\
G_{q}(p, p') = J(p, p'-q; p', p-q) \\
-J(p, p'-q, p-q, p') \\
+J(p, -p'; -p'+q, p-q).
\end{cases}$$
(82)

We shall now elucidate the physical meaning of the functions θ and ϑ . We consider thereto the expressions for the number density of the particles $\rho(\mathbf{r})$ and the momentum density $\mathbf{p}(\mathbf{r})$.

We have:

$$p(r) = \left\langle \sum_{(\sigma)} \overset{*}{\Psi}_{\sigma}(r) \Psi_{\sigma}(r) \right\rangle = \frac{1}{V} \sum_{(p_1, p_2, \sigma)} \left\langle \overset{*}{a}_{p_1 \sigma} a_{p_2 \sigma} \right\rangle e^{i (p_2 - p_1) r}$$
$$= \frac{1}{V} \sum_{(p_1, p_2, \sigma)} F_{\sigma \sigma}(p_1, p_2) e^{i (p_2 - p_1) r}$$
(83)

and

$$\mathbf{p}(r) = \left\langle \sum_{\langle \sigma \rangle} \left\{ \stackrel{+}{\Psi}_{\sigma}(r) \left(-i \frac{\partial}{\partial \mathbf{r}} \Psi_{\sigma}(r) \right) + i \frac{\partial \stackrel{+}{\Psi}_{\sigma}(r)}{\partial \mathbf{r}} \Psi_{\sigma}(r) \right\} \right\rangle$$
$$= \frac{1}{V} \sum_{(p_1, p_2, \sigma)} \left\langle \stackrel{+}{a}_{p_1 \circ} a_{p_2 \sigma} \right\rangle (\mathbf{p}_1 + \mathbf{p}_2) e^{i (p_2 - p_1) r}$$
$$= \frac{1}{V} \sum_{(p_1, p_2, \sigma)} F_{\sigma \sigma}(p_1, p_2) e^{i (p_2 - p_1) r} (\mathbf{p}_1 + \mathbf{p}_2).$$

We introduce the Fourier components for these densities

$$p(r) = \sum_{(q)} p_q e^{i(qt)}, \quad \mathbf{p}(r) = \sum_{(q)} \mathbf{p}_q e^{i(qr)}$$

and note that our ground state is uniform in space and carries no current.

We have thus from (83)

$$\rho_{0} = \frac{1}{V} \sum_{(p)} 2v_{p}^{2}, \ \rho_{q} = \frac{1}{V} \sum_{(p_{2} - p_{1} = q)} \{\delta F_{++}(p_{1}, p_{2}) + \delta F_{--}(p_{1}, p_{2})\}, \ q \neq 0,$$

$$\mathbf{p}_{q} = \frac{1}{2V} \sum_{(p_{2} - p_{1} = q)} (\mathbf{p}_{1} + \mathbf{p}_{2}) \{\delta F_{++}(p_{1}, p_{2}), \delta F_{--}(p_{1}, p_{2})\}.$$
(84)

On the other hand, writing out Eq. (64) in detail we get

$$\delta F_{--}(p_1, p_2) = v(p_1) u(p_2) \lambda(p_2, -p_1) + u(p_1) v(p_2) \lambda^*(p_1, -p_2), \delta F_{++}(p_1, p_2) = v(p_1) u(p_2) \lambda(-p_1, p_2) + u(p_1) v(p_2) \lambda^*(-p_2, p_1).$$
(85)

Substituting these expressions into (84) we find after some obvious simplifications:

$$\rho_{q} = \sum_{\substack{(p_{1}+p_{2}=q) \\ +\lambda^{*}(-p_{2}, -p_{1})\}, \\ p_{g} = \frac{1}{2V} \sum_{\substack{(p_{1}+p_{2}=q) \\ -v(p_{1})u(p_{2})\}} \{\lambda(p_{1}, -p_{2}) + v(p_{1})u(p_{1}) \\ -v(p_{1})u(p_{2})\} \{\lambda(p_{1}, p_{2}) - \lambda^{*}(-p_{2}, -p_{1})\}.$$
(86)

Hence, from (73)

$$\rho_{q} = \sum_{(E)} \rho_{q}^{(E)} e^{-iEt}, \quad \mathbf{p}_{q} = \sum_{(E)} \mathbf{p}_{q}^{(E)} e^{-iEt},$$

$$\rho_{q}^{(E)} = \frac{1}{V} \sum_{(p)} \{u(p) v(p-q) + v(p) u(p-q)\} \vartheta_{q}(p),$$

$$\mathbf{p}_{q}^{(E)} = \frac{1}{2V} \sum_{(p)} (2\mathbf{p} - \mathbf{q})$$

$$\times \{u(p) v(p-q) - v(p) u(p-q)\} \vartheta_{q}(p).$$
(87)

The contribution of an elementary excitation to the oscillations in the particle number density is thus determined by the function ϑ and the corresponding contribution to the oscillations of the momentum density by the function θ .

We turn now to Eqs. (81). In them we put

$$\left\{ \begin{array}{l} \vartheta\left(p\right) = S_1 \delta\left(p - p_0\right), \\ \vartheta\left(p\right) = S_2 \delta\left(p - p_0\right), \end{array} \right\}$$

$$(88)$$

where S_1 and S_2 are constant and p_0 is an arbitrary, fixed momentum.

Dropping terms of the order V^{-1} , which vanish when we take the limit $V \rightarrow \infty$ and which produce only local changes in the wave functions, we see that (88) will be a possible set of solutions, if S_1 and S_2 are connected by the relations:

$$S_{1} \{ \Omega (p_{0}) + \Omega (p_{0} - q) \} = ES_{2},$$

$$S_{2} \{ \Omega (p_{0}) + \Omega (p_{0} - q) \} = ES_{1},$$
(89)

whence we see that

$$E^{2} = \{ \Omega(p_{0}) + \Omega(p_{0} - q) \}^{2}.$$

We satisfy ourselves therefore of the existence of

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a continuous spectrum*

$$E = \Omega(p_0) + \Omega(p_0 - q),$$
 (90)

separated by a gap. The energy E depends here, for given q, continuously on the momentum p_0 .

We construct also the asymptotic part of the wave function of an elementary excitation of this type; to do this we write out Eq. (65) in detail. We find

$$\delta \Phi_{-+}(p_1, p_2) = u(p_1) u(p_2) \lambda(p_1, p_2) - v(p_1) v(p_2) \lambda^*(-p_2, -p_1),$$

and thus for the case under consideration with a δ -shaped component

$$\delta \Phi_{\to} (p_1, p_2) = \delta (p_1 - p_0) \delta (p_2 + p_0 - q) S$$

$$\times \exp \{ -i [\Omega (p_0) + \Omega (p_0 - q)] t \},$$

where the constant S will be

$$S = u(p_0) u(p_0 - q) \frac{S_1 + S_2}{2} + v(p_0) v(p_0 - q) \frac{S_1 - S_2}{2}.$$

We have thus in the r-representation

$$\begin{split} \delta \Phi_{-+} (r_1, r_2) &= \mathrm{const} \cdot \exp\{ - i \left(\Omega \left(p_0 \right) + \Omega \left(p_0 - q \right) \right) t \} \\ &\times \exp\{ i p_0 r_1 + i \left(q - p_0 \right) r_2 \}. \end{split}$$

Let us compare this expression with the wave function for a (-, +) pair in the ground state:

$$\Phi_{-+}^{0}(r_{1}, r_{2}) = \text{const} \int e^{ip(r_{1}-r_{2})} u(p) v(p) dp.$$

It is clear that such a Φ_{-+}^0 corresponds to a bound state of a pair of particles and, in particular, that this function tends to zero as $|\mathbf{r}_1 - \mathbf{r}_2| \to \infty$. The expression $\delta \Phi_{-+}$, on the other hand, splits into a product of two plane waves and corresponds to the independent motion of two particles with momenta p_0 and $q - p_0$.

We see thus that the elementary excitation from the continuous spectrum can be interpreted physically as the corresponding dissociation of the quasimolecule into separate states of its particles.

We now proceed to study the spectrum of the collective oscillations, which will be determined using the solutions of Eq. (81) corresponding (for fixed q) to discrete values of E.

We first consider the case where the particles do not have an electrical charge. Since there is

$$\sum_{(p)} \vartheta(p) \vartheta(p) > 0.$$
(76)

Substituting the solution (88) into this condition we see that S_1 and S_2 must have the same sign. Therefore Eq. (89) leads to a positive sign for E.

no Coulomb interaction, we consider all kernels

I, J, and G to be finite. From Eq. (35) it follows further that

$$L_0(\theta) = 0$$
 for $\theta = u(p)v(p)$.

The inhomogeneous equation

$$L_0(\theta) = f(p)$$

can therefore be solved only if

$$\sum_{(p)} f(p) u(p) v(p) = 0.$$
(91)

We see now that the set (81) has a solution

$$\theta = u(p)v(p), \quad \vartheta = 0, \quad E = 0, \quad (92)$$

when q = 0 and we shall therefore write its solution for small |q| as an expansion in powers of |q|:

$$\begin{aligned} \theta &= u(p) v(p) + |q| \theta_1(p, e) + |q|^2 \theta_2(p, e) + \dots, \\ \theta &= |q| \theta_1(p, e) + \dots, \\ E &= |q| E_1 + \dots, \end{aligned}$$
(93)

where

$$\mathbf{e} = \frac{\mathbf{q}}{|\mathbf{q}|} \, .$$

Substituting these expansions into Eq. (81) we get

$$L_{0}(\theta_{1}) = -\sum_{(1 \leq \alpha \leq 3)} e_{\alpha} \left\{ \frac{\partial L_{q}(uv)}{\partial q_{\alpha}} \right\}_{q=0}, \qquad (94)$$

$$M_{0}(\vartheta_{1}) = E_{1}u(p)v(p), \qquad (95)$$

$$L_{0}(\theta_{2}) = E_{1}\vartheta_{1} - \sum_{\substack{(1 \leq \alpha \leq 3) \\ \left\{\frac{1}{2} \leq \alpha \leq 3\right\}}} e_{\alpha} \left\{\frac{\partial L_{q}}{\partial q^{\alpha}}(\theta_{1})\right\}_{q=0} - \frac{1}{2} \sum_{\substack{(1 \leq \alpha \leq 3) \\ \left\{\frac{1}{2} \leq \alpha \leq 3\right\}}} e_{\alpha}e_{\beta} \left\{\frac{\partial^{2}L_{q}(uv)}{\partial q^{\alpha}\partial q^{\beta}}\right\}_{q=0}.$$
(96)

Equation (94) can be solved since the function f(p) occurring on the right hand side has the property f(-p) = -f(p) so that the condition (91) is satisfied trivially.

In order that Eq. (96) be soluble we must demand, on the basis of (91), that

$$E_{1} \sum_{(p)} \vartheta_{1}(p, e) u(p) v(p)$$

$$= \sum_{(p)} u(p) v(p) \left\{ \sum_{(1 \leq \alpha \leq 3)} e_{\alpha} \left\{ \frac{\partial L_{\eta}}{\partial q^{\alpha}} (\theta_{1}) \right\}_{q=0} + \frac{1}{2} \sum_{(\alpha, \beta)} e_{\alpha} e_{\beta} \left\{ \frac{\partial^{2} L_{\eta}(uv)}{\partial q^{\alpha} \partial q^{\beta}} \right\}_{q=0} \right\}.$$
(97)

From Eq. (95) we see that ϑ_1 is proportional to E_1 so that condition (97) gives us the possibility to determine E_1^2 , and so on.

Carrying out in practice the program of calculations given here for the spherically symmetric

^{*}The positive sign is chosen by us on the basis of the general normalization condition (76), which in the case under consideration will be

case we can verify that for small |q|:

$$E = \frac{|q|s}{\sqrt{3}},$$

where, if we disregard the corrections due to the interaction, s will be equal to the value of the particle velocity at the Fermi surface.

We thus find collective oscillations of quasiacoustic character. Their region of existence is bounded by momenta q for which the corresponding E lies below the threshold of excitation for the continuous spectrum.

Let us now see what happens with oscillations of this type in a dynamical system of electrons, such as is considered in superconductivity theory. We note first that the presence of the Coulomb interaction causes here an important singularity in

the kernel $G_q: G_q = \frac{8\pi e^2}{|q|^2} + G'_q.$

It is therefore convenient to construct now an operator M_q of the form

$$M_{q}(\vartheta) = M'_{q}(\vartheta) + \frac{8\pi e^{2}}{|q|^{2}} \{v(p) u(p-q) + u(p) v(p-q)\}$$

$$\times \frac{1}{V} \sum_{(p')} \vartheta(p') \{v(p') u(p'-q) + u(p') v(p'-q)\}, \quad (98)$$

in which we have split off the part with the singularity* at q = 0 explicitly.

To regularize (81) we introduce a new unknown by putting

$$\frac{1}{V} \sum_{p'} \vartheta(p') \{ v(p') u(p'-q) + u(p') v(p'-q) \} = \frac{|q|^2}{16\pi e^2} \Psi.$$

Our system of equations can then be written in the form

$$L_{q}(\theta) = E\vartheta,$$

$$M'_{q}(\theta) + \{v(p)u(p-q) + u(p)v(p-q)\}\frac{\Psi}{2} = E\theta,$$

$$\frac{1}{V}\sum_{p'} \vartheta(p')\{v(p')u(p'-q) + u(p')v(p'-q)\} = \frac{|q|^{2}}{16\pi e^{2}}\Psi.$$
(99)

*One should not think that a more rigorous treatment would have yielded the screening effect in the factor G_a and thereby would have eliminated this singularity. This is because we are dealing with oscillations of the electric charge density which is clear at least from the fact that precisely the amplitude of these oscillations [see (87)] enters into (98). The screening effect appears, generally speaking, in expressions corresponding to allowances for correlations. To consider the influence of spatial inhomogeneities, however, we must always take the long range character of the Coulomb forces into account. We must therefore also expect that in a more rigorous treatment the singularity at q = 0 will remain in the expressions mentioned. In investigating the non-uniformity in the charge distribution, the Coulomb forces are long range in character and the q-representation must thus always have the above-mentioned singularity at q = 0.

We see that for arbitrary E it has, for q = 0, the solution

$$\theta = u(p)v(p), \quad \vartheta = 0, \quad \Psi = E,$$

so that we can write its solution for small |q| using the expansion

$$\begin{aligned} \theta &= u(p)v(p) + |q|\theta_{1}(p, e) + |q|^{2}\theta_{2}(p, e) + \dots, \\ \theta &= |q|\theta_{1}(p, e) + \dots, \quad \Psi = E_{0} + |q|\Psi_{1} + \dots, \\ E &= E_{0} + |q|E_{1} + \dots, \end{aligned}$$
(100)

and substituting this into (99) we find

$$L_0(\theta_1) = E_0 \vartheta_1 - \sum_{\substack{(1 \leq \alpha \leq 3)}} e_\alpha \left\{ \frac{\partial L_q(uv)}{\partial q_\alpha} \right\}_{q=0}, \quad (101)$$

$$M'_{0}(\vartheta) = u(p)v(p)(E_{1} - \Psi_{1}) + E_{0}\theta_{1} + \frac{E_{0}}{2} \sum_{(\alpha)} e_{\alpha} \left\{ u(p) \frac{\partial v(p)}{\partial p_{\alpha}} + v(p) \frac{\partial u(p)}{\partial p_{\alpha}} \right\},$$
(102)

$$\frac{1}{V} \sum_{(p')} \vartheta_1(p') u(p') v(p') = 0,$$
(103)

$$L_{0}(\theta_{2}) = E_{0}\theta_{2} + E_{1}\theta_{1} - \sum_{(\alpha)} e_{\alpha} \left\{ \frac{\partial L_{q}}{\partial q_{\alpha}}(\theta_{1}) \right\}_{q=0}$$
$$-\frac{1}{2} \sum_{(\alpha,\beta)} e_{\alpha}e_{\beta} \left\{ \frac{\partial^{2}L_{q}(uv)}{\partial q_{\alpha}\partial q_{\beta}} \right\}_{q=0}, \qquad (104)$$

$$2 \frac{1}{V} \sum_{(p)} \vartheta_2(p) u(p) v(p) = \frac{E_0}{16\pi e^2} + \frac{1}{V} \sum_{(\alpha, p)} \vartheta_1(p) e_\alpha \left\{ u(p) \frac{\partial v(p)}{\partial p_\alpha} + v(p) \frac{\partial u(p)}{\partial p_\alpha} \right\}.$$
 (105)

In Eq. (102) we take

$$E_1 - \Psi_1 = 0,$$

and we can conclude from (100) and (102) that θ_1 and ϑ_1 must be antisymmetric with respect to a change in the sign of p, and Eq. (103) is thus satisfied automatically.

We write down our usual condition for the solubility of (104):

$$E_{0} \sum \vartheta_{2}(p) u(p) v(p) = \sum u(p) v(p) \left\{ \sum_{(\alpha)} e_{\alpha} \left(\frac{\partial L_{q}}{\partial q_{\alpha}} (\theta_{1}) \right)_{q=0} + \frac{1}{2} \sum_{(\alpha,\beta)} e_{\alpha} e_{\beta} \left[\frac{\partial^{2} L_{q}(uv)}{\partial q_{\alpha} \partial q_{\beta}} \right]_{q=0} \right\}.$$
(106)

The left hand side of this equation will be, if we use (105):

$$V\left\{\frac{E_{\partial}^{2}}{32\pi e^{2}}+\frac{1}{V}\sum_{(\alpha, p)}\vartheta_{1}(p)e_{\alpha}\left\{u\left(p\right)\frac{\partial v\left(p\right)}{\partial p_{\alpha}}+v\left(p\right)\frac{\partial u\left(p\right)}{\partial p_{\alpha}}\right\}\right\}.$$
(107)

We see now that Eq. (106), which determines E_0 , does not have a zero root. Indeed, it follows from (101) and (102) that the left hand side of (106), which is expression (107), vanishes for $E_0 = 0$. The right hand side of (106), however, is the same as the right hand side of (97) for $E_0 = 0$, and will therefore be different from zero.

We now evaluate E_0 for the spherically symmetric case. We take

$$E\left(p\right) = \frac{p^2}{2m}$$

and also assume that

$$J(p_1, p_2; p'_2, p'_1) = J(p_1 - p'_1)$$
 and $p_1 + p_2 = p'_1 + p'_2$. (108)

We can then verify the existence of the identity

$$L_{q}(\chi_{q}) = \left\{ \frac{(p-q)^{2}}{2m} - \frac{p^{2}}{2m} \right\} (v(p) u(p-q) - u(p) v(p-q)),$$
(109)

where

$$\chi_{q}(p) = u(p)v(p-q) + u(p-q)v(p).$$
(110)

We note that the case (108) is realized if the interaction does not depend on the velocities and is determined by a potential $U(r_1 - r_2)$. In that case

$$J(p) = J(-p) = \int U(r) e^{i(rp)} dr.$$

In superconductivity theory one must take into account, apart from the Coulomb forces for which Eq. (108) is, of course, satisfied, also the Fröhlich interaction produced by the exchange of phonons. Such an interaction is effective only in a narrow layer near the Fermi surface and in that region its contribution to J will be

$$J_{ph}(p_1, p_2; p'_2, p'_1) = -g^2(p_1 - p'_1)$$

if $p_1 + p_2 = p'_1 + p'_2$, (111)

where g(q) is a quantity characterizing the coupling of the electrons and the phonons. We can thus also use here Eq. (109). Strictly speaking, in order that it be <u>rigorously</u> true it is necessary to change Eq. (110). We would then note a deviation of the order of the ratio C/ω , where ω is the average phonon energy, i.e., a deviation of the order of the magnitude of the electron-phonon interaction timelag effects.

Because of this fact it is not expedient to make this refinement in the model considered here, in which the electron-phonon interaction is replaced by a direct interaction between the electrons, since this replacement itself is possible only if we neglect time-lag effects.

We now use Eqs. (109) and (110) to determine the value of E_0 . Because the operator L_q is Hermitian, we have

$$\sum_{(p)} \{ L_q(\theta) \chi_q - L_q(\chi_q) \theta \} = 0, \qquad (112)$$

so that

$$E \frac{1}{V} \sum_{(p)} \vartheta(p) \{ u(p) v(p-q) + v(p) u(p-q) \}$$

= $\frac{1}{V} \sum_{(p)} \vartheta(p) \left\{ \frac{(p-q)^2}{2m} - \frac{p^2}{2m} \right\}$
× $\{ v(p) u(p-q) - u(p) v(p-q) \}.$ (113)

We shall now evaluate both sides of this equation up to terms of the order $|q|^2$, <u>inclusive</u>. From (110) we see that

$$\theta(p) = u(p)v(p) + |q|\theta_1 + \dots$$

From (99) and (100) we have, furthermore,

$$\frac{-1}{V} \sum_{p} \vartheta(p) \{ u(p) v(p-q) + v(p) u(p-q) \}$$

= $\frac{|q|^2}{16\pi e^2} \{ E_0 + |q| \Psi_1 + \ldots \},$

so that we get from (113)

$$E_{0}^{2} = 16\pi e^{2} \frac{1}{V} \sum_{(p)} u(p) v(p) \frac{(pe)}{m} \times \left\{ v(p) \left(e^{\frac{\partial u(p)}{\partial p}} \right) - u(p) \left(e^{\frac{\partial v(p)}{\partial p}} \right) \right\}, \quad (114)$$

where $\mathbf{e} = \mathbf{q}/|\mathbf{q}|$. Substituting Eqs. (36) for u and v into (114) we find finally,

$$E_{0} = \sqrt{\frac{4e^{2}}{3\pi} \frac{p_{F}^{3}}{m}},$$
 (115)

where p_F is the Fermi momentum.

It is clear that we have here obtained the usual energy value for the well-known plasma oscillations; the special character of the superconducting state has completely disappeared.* Since E_0 is appreciably larger than the energy of the continuous spectrum (for small q) the stationary solution found here turns out to be only quasi-stationary in a more rigorous treatment.

We note, however, one curious fact, namely that notwithstanding the result obtained here the value E = 0 can be considered to be an approximate eigenvalue for the set (81).

Indeed, taking (109) into account one notes easily that, taking

$$\theta_q(p) = \chi_q(p), \quad \vartheta_q(p) = 0, \quad E = 0,$$

we satisfy Eqs. (81) up to terms of the order $|q|^2$. After this we note that this fact turns out to be very essential in order to guarantee the gauge invariance of the theory.

We noted just now that the plasma oscillations with their high value for E are not typical of the

^{*}This result had been obtained before by Anderson.⁶ The earlier statement (see Sec. 7 of reference 1) of the importance of the influence of the superconducting state was not confirmed.

superconducting state. In that connection we can raise the problem whether there are in general collective oscillations that are characteristic of this state.

As we see now, we can look for them only among oscillations which do not change the electrical charge distribution density.

In other words, we must look for solutions of (81) for which the expression

$$\frac{1}{V}\sum_{p}\vartheta(p)\{u(p)v(p-q)+v(p)u(p-q)\},\$$

with which the occurrence of the singularity at q = 0 [see (98)] is also connected, vanishes.

We now consider the spherically symmetric case. We take the z-axis in the direction of the vector \mathbf{q} and introduce cylindrical coordinates. We seek solutions of the form

$$\begin{split} \theta_q(p) &= e^{in\varphi}\, \theta\left(p^2, \ p_z\right), \\ \vartheta_q(p) &= e^{in\varphi}\, \vartheta\left(p^2, \ p_z\right), \end{split} \qquad n \neq 0.$$

Such solutions will formally exist, and the above mentioned expression is identically equal to zero for these solutions. The question is only whether the corresponding values of E lie below the threshold for excitation of the continuous spectrum.

One should also analyze oscillations of the branch of the spectrum not considered here, for which

$$\lambda_{-+} = \lambda_{+-} = 0.$$

5. PROBLEMS OF THE ELECTRODYNAMICS OF THE SUPERCONDUCTING STATE

We consider the problem of the change in the superconducting ground state under the action of a constant external field A(r).

To work in the linear approximation, we assume A(r) to be infinitesimally small, of the first order, and use the general Equations (77).

If we do not take the paramagnetic term* into account we get then

$$\lambda_{-+}(p_1, p_2) = \frac{1}{2} \theta_q(p); \ \lambda_{-+}^*(-p_2, -p_1) = -\frac{1}{2} \theta_q(p)$$
 (116)
and

$$L_{\mathbf{q}}(\boldsymbol{\theta}_{q}) = -\frac{e}{m} (2\mathbf{p} - \mathbf{q}) \Lambda (q) \{ \boldsymbol{v}(p) \, \boldsymbol{u}(p-q) - \boldsymbol{u}(p) \, \boldsymbol{v}(p-q) \}.$$
(117)

We now investigate the properties of this equation. We take

$$e\mathbf{A}\left(q\right) = i\mathbf{q}\boldsymbol{\varphi}\left(q\right). \tag{118}$$

We must then have, in the r-representation,

$$F(r_1, r_2) = e^{i(\varphi(r_2) - \varepsilon(r_1))} F_0(r_1, r_2)$$

if there is gauge invariance, or, since in our case φ is infinitesimally small:

$$\delta F(r_1, r_2) = i \{\varphi(r_2) - \varphi(r_1)\} F_0(r_1, r_2).$$

Going over to the p-representation and using Eq. (85) we get

$$\lambda(p_1, p_2) = i\varphi(p_1 + p_2) \{u_{p_1} v_{p_2} + v_{p_1} u_{p_2}\}$$

and

$$\theta_q(p) = 2i\varphi(q) \{ u(p) v(p-q) + v(p) u(p-q) \} = 2i\varphi(q) \chi_q(p).$$

On the other hand, the $\theta_q(p)$ which we have found must satisfy Eq. (117) in the case (118), and thus

$$2i\boldsymbol{\varphi}(q) L_q \{\chi_q\} = \frac{1}{im} \{(2\mathbf{p} - \mathbf{q}) \, \mathbf{q}\} \, \boldsymbol{\varphi}(q) \{ v(p) \, u(p-q) - u(p) \, v(p-q) \}.$$

But this is none other than Eq. (109).

The property of gauge invariance is thus true with the same degree of accuracy as Eq. (109), i.e., up to electron-phonon interaction time-lag effects.

Let us now imagine the situation that results if we proceed as follows. We first consider the Hamiltonian of the system without the external field; we perform the canonical transformation

$$a_{k_1+} = u_k a_{k_0} + v_k a_{k_1}, \quad a_{-k} = u_k a_{k_1} - v_k a_{k_0}$$

and determine u, v from the condition of compensating dangerous diagrams with momenta k, -k.

We shall then introduce into the Hamiltonian the small external field and transform all expressions in terms of the amplitudes α , $\dot{\alpha}$, after which we apply the usual perturbation theory without bothering to compensate the new dangerous diagrams with momenta k, -k+q, arising from the external field.

We then obtain instead of (117)

$$\{ \mathfrak{Q}(p) + \mathfrak{Q}(p-q) \} \theta_q(p) = -\frac{e}{m} (2\mathbf{p} - \mathbf{q}) \mathbf{A}(q) \{ v(p) u(p-q) - u(p) v(p-q) \},$$

whence

$$\theta_{q}(p) = \frac{-\frac{-w}{m}(2p-q)\mathbf{A}(q)}{\Omega(p)+\Omega(p-q)} \{v(p)u(p-q) - u(p)v(p-q)\}.$$
(119)

This result is clearly no longer gauge invariant in any reasonable approximation. By replacing $L_q(\theta)$ with

^{*}In the linear approximation its effect can always be considered separately.

$$\Omega(p) + \Omega(p-q) \} \theta,$$

we have violated the very basic property of this operator, namely that we have a zero eigenvalue for q = 0.

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It is of interest to note that Eq. (117) can also be obtained as follows. We perform in the total Hamiltonian the usual canonical transformation mixing up amplitudes with momenta $\pm q$. We then apply the method of approximate second quantization by introducing Bose amplitudes in place of the operator products $\alpha_{\nu}\alpha_{\mu}$. Then, as Galasiewicz has shown, as we study the "static deformation" of the system due to the action of a constant vector potential, we arrive at just Eq. (117). The integral term in the expression for L can thus be interpreted in some sense as being produced by a collective effect. We note that an analogous approach was developed in a paper by Blatt and Matsubara.⁹

We now proceed to study the dependence of the current density on the vector potential. From (84) we have

$$\boldsymbol{m} \mathbf{j}_{q} = e \mathbf{p}_{q} - e^{2} \mathbf{A} \left(q \right) \frac{2}{V} \sum v_{p}^{2},$$

and thus, because of (87)

$$m\mathbf{j}_{q} = \frac{1}{V} \sum_{(p)} e\left(\mathbf{p} - \frac{\mathbf{q}}{2}\right) \theta_{q}(p) \{u(p) v(p-q) - v(p) u(p-q)\}$$
$$- e^{2} \mathbf{A}(q) \frac{2}{V} \sum_{(p)} v_{p}^{2}.$$
(120)

We now denote the solution of the equation

$$L_{q}(T_{\alpha}) = -\frac{2p_{\alpha} - q_{\alpha}}{m} \{v(p) u(p-q) - u(p) v(p-q)\},$$

$$\alpha = 1, 2, 3.$$
(121)

by $T_{\alpha}(p, q)$. We find then from (117) and (120):

$$\theta_{q}(p) = e \sum_{\alpha} T_{\alpha}(p, q) A_{\alpha}(q),$$

$$i_{\alpha}^{\alpha} = \frac{e^{2} \rho_{0}}{m} \sum_{\beta} \{S_{\alpha\beta}(q) - \delta(\alpha - \beta)\} A_{\beta}(q), \qquad (122)$$

where

$$\rho_{0} = \frac{2}{V} \sum_{p} v_{p}^{2},$$

$$S_{\alpha\beta}(q) = \frac{1}{V} \sum_{p} \frac{(2p_{\alpha} - q_{\alpha})}{2\rho_{0}} \{u(p) v(p - q) - v(p) u(p - q)\} T_{\beta}(p, q).$$
(123)

Because of (121) we can also write

$$S_{\alpha\beta}(q) = \frac{1}{V} \frac{m}{\rho_0} \sum_{(p)} L_q(T_a) T_{\beta}$$

From this we can satisfy ourselves that $S_{\alpha\beta}$ is symmetrical:

 $S_{\alpha\beta}(q) = S_{\beta\alpha}(q). \tag{124}$

From (123) we have also

$$\begin{split} \sum_{(\alpha)} q_{\alpha} S_{\alpha\beta}(q) &= \frac{m}{p_{0} V} \sum_{(p)} L_{q}(\chi_{q}) T_{\beta} = \frac{1}{V} \frac{m}{p_{0}} \sum_{(p)} \chi_{q} L_{q}(T_{\beta}) \\ &= \frac{1}{V \rho_{0}} \sum_{(p)} (2p_{\beta} - q_{\beta}) \{ u(p) v(p-q) - v(p) u(p-q) \} \\ &\times \{ u(p) v(p-q) + v(p) u(p-q) \} \\ &= \frac{1}{V \rho_{0}} \sum_{(p)} (2p_{\beta} - q_{\beta}) \{ u^{2}(p) v^{2}(p-q) - v^{2}(p) u^{2}(p-q) \} \\ &= \frac{1}{V \rho_{0}} \sum_{(p)} (2p_{\beta} - q_{\beta}) \{ v^{2}(p-q) - v^{2}(p) \} \\ &= \frac{1}{V \rho_{0}} \sum_{(p)} (2p_{\beta} - q_{\beta}) v^{2}(p-q) - \frac{1}{V \rho_{0}} \sum_{(p)} (2p_{\beta} - q_{\beta}) v^{2}(p) \\ &= \frac{1}{V \rho_{0}} \sum_{(p)} (2p_{\beta} + q_{\beta}) v^{2}(p) - \frac{1}{V \rho_{0}} \sum_{(p)} (2p_{\beta} - q_{\beta}) v^{2}(p). \end{split}$$

We get in this way Buckingham's relations:⁷

$$\sum_{(\alpha)} q_{\alpha} S_{\alpha\beta}(q) = q_{\beta}.$$
 (125)

Because of (125) and (122) we convince ourselves that the conservation law $qj_a = 0$ is satisfied. We see also that j_q depends practically only on the transverse part \mathfrak{A} of the vector potential A:

$$\begin{split} f_{q}^{a} &= \frac{e^{2}\rho_{0}}{m} \sum_{\beta} \left\{ S_{\alpha\beta}\left(q\right) - b\left(\alpha - \beta\right) \right\} \mathfrak{A}_{\beta}\left(q\right), \\ \mathfrak{A}_{\alpha}\left(q\right) &= A_{\alpha}\left(q\right) - \frac{\left(\mathbf{q} \cdot \mathbf{A}_{-}\left(q\right)\right)}{q^{2}} q_{\alpha} \,. \end{split}$$

We now study the dependence of j_q on $\mathfrak{A}(q)$ for small q. Since now $\mathbf{q} \cdot \mathfrak{A}(q) = 0$, we can write (117) in the form

$$L_q(\boldsymbol{\theta}_q) = 2 \frac{e}{m} (\mathbf{p}_{\perp} \mathfrak{A}) \{ u(p) v(p-q) - v(p) u(p-q) \},$$

where \mathbf{p}_{\perp} is the component of \mathbf{p} perpendicular to the vector \mathbf{q} . Taking the z axis in momentum space along the direction of $\mathfrak{A}(\mathbf{q})$ and the x axis along the direction of \mathbf{q} we then get

$$\theta_q(p) = e\mathfrak{A}(q)\,\tau(p,\,q),\tag{126}$$

where

$$L_{q}(\tau) = f(p, q)$$

= $\frac{2}{m} p_{z} \{ u(p) v(p-q) - v(p) u(p-q) \}.$ (127)

It is clear that here f(p, q) must be an antisymmetric function of p_z :

$$f(p_x, p_y, -p_z; q) + f(p_x, p_y, +p_z; q) = 0.$$
(128)

Such a function will be orthogonal to u(p)v(p).

We can thus always* look for the solution of Eq. (127) in the form

$$\tau(p, q) = q\tau_1(p) + q^2\tau_2(p) + \ldots,$$

where τ_1, τ_2, \ldots are antisymmetric functions of the variable p in the sense of (128).

On the other hand, substituting (126) into (120) we find

$$\mathbf{j}_{q} = \frac{e^{2} \boldsymbol{\rho}_{0}}{m} \{ \mathbf{S}(q) - \mathbf{e}_{z} \} \mathfrak{A}(q),$$

where \mathbf{e}_{z} is a unit vector along the z axis, and

$$S(q) = \sum \frac{2\mathbf{p} - \mathbf{q}}{2\rho_0} \tau(p, q) \{ u(p) v(p-q) - v(p) u(p-q) \}.$$

However, as $q \rightarrow 0$ the function τ will be of first order of smallness and S(q) must thus vanish as q^2 .

For sufficiently small q we have thus

$$\mathbf{j}_{q} = -\frac{e^{2}\rho_{0}}{m} \mathfrak{A}(q)$$
 (129)

and we have the Meissner effect in its exact form.^{8,9}

We saw that for a consideration of the influence of a vector potential, only the operator¹⁰ $L_q(\theta)$ was of importance.

If we had wanted to consider the influence of an external scalar potential U, we would have arrived in the linear approximation at the equation

$$M_{q}(\vartheta) = -2eU(q)\{u(p)v(p-q) + v(p)u(p-q)\}$$

with the operator M_q . Since this operator contains a singular term due to the deformation of the charge density, we can easily verify that there is no typical effect for the superconducting state (in the linear approximation) and that the screening effect will occur as in the normal state.

We note finally that if we study the influence of the term proportional to $\mathbf{H} \times \boldsymbol{\sigma}$ we are led to a

new operator, namely just the one which enters into the equation for the oscillations for that branch of the spectrum where $\lambda_{-+} = 0$.

Note added in proof. We recently saw a new interesting paper by May and Schafroth¹¹ in which they used our old method of compensating only diagrams with opposite momenta and also obtained convincing results about gauge invariance of the Meissner effect. Because of this they had to consider all orders of perturbation theory because, as we showed in the present paper, one must apply the generalized compensation principle when an electromagnetic field is present. In contradistinction to our approach, however, May and Schafroth considered at once the situation with the threefold Hamiltonian, which gives additional advantages.

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⁷ M. J. Buckingham, Nuovo cimento **5**, 1763 (1957).

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¹⁰ J. Bardeen, Nuovo cimento 5, 1766 (1957).

¹¹R. M. May and M. R. Schafroth, in press.

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^{*}From a purely mathematical point of view there is the possibility, finally, that the equation $L_0(\theta) = 0$ possesses apart from the symmetrical solution $\theta = u(p)v(p)$ also another eigensolution which is antisymmetrical with respect to p_z . There is, however, physically no ground for considering such a solution and we shall not take it into account.