

# Quantum Condensation, Thermodynamic Limit, and Dimensionality

## II. Interacting Fermion Gas

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(Z. Naturforsch. 27 a, 881—889 [1972]; received 24 March 1972)

The analysis presented recently for the interacting boson gas is repeated for the interacting fermion gas. It is shown that quantum condensation does not occur in finite systems and even not if the thermodynamic limit is formed with respect to one or two space dimensions only.

Quantum condensation of an interacting fermion or boson gas is formulated with the help of the method of the quasi-expectation value<sup>1</sup>. A convenient version of this method was, for the boson gas, given recently by the author<sup>2,3</sup>. It is adapted to the fermion case in Section 1 of the present paper. This method leads to the introduction of new building blocks into a diagrammatic perturbation analysis. The new elements disappear again when, in the end of the calculation, quasi-expectation values are obtained by a limiting procedure. But they may still leave a trace. This is quantum condensation.

As shown in I, quantum condensation of the interacting boson gas cannot occur in a finite system and even not if the thermodynamic limit is formed with respect to one or two space dimensions only. These considerations are, with the same results, repeated for the fermion case in Section 2 to 4 of the present paper.

Quantum condensation of the interacting fermion gas essentially consists in the formation of a condensate of particle pairs. This physical aspect is obscured in the conventional formulation of the condensation problem as given in Section 1. Therefore, a reformulation is developed in Section 2. The interaction between two particles is emphasized in this alternative formulation. It is subsequently shown in Section 3 that a certain class of diagrams, essentially representing the propagation of two interacting particles, would not exist if quantum condensation occurred in a finite system. Since the irreducible self-energy parts are immediately derived from this class of diagrams, quantum condensation of the interacting fermion gas cannot occur in a finite system. As finally pointed out in Section 4, quantum condensation does still not occur if the

thermodynamic limit is formed with respect to one or two space dimensions only provided that a certain assumption about the spectrum of an eigenvalue equation is true. That quantum condensation of the fermion gas does not occur in strictly one or two-dimensional systems (with no spatial extension in other dimensions) was shown earlier by HOHENBERG<sup>4</sup>.

All this is quite analogous to the analysis given and the results obtained in I. Some formulae are more lengthy and complicated in the present fermion case. Some details will, therefore, be suppressed whenever this seems appropriate. Especially in Section 4 the detailed arguments would practically be the same as in I. Also the statement on the possible physical meaning of the results given in the introduction of I could be repeated word by word.

One difference between the boson and the fermion case deserves special mentioning. In the boson case, the singularity preventing quantum condensation in a finite system appeared in the one-particle propagator. It turned up already in a low order approximation, e.g., the Bogoljubov approximation. In the fermion case, the singularity occurs primarily in an object of less direct physical meaning. Though the singularity is in principle also noticeable in the normal and anomalous self-energy part, it does not turn up as long as the self-energy parts are approximated by a finite number of skeleton graphs.

The singularity in question is doubtless related to excitations (pair states, collective excitations) of the quantum condensed fermion gas. A reexamination of this problem shall, however, be reserved for a separate publication.



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### 1. Quasi-Expectation Value and Quantum Condensation

The system under discussion is a gas of identical spin-one-half fermions contained in a finite volume. The particle annihilation and creation operators are denoted by  $\psi_\alpha(\mathbf{r})$  and  $\psi_\alpha^*(\mathbf{r})$ , respectively.  $\alpha$  is a spin subscript for which occasionally the explicit symbols  $\uparrow$  (up) and  $\downarrow$  (down) will be used. The annihilation and creation operators satisfy the customary anti-commutation relations and vanish on the surface. For a local and spin independent interaction it is

$$H - \mu N = \int \sum_\alpha \left[ \frac{1}{2m} \text{grad } \psi_\alpha^*(\mathbf{r}) \cdot \text{grad } \psi_\alpha(\mathbf{r}) - \mu \psi_\alpha^*(\mathbf{r}) \psi_\alpha(\mathbf{r}) \right] d^3 \mathbf{r} + \frac{1}{2} \int \sum_{\alpha\beta} \psi_\alpha^*(\mathbf{r}) \psi_\beta^*(\mathbf{r}') v(\mathbf{r} - \mathbf{r}') \psi_\beta(\mathbf{r}') \psi_\alpha(\mathbf{r}) d^3 \mathbf{r} d^3 \mathbf{r}'. \quad (1.1)$$

Here,  $H$  is the Hamiltonian operator and  $N$  the particle-number operator.  $\mu$  is the chemical potential and  $m$  the particle mass.  $v(\mathbf{r} - \mathbf{r}')$  is the interaction potential. All spatial integrals are extended over the volume of the system.

The concept of the quasi-expectation value<sup>2,3</sup> is now introduced by adding the operator

$$\tilde{H} = -\frac{1}{2} \int \sum_{\alpha\beta} \varepsilon_{\alpha\beta} [\zeta_0^*(\mathbf{r}, \mathbf{r}') \psi_\alpha(\mathbf{r}) \psi_\beta(\mathbf{r}') + \text{h.c.}] d^3 \mathbf{r} d^3 \mathbf{r}' \quad (1.2)$$

to  $H - \mu N$ .  $\varepsilon_{\alpha\beta}$  is a skew-symmetric quantity with

$$\varepsilon_{\uparrow\uparrow} = +1. \quad (1.3)$$

It is a consequence of the anti-commutation relations that the  $c$ -number function  $\zeta_0(\mathbf{r}, \mathbf{r}')$  may be chosen symmetric with respect to its arguments. The expression (1.2) is appropriate if the condensate consists of singlett pairs. Quasi-expectation values are expectation values for  $\zeta_0(\mathbf{r}, \mathbf{r}') \neq 0$  in the limit  $\zeta_0(\mathbf{r}, \mathbf{r}') \rightarrow 0$ .

The building blocks entering into a diagrammatic perturbation analysis are summarized in Figure 1. The free-particle propagator,  $G_0(\mathbf{r}, \mathbf{r}'; iz)$ , satisfies the differential equation

$$\begin{aligned} \overrightarrow{\mathbf{r} \xrightarrow{z} \mathbf{r}'} &= G_0(\mathbf{r}, \mathbf{r}'; iz) \\ \overleftarrow{\mathbf{r} \xrightarrow{z} \mathbf{r}'} &= -v(\mathbf{r} - \mathbf{r}') \end{aligned} \quad \left( -\frac{1}{2m} \Delta - \mu - iz \right) G_0(\mathbf{r}, \mathbf{r}'; iz) = \delta(\mathbf{r} - \mathbf{r}') \quad (1.4)$$

$$\begin{aligned} \overleftarrow{\mathbf{r} \circ \mathbf{r}'} &= -\xi_0(\mathbf{r}, \mathbf{r}') \\ \overrightarrow{\mathbf{r} \circ \mathbf{r}'} &= +\xi_0^*(\mathbf{r}, \mathbf{r}') \end{aligned}$$

and vanishes when the first spatial argument is situated on the surface.

A similar formulation may be applied to the boson case. This alternative to the formulation presented in I is pointed out in Appendix 1.

Fig. 1. Building blocks of a diagrammatic perturbation analysis.

Normal and anomalous one-particle propagators,  $G(\mathbf{r}, \mathbf{r}'; iz)$  and  $F(\mathbf{r}, \mathbf{r}'; iz)$ , are now introduced by

$$\begin{aligned} \langle \mathcal{T} \psi_\alpha(\mathbf{r}, -i\tau) \psi_\gamma^*(\mathbf{r}', -i\tau') \rangle &= \delta_{\alpha\gamma} \frac{1}{\beta} \sum_z G(\mathbf{r}, \mathbf{r}'; iz) \exp[iz(\tau' - \tau)], \\ \langle \mathcal{T} \psi_\alpha^*(\mathbf{r}, -i\tau) \psi_\gamma(\mathbf{r}', -i\tau') \rangle &= \varepsilon_{\alpha\gamma} \frac{1}{\beta} \sum_z F(\mathbf{r}, \mathbf{r}'; iz) \exp[iz(\tau' - \tau)]. \end{aligned} \quad (1.5)$$

The expectation values are formed with respect to the grand canonical ensemble determined by  $H + \tilde{H} - \mu N$  [cf. Eqs. (1.1) and (1.2)]. The same operator also governs the time dependence of the annihilation and creation operators. The variables  $\tau$  and  $\tau'$  are restricted to the interval between zero and  $\beta$  where  $\beta$  is the inverse absolute temperature with Boltzmann's constant put equal to one.  $\mathcal{T}$  is the time ordering symbol for imaginary times. The  $z$  summation is extended over all odd multiples of  $\pi/\beta$ . Graphical symbols corresponding to normal and anomalous propagators are shown in Figure 2. They are building blocks of skeleton graphs.

$$\begin{aligned} \overleftarrow{\mathbf{r} \xleftarrow{z} \mathbf{r}'} &= G(\mathbf{r}, \mathbf{r}'; iz) \\ \overrightarrow{\mathbf{r} \xrightarrow{z} \mathbf{r}'} &= F(\mathbf{r}, \mathbf{r}'; iz) \\ \overleftarrow{\mathbf{r} \xrightarrow{z} \mathbf{r}'} &= -F^*(\mathbf{r}, \mathbf{r}'; iz) \end{aligned}$$

Fig. 2. One-particle propagators.

The propagators satisfy Gorkov's equations<sup>5</sup>

$$\begin{aligned}
 \overleftrightarrow{\text{---}} &= \overleftrightarrow{\text{---}} + \overleftrightarrow{\text{---}} \boxed{-\Sigma} \overleftrightarrow{\text{---}} + \overleftrightarrow{\text{---}} \boxed{-\Delta} \overleftrightarrow{\text{---}} \\
 \overleftrightarrow{\text{---}} &= \overleftrightarrow{\text{---}} \boxed{+\Delta^*} \overleftrightarrow{\text{---}} + \overleftrightarrow{\text{---}} \boxed{-\Sigma^*} \overleftrightarrow{\text{---}}
 \end{aligned} \tag{1.6}$$

$-\Sigma$  is the normal irreducible self-energy part (i.e. the sum over all irreducible self-energy graphs with one ingoing and one outgoing particle line).  $-\Delta$  is the corresponding anomalous irreducible self-energy part. The reversal of arrows in the anomalous self-energy part is a consequence of the introduction of the operator (1.2).

Equations (1.6) may be translated into a system of integral equations. If, furthermore, use is made of Eq. (1.4), Gorkov's equations assume the form

$$\begin{aligned}
 \left(-\frac{1}{2m}\Delta - \mu - iz\right) G(\mathbf{r}, \mathbf{r}'; iz) + \int [\Sigma(\mathbf{r}, \mathbf{r}''; iz) G(\mathbf{r}'', \mathbf{r}'; iz) \\
 + \Delta(\mathbf{r}, \mathbf{r}''; iz) F(\mathbf{r}'', \mathbf{r}'; iz)] d^3\mathbf{r}'' = \delta(\mathbf{r} - \mathbf{r}'), \\
 \left(-\frac{1}{2m}\Delta - \mu + iz\right) F(\mathbf{r}, \mathbf{r}'; iz) + \int [-\Delta^*(\mathbf{r}, \mathbf{r}''; iz) G(\mathbf{r}'', \mathbf{r}'; iz) \\
 + \Sigma^*(\mathbf{r}, \mathbf{r}''; iz) F(\mathbf{r}'', \mathbf{r}'; iz)] d^3\mathbf{r}'' = 0.
 \end{aligned} \tag{1.7}$$

These integro-differential equations are supplemented by a boundary condition: the propagators vanish when the first spatial argument is situated on the surface. In Eq. (1.7) and elsewhere, the asterisk denotes complex conjugation.

The irreducible self energy parts may be represented by skeleton graphs. If only the first terms of the infinite series are drawn explicitly, we obtain

$$\begin{aligned}
 \boxed{-\Sigma} &= \text{---} \overleftrightarrow{\text{---}} \text{---} + \text{---} \overleftrightarrow{\text{---}} \text{---} + \dots \\
 \boxed{-\Delta} &= \text{---} \overleftrightarrow{\text{---}} \text{---} + \text{---} \overleftrightarrow{\text{---}} \text{---} + \dots
 \end{aligned} \tag{1.8}$$

The equation for the anomalous self-energy part,  $-\Delta(\mathbf{r}, \mathbf{r}'; iz)$ , contains the function  $-\zeta_0(\mathbf{r}, \mathbf{r}')$  as an inhomogeneity.

The problem of quantum condensation may now be formulated in the following way: does there exist a common solution of the Eqs. (1.7) and (1.8) with the anomalous propagator and the anomalous self-energy part not vanishing identically even for  $\zeta_0(\mathbf{r}, \mathbf{r}') \rightarrow 0$ ? This formulation is very convenient for practical calculations. It is, however, not suitable for answering the questions to be studied in this paper. The reason is that physics of quantum condensation of an interacting fermion gas, i.e., the formation of a condensate of pairs, is not exhibited in the above self-energy-like formulation. Therefore, an alternative formulation will be developed in the subsequent section.

## 2. Alternative Formulation: Interacting Particles

The second Eq. (1.8) may also be drawn in the form

$$\boxed{-\Delta} = \text{---} \overleftrightarrow{\text{---}} \text{---} + \boxed{-\Gamma} + \boxed{-\Gamma'} \tag{2.1}$$

where  $-\Gamma$  and  $-\Gamma'$  denote irreducible particle-particle interactions. Some contributions to  $-\Gamma$  are shown in Figure 3a. The diagram given in Figure 3b is not irreducible but is a repetition of a diagram

shown in Figure 3a. No diagrams with crossing particle lines (Figure 3c) or with returning particle lines (Figure 3d) are admitted to the set  $-I$ . Similar statements hold for  $-I'$ .

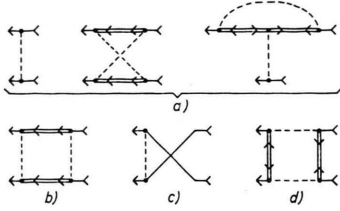
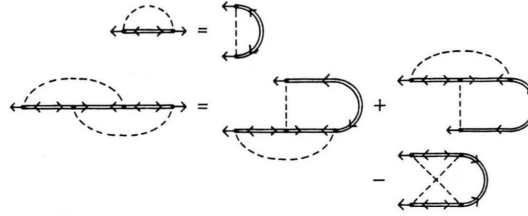


Fig. 3. a) Contributions to the irreducible particle-particle interaction  $-I$ . The diagrams b) to d) are excluded because they are either reducible or contain crossing or returning particle lines.

The proof of Eq. (2.1) is based upon the following simple observation. In the particle line connecting the two open ends of any contribution to  $-\Delta$ , the number of  $F^*$  pieces always exceeds by one, the number of  $F$  pieces. E.g., it is



But in contributions to  $-\Sigma$ , the numbers of  $F^*$  pieces and of  $F$  pieces are always equal. Consequently it is

$$0 = \text{[diagram with box and loop]} - \text{[diagram with box and loop]} \quad (2.2)$$

where the boxes again stand for irreducible interactions. Equation (2.2) will be used in Section 3.

Applying the rules for the translation of graphs we obtain

$$\begin{aligned} \Delta(\mathbf{r}, \mathbf{r}'; iz) = & \zeta_0(\mathbf{r}, \mathbf{r}') - \frac{1}{\beta} \sum_{z''} \int [(\mathbf{r}, \mathbf{r}'; iz | I | iz''; \mathbf{r}'', \mathbf{r}'') F^*(\mathbf{r}'', \mathbf{r}'''; iz'') \\ & + (\mathbf{r}, \mathbf{r}'; iz | I' | iz''; \mathbf{r}'', \mathbf{r}'') F(\mathbf{r}'', \mathbf{r}'''; iz'')] d^3 \mathbf{r}'' d^3 \mathbf{r}''' \end{aligned} \quad (2.3)$$

from Equation (2.1). Both Eq. (2.1) and Eq. (2.3) exhibit the role of the interaction between particles for the phenomenon of quantum condensation of the fermion gas. But these equations are not yet in a form suitable for our analysis.

Use has also to be made of the relations which are a consequence of Gorkov's Eq. (1.6) or (1.7). An explicit proof is given in Appendix 2. The first Eq. (2.4) is translated in the following way

$$\begin{aligned} \longleftrightarrow &= \longleftrightarrow \boxed{-\Delta} \longleftrightarrow - \longleftrightarrow \boxed{+\Delta^*} \longleftrightarrow \\ -\longleftrightarrow &= \longleftrightarrow \boxed{-\Delta} \longleftrightarrow - \longleftrightarrow \boxed{+\Delta^*} \longleftrightarrow \\ 0 &= \longleftrightarrow \boxed{-\Delta} \longleftrightarrow - \longleftrightarrow \boxed{+\Delta^*} \longleftrightarrow \\ 0 &= \longleftrightarrow \boxed{-\Delta} \longleftrightarrow - \longleftrightarrow \boxed{+\Delta^*} \longleftrightarrow \end{aligned} \quad (2.4)$$

$$\begin{aligned} F^*(\mathbf{r}, \mathbf{r}'; iz) = & \int [G(\mathbf{r}, \mathbf{r}''; iz) \Delta(\mathbf{r}'', \mathbf{r}'''; iz) G^*(\mathbf{r}''', \mathbf{r}'; iz) \\ & + F^*(\mathbf{r}, \mathbf{r}''; iz) \Delta^*(\mathbf{r}'', \mathbf{r}'''; iz) F^*(\mathbf{r}'', \mathbf{r}'; iz)] d^3 \mathbf{r}'' d^3 \mathbf{r}''' \\ = & \int [G(\mathbf{r}, \mathbf{r}''; iz) G(\mathbf{r}', \mathbf{r}'''; -iz) \Delta(\mathbf{r}'', \mathbf{r}'''; iz) \\ & + F^*(\mathbf{r}, \mathbf{r}''; iz) F^*(\mathbf{r}', \mathbf{r}'''; -iz) \Delta^*(\mathbf{r}'', \mathbf{r}'''; iz)] d^3 \mathbf{r}'' d^3 \mathbf{r}''' . \end{aligned} \quad (2.5)$$

After the second equality sign use has been made of symmetry properties of the propagators,

$$G(\mathbf{r}', \mathbf{r}'''; -iz) = G^*(\mathbf{r}'', \mathbf{r}'; iz), F(\mathbf{r}', \mathbf{r}'''; -iz) = F(\mathbf{r}'', \mathbf{r}'; iz). \quad (2.6)$$

The remaining three lines of Eq. (2.4) may be translated in a similar way. When, finally, Gorkov's Eq. (1.7) and their complex conjugates are applied, the result is

$$\int \left\{ \left[ \left( -\frac{1}{2m} \Delta - \mu - iz \right) \delta(\mathbf{r} - \mathbf{r}'') + \Sigma(\mathbf{r}, \mathbf{r}''; iz) \right] \left[ \left( -\frac{1}{2m} \Delta' - \mu + iz \right) \delta(\mathbf{r}' - \mathbf{r}''') + \Sigma(\mathbf{r}', \mathbf{r}'''; -iz) \right] F^*(\mathbf{r}'', \mathbf{r}'''; iz) + \Delta(\mathbf{r}, \mathbf{r}''; iz) \Delta(\mathbf{r}', \mathbf{r}'''; -iz) F(\mathbf{r}'', \mathbf{r}'''; iz) \right\} d^3\mathbf{r}'' d^3\mathbf{r}''' = \Delta(\mathbf{r}, \mathbf{r}'; iz). \quad (2.7)$$

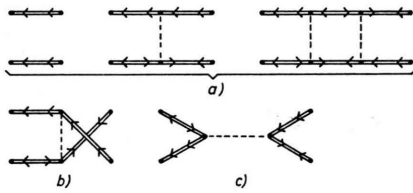
Here,  $\Delta'$  denotes the Laplacian with respect to  $\mathbf{r}'$ .

A combination of Eqs. (2.3) and (2.7) leads to an integro-differential equation for the anomalous propagator and its complex conjugate. The somewhat lengthy equation is, apart from the inhomogeneity, essentially of the Bethe-Salpeter type<sup>6</sup>. This resulting equation is, in the fermion case, the closest analogue to Eq. (I.1.14) in the boson case [cf., also, Eq. (A1.3) in Appendix 1]. We do not propose to start actual calculations from Eqs. (2.3) and (2.7). But these equations form the basis of our further arguing.

*Note added in proof:* W. MOOMANN kindly pointed out to the author that essentially the same formulation was given earlier in the last chapter of a book by NOZIERES<sup>8</sup>.

### 3. Propagation of Interacting Particles

We consider the propagation of two particles without or with interaction between them. A few examples are given in Figure 4a. Diagrams with crossing particle lines (Figure 4b) or with returning particle lines (Figure 4c) are excluded from the considerations. The sum of all admitted diagrams is denoted by  $(\mathbf{r}, \mathbf{r}'; iz; k | R | l; iz''; \mathbf{r}'', \mathbf{r}'')$  where most symbols find their explanation in Figure 5. The letters  $k$  and  $l$



← Fig. 4. a) Contributions to  $R$  (for ingoing arrows on the right and outgoing arrows on the left side). The diagrams b) (with crossing particle lines) and c) (with returning particle lines) are not to be included.

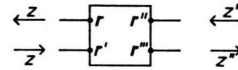


Fig. 5. Labels entering into the definition of matrix elements of  $R$ .

1 = $\leftarrow$	2 = $\leftarrow$
3 = $\rightarrow$	4 = $\rightarrow$

Table 1.

denote the direction of arrows on the left and right end. The key is given in Table 1. It is explicitly assumed that the total flow from right to left, of the variable  $z$ , is equal to zero.

The matrix  $R$  obeys an inhomogeneous integral equation whose kernel is essentially given by irreducible particle-particle interactions (cf. Figure 3a). It is convenient to remove the particle lines on the left side of  $R$  with the help of Gorkov's Equations (1.7). This procedure is similar to the transition from Eq. (2.5) (and from similar equations not written down explicitly) to Eq. (2.7). In this way an integro-differential equation is obtained which, in a matrix notation, may be written as

$$(\Omega + I) R = I. \quad (3.1)$$

The symbol  $I$  on the righthand side stands for the unit matrix with matrix elements

$$(\mathbf{r}, \mathbf{r}'; iz; k | I | l; iz''; \mathbf{r}'', \mathbf{r}'') = \delta(\mathbf{r} - \mathbf{r}'') \delta(\mathbf{r}' - \mathbf{r}''') \beta \delta_{zz''} \delta_{kl}. \quad (3.2)$$

The matrix  $\Omega$  stems from the application of Gorkov's equations. Instead of a complete compilation we only give a few examples,

$$\begin{aligned} (\mathbf{r}, \mathbf{r}'; iz; 1 | \Omega | 1; iz''; \mathbf{r}'', \mathbf{r}'') &= \left[ \left( -\frac{1}{2m} \Delta - \mu - iz \right) \delta(\mathbf{r} - \mathbf{r}'') + \Sigma(\mathbf{r}, \mathbf{r}''; iz) \right] \\ &\quad \left[ \left( -\frac{1}{2m} \Delta' - \mu + iz \right) \delta(\mathbf{r}' - \mathbf{r}''') + \Sigma(\mathbf{r}', \mathbf{r}'''; -iz) \right] \beta \delta_{zz''}, \\ (\mathbf{r}, \mathbf{r}'; iz; 2 | \Omega | 1; iz''; \mathbf{r}'', \mathbf{r}'') &= \left[ \left( -\frac{1}{2m} \Delta - \mu - iz \right) \delta(\mathbf{r} - \mathbf{r}'') + \Sigma(\mathbf{r}, \mathbf{r}''; iz) \right] \\ &\quad \left[ -\Delta^*(\mathbf{r}'', \mathbf{r}'''; -iz) \right] \beta \delta_{zz''}. \end{aligned}$$



Because of the differentiations introduced by  $\Omega$ , boundary conditions are required: the matrix elements of  $R$  vanish when at least one of the left spatial arguments is situated on the surface. —  $I$  is the irreducible particle-particle interaction. Examples are given by

$$\begin{aligned}(\mathbf{r}, \mathbf{r}'; iz; 1 | I | 1; iz''; \mathbf{r}''', \mathbf{r}'') &= (\mathbf{r}, \mathbf{r}'; iz | I | iz''; \mathbf{r}''', \mathbf{r}''), \\(\mathbf{r}, \mathbf{r}'; iz; 1 | I | 2; iz''; \mathbf{r}''', \mathbf{r}'') &= (\mathbf{r}, \mathbf{r}'; iz | I' | iz''; \mathbf{r}''', \mathbf{r}''),\end{aligned}$$

where the matrix elements on the righthand side are those appearing in Equation (2.3). The matrix product in Eq. (3.1) is done by an integration of the two spatial arguments over the volume of the system, multiplication by  $\beta^{-1}$  and summation of the variable  $z$  over all odd multiples of  $\pi/\beta$ , and summation of the variable  $k$  (cf. Table 1) from 1 to 4. The matrix  $I$  given in Eq. (3.2) is the unit matrix with respect to exactly this multiplication.

The main result of Section 2 may now be summarized by stating that it is

$$(\Omega + I) u_0 = 0 \quad (3.3)$$

with

$$u_0^*(\mathbf{r}, \mathbf{r}'; iz; 1) = u_0(\mathbf{r}, \mathbf{r}'; iz; 4) = \mathcal{N} F(\mathbf{r}, \mathbf{r}'; iz), \quad u_0(\mathbf{r}, \mathbf{r}'; iz; 2) = u_0(\mathbf{r}, \mathbf{r}'; iz; 3) = 0. \quad (3.4)$$

$\mathcal{N}$  is an appropriate normalization factor which will be of relevance only in Section 4. The boundary condition satisfied by  $u_0(\mathbf{r}, \mathbf{r}'; iz; k)$  is again the usual one. Strictly speaking, also Eq. (2.2), together with the complex conjugate of this and a few other equations, was used for the derivation of Equation (3.3).

No direct conclusion may be drawn from a comparison of Eqs. (3.3) and (3.1) since  $\Omega + I$  is not a Hermitian matrix. In order to produce a Hermitian matrix we define a matrix,  $\Pi$ , by its matrix elements

$$(\mathbf{r}, \mathbf{r}'; iz; k | \Pi | l; iz''; \mathbf{r}''', \mathbf{r}'') = \varepsilon_k \delta(\mathbf{r} - \mathbf{r}'') \delta(\mathbf{r}' - \mathbf{r}''') \beta \delta_{z-z'} \delta_{kl}. \quad (3.5)$$

Here, the factor  $\varepsilon_k$  is defined by

$$\varepsilon_1 = -\varepsilon_2 = -\varepsilon_3 = \varepsilon_4 = +1. \quad (3.6)$$

Now it can be shown that the matrix operator  $\Pi(\Omega + I)$  is indeed Hermitian. Eqs. (3.1) and (3.3) may be written as

$$\Pi(\Omega + I) R = \Pi, \quad (3.7)$$

$$\Pi(\Omega + I) u_0 = 0. \quad (3.8)$$

Since now the matrix is Hermitian we may conclude that Eq. (3.7) or (3.1) admits a solution

$(\mathbf{r}, \mathbf{r}'; iz; k | R | l; iz''; \mathbf{r}''', \mathbf{r}'')$  for a finite system only for  $l = 2$  or  $3$  or for such values of  $\mathbf{r}''$ ,  $\mathbf{r}'''$ , and  $z''$  for which it is

$$F(\mathbf{r}'', \mathbf{r}'''; -iz'') = 0. \quad (3.9)$$

The general solution does, however, not exist.

Normal and anomalous self-energy parts may be calculated from  $R$  in a straightforward manner. The proof of this assertion is postponed to Appendix 3 in order not to interrupt the flow of arguments. The self-energy parts do not exist if  $R$  does not exist. Consequently, also normal and anomalous one-particle propagator do not exist in this case. We conclude that quantum condensation of the interacting fermion gas does not occur in a finite system. Only if the thermodynamic limit is done prior to the limit  $\zeta_0(\mathbf{r}, \mathbf{r}') \rightarrow 0$ , quantum condensation could possibly occur.

#### 4. Thermodynamic Limit and Dimensionality

Let the volume of the system still be finite. Then a complete orthonormal set of functions,  $u_n(\mathbf{r}, \mathbf{r}'; iz; k)$ , may be defined by the Hermitian eigenvalue equation

$$\Pi(\Omega + I) u_n = \lambda_n u_n \quad (4.1)$$

together with the usual boundary condition. A special solution, with  $\lambda_0 = 0$ , was already presented in Equation (3.4). For appropriate normalization of the eigenfunctions, the completeness relation is given by

$$\sum_n u_n(\mathbf{r}, \mathbf{r}'; iz; k) u_n^*(\mathbf{r}'', \mathbf{r}'''; iz''; l) = (\mathbf{r}, \mathbf{r}'; iz; k | I | l; iz''; \mathbf{r}'', \mathbf{r}'''), \quad (4.2)$$

where the righthand side was defined in Eq. (3.2). With the help of Eqs. (4.1) and (4.2) the solution

$$(\mathbf{r}, \mathbf{r}'; iz; k | R | l; iz''; \mathbf{r}'', \mathbf{r}''') = \varepsilon_l \sum_n \lambda_n^{-1} u_n(\mathbf{r}, \mathbf{r}'; iz; k) u_n^*(\mathbf{r}'', \mathbf{r}'''; -iz''; l) \quad (4.3)$$

of Eq. (3.7) may be derived. The non-existence of  $R$  is a direct consequence of  $\lambda_0 = 0$ .  $\lambda_0$  may only be different from zero as long as the limit  $\zeta_0(\mathbf{r}, \mathbf{r}') \rightarrow 0$  has not yet been made.

The thermodynamic limit shall again (as in I for the boson case) first be formed with respect to one space dimension. The geometry is the same as in I, Figure 3. The eigenfunctions are postulated to vanish on the cylinder mantle and to be periodic on the plane surfaces perpendicular to the cylinder axis. Finally the length,  $L$ , of the axis goes to infinity. In order to avoid confusions with the discrete variable  $z$ , the Cartesian coordinates shall be denoted by  $\xi$ ,  $\eta$ , and  $\zeta$ , respectively.

An exponential  $\zeta$  dependence of the centre-of-mass coordinate may be split off from the eigenfunctions  $u_n$ . Therefore, we replace

$$u_n(\mathbf{r}, \mathbf{r}'; iz; k) \rightarrow u_{nP}(\xi, \eta, \xi', \eta', \zeta - \zeta') \exp[iP(\zeta + \zeta')/2], \quad (4.4)$$

where  $P$  is the  $\zeta$  component of the total momentum. The periodic boundary conditions select discrete values of  $P$ . Also the first factor on the righthand side of Eq. (4.4) satisfies a periodic boundary condition,

$$u_{nP}(\xi, \eta, \xi', \eta', \zeta - \zeta' + L) = u_{nP}(\xi, \eta, \xi', \eta', \zeta - \zeta'). \quad (4.5)$$

Equation (4.1) becomes an integro-differential equation for  $u_{nP}$  which shall not be written down. For  $\zeta_0(\mathbf{r}, \mathbf{r}') \rightarrow 0$ , the following statements concerning the eigenvalues  $\lambda_{nP}$  can be made. It is

$$\lambda_{00} = 0 \quad (4.6)$$

and

$$\lambda_{0P} = O(P^2) \quad \text{for } P \rightarrow 0. \quad (4.7)$$

It is now explicitly assumed that there are no neighbouring eigenvalues to  $\lambda_{0P}$  so that this eigenvalue does not merge into a continuum for  $L \rightarrow \infty$ . For  $n = 0$  the  $P$  summation in Eq. (4.3) is replaced by an integration in the limit  $L \rightarrow \infty$ . This integral does, however, not converge as a consequence of Equation (4.7). It does also not converge if the thermodynamic limit is formed with respect to two space dimensions. But the  $P$  integral may converge if the thermo-dynamic limit is formed with respect to all three space dimensions.

The above assumption on the behaviour of the spectrum  $\lambda_{nP}$  in the limit  $L \rightarrow \infty$  seems plausible to the author. It shall be discussed in detail at a later occasion. But a rigorous proof cannot be presented.

That quantum condensation of the interacting fermion gas does not occur in strictly one and two-dimensional systems was shown earlier by HOHENBERG<sup>4</sup>.

Discussions on the subject with members of the Institute are gratefully acknowledged.

### Appendix 1. Boson Case Reconsidered

An alternative formulation of the method of the quasi-expectation value is obtained if Eq. (I.1.2) is replaced by

$$\tilde{H} = - \int [\zeta_0^*(\mathbf{r}) \psi(\mathbf{r}) + \psi^*(\mathbf{r}) \zeta_0(\mathbf{r})] d^3\mathbf{r}. \quad (A1.1)$$

The new building blocks of a diagrammatic perturbation analysis are shown in Figure 6a. The small circles are always connected to  $G_0$  lines. Therefore, the stumps of I are introduced if we put

$$\int G_0(\mathbf{r}, \mathbf{r}'; 0) \zeta_0(\mathbf{r}') d^3\mathbf{r}' = \xi(\mathbf{r}). \quad (A1.2)$$

This is shown graphically in Figure 6b. Eq. (I.1.14) is replaced by

$$\left(-\frac{1}{2m} \Delta - \mu\right) \xi(\mathbf{r}) + \int \tilde{\Sigma}(\mathbf{r}, \mathbf{r}'; 0) \xi(\mathbf{r}') d^3\mathbf{r}' = \zeta_0(\mathbf{r}). \quad (A1.3)$$

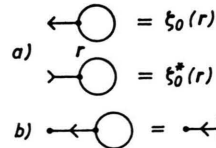


Fig. 6. a) Building blocks in the alternative formulation of the boson condensation problem. b) Introduction of stumps.

We use this occasion to point out that Eq. (A1.3) may be used for an analytic continuation in  $\mu$  from negative values to positive ones as required in connection with quantum condensation. The procedure of adding a small imaginary part to  $\mu$  which was proposed earlier<sup>2</sup> is not correct.

### Appendix 2. Proof of Eqs. (2.4)

These equations are an immediate consequence of Gorkov's equations. An analytic proof may be based upon Eq. (1.7). Here we present a diagrammatic proof.

The following two relations are readily obtained from the first Eq. (1.6),

$$\begin{aligned} \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} &= \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} \\ \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} &= \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} \end{aligned} \quad (\text{A2.1})$$

The boxes represent irreducible self-energy parts. Whether an individual self-energy part is to be labeled by  $-\Sigma$ ,  $-\Delta$ ,  $-\Sigma^*$ , or  $+\Delta^*$  follows unambiguously from the directions of neighbouring arrows. When the second Eq. (1.6) is reformulated as

$$\begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} = \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} \quad (\text{A2.2})$$

also the relations

$$\begin{aligned} \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} &= \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} \\ \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} &= \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} \end{aligned} \quad (\text{A2.3})$$

are derived. If, finally, the two Eqs. (A2.1) are added and the two Eqs. (A2.3) subtracted, and if use is also made of Eq. (A2.2), the second Eq. (2.4) is obtained. The other three equations are derived in an analogous manner.

### Appendix 3. Particle-Particle Interaction and Self-Energy Parts

The normal and anomalous self-energy part may be derived from the matrix  $R$  introduced in Section 3. The normal self-energy part is given by

$$\begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} = \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} - 2 \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} + \begin{array}{c} \text{---} \square \text{---} \\ \text{---} \square \text{---} \end{array} \quad (\text{A3.1})$$

A similar equations holds for the anomalous self-energy part. The boxes in Eq. (A3.1) essentially represent the matrix  $R$ . The upper right particle line has, however, been extracted with the help of Gorkov's equations. The other three particle lines are exhibited.

Eq. (A3.1) is derived by collecting all self-energy skeleton graphs with two or more interaction lines. The 'last' interaction may be an interaction with a closed loop (third term on the righthand side) or with the particle line itself (fourth term).

Eq. (A3.1) can only be evaluated if all matrix elements of  $R$  exist. Otherwise, also the self-energy parts do not exist.



- <sup>1</sup> N. N. BOGOLUBOV, *Physica* **26**, S 1 [1960]; Dubna Report 1962. German transl. *Phys. Abh. S. U.* **6**, 1, 113, 229 [1962]; *Lectures on Quantum Statistics*, Vol. 2, Gordon and Breach Science Publishers, New York 1970.
- <sup>2</sup> G. LÜDERS in: H. P. DÜRR (ed.), *Quanten und Felder — Physikalische und philosophische Betrachtungen zum 70. Geburtstag von Werner Heisenberg*, Vieweg, Braunschweig 1971.
- <sup>3</sup> G. LÜDERS, *Z. Naturforsch.* **27 a**, 175, [1972]. This paper will henceforth be referred to as I. Eq. (m. n) of I will be quoted as Eq. (I. m. n).
- <sup>4</sup> P. C. HOHENBERG, *Phys. Rev.* **158**, 383 [1966].
- <sup>5</sup> L. P. GORKOV, *Zh. Eksperim. Teor. Fiz. (USSR)* **34**, 735 [1959]; Engl. transl. *Soviet Phys. JETP* **9**, 636 [1959]. GORKOV himself formulated the equations in connection with essentially the following approximations:  $\Sigma$  is put equal to zero. In  $\Delta$  only the first diagram beyond  $\zeta_0$  is retained on the righthand side of Equation (1.8).
- <sup>6</sup> E. E. SALPETER and H. A. BETHE, *Phys. Rev.* **84**, 1232 [1951].
- <sup>7</sup> H. J. SOMMERS, private communication.
- <sup>8</sup> P. NOZIÈRES, *Theory of Interacting Fermion Systems*, Benjamin, New York 1964.

## The Ground State Energy of the Hubbard Model in Hubbard's Approximation

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(*Z. Naturforsch.* **27 a**, 889—893 [1972]; received 24 March 1972)

We have calculated the ground state energy of the Hubbard model in the approximation of Hubbard's first paper<sup>1</sup>. For the neutral model with nearest neighbour interaction the energy resulting from the selfconsistent paramagnetic solution is compared with those ones following from the (ferromagnetic) Hartree-Fock and an (antiferromagnetic) single particle theory. The energy of the latter one turns out to be the best approximation of the true ground state energy of the model for all values of the coupling constant  $V_0$ , but the energy derived from Hubbard's approximation, in spite of the absence of magnetic ordering, is a reasonable approximation at least for sufficiently large values of  $V_0$ .

### 1. Introduction

During the last years the Hubbard model<sup>1</sup> of electron interactions in narrow energy bands has been the object of detailed investigations both with respect to its magnetic and its conductivity properties.

This model is stated by the Hamiltonian

$$H = \sum_{j,k,\sigma} T_{jk} c_{j\sigma}^{\dagger} c_{k\sigma} + \frac{V_0}{2} \sum_{j,\sigma} n_{j\sigma} n_{j,-\sigma} \quad (1)$$

where  $c_{j\sigma}^{\dagger}$  generates an electron of spin  $\sigma$  in a Wannier state centred at the lattice site  $j$ ,  $n_{j\sigma} = c_{j\sigma}^{\dagger} c_{j\sigma}$ ,  $T_{jk}$  is the hopping constant for electron transitions from the site  $j$  to  $k$  and  $V_0$  is the matrix element of the Coulomb repulsion, which electrons of opposite spin feel, when they are brought together to the same lattice site.

Hubbard himself in a series of papers<sup>1,2</sup> not only discusses the usual Hartree-Fock (HF) approach to this Hamiltonian (1) but also takes into account correlations between the electrons by introducing different decouplings of quantum statistical Greens functions. In his first paper<sup>1</sup>,\* he uses a decoupling

which gives interesting results for the band-splitting but does not yield a selfconsistent solution for ferromagnetism for reasonable shapes of the density of states of the free electrons, whereas, on the other hand the HF approach yields ferromagnetism for sufficiently strong coupling  $V_0$ . Later on a single particle (SP) approach<sup>3,4</sup> to the Hamiltonian (1) was set up allowing for antiferromagnetic ordering of the electron-spins, which for the neutral model (i. e. number of electrons  $N_e$  = number of lattice sites  $N$ ) led to the prediction of antiferromagnetism for all values of  $V_0 > 0$ . This theory may be deduced from a variational principle<sup>3,5</sup>, such giving an upper bound for the true groundstate energy of the problem and may be shown to yield a much better approximation to the groundstate energy than the HF approach does.

Recently this approach was extended to an investigation of the stability of antiferromagnetism versus ferromagnetism<sup>5</sup> with the result that (at least) for the neutral Hubbard model with nearest neighbour interactions the antiferromagnetic phase is stable for all values of the coupling  $V_0$ .

Contrary to these theories the decoupling of H I goes beyond a single particle approach and takes into account correlations between the band electrons.

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\* This paper will be hereafter referred to as H I.