Zeitschrift: Helvetica Physica Acta
Band: 50 (1977)
Heft: 3

Artikel: Higher order decoupling in the Gorkov theory of superconductivity
Autor: Giovannini, B.
DOI: https://doi.org/10.5169/seals-114865

Higher order decoupling in the Gorkov theory of superconductivity

By **B. Giovannini**

Département de Physique de la Matière Condensée, 24, quai Ernest Ansermet, 1211-Genève-4, Switzerland

(26. I. 1977)

Abstract. In order to get an insight into higher order decoupling procedures in the theory of superconductivity, the Gorkov equations are calculated one step further than usual and then decoupled following the moment conserving procedure introduced by Takir-Kehli and Jarrett. The results are compatible with the BCS results.

I. Introduction

The approximation procedures in the calculation of Green's function in many body problems fall into two categories (i) the selection of a certain subset of diagrams, (ii) the decoupling of the equation of motion.

In this context, A. Theumann and R. D. Mattuck [1] have shown that to any given decoupling of the equation of motion for an interacting Fermi system, there exists an equivalent partial sum of Feynman diagram.

The selection of the decoupling procedure is of course not unique. R. A. Tahir-Kheli and H. S. Jarrett [2] have proposed a well defined decoupling procedure, which is based on the preservation of the first several moments of the spectral function.

Another procedure, introduced by L. M. Roth [3] was shown by R. A. Young [4] to be essentially equivalent to the method of Reference [2].

The purpose of this paper is to show that the moment conserving procedure of Reference [2] applied to higher order Gorkov equations yields the BCS theory again, provided one makes two approximations. Firstly one has to neglect correlations between the order parameter and the fluctuations of the number of particles, and secondly one has to introduce for an order parameter of higher order a special *ad hoc* decoupling which is not specified by the moment conserving procedure. In Section II we calculate the higher order equations of motion for a BCS superconductor, in Section III we review briefly the method of Reference [2], which we apply then in Section IV to the equations divided in Section II.

II. Higher order Gorkov equations

We start from the BCS Hamiltonian

$$\mathscr{H} = \sum \varepsilon_k a_{k\sigma}^{+} a_{k\sigma} + \sum' V B_l^{+} B_m \tag{1}$$

where $B_l^+ = a_{l\uparrow}^+ a_{-l\downarrow}^+$, $\sum'$ means that the sum is restricted to an energy shell around the Fermi surface, and the other symbols have their usual meaning. We introduce the Green's function

$$G_\sigma(kt) = -i\langle T\{a_{k\sigma}(t)a_{k\sigma}^+(0)\}\rangle \tag{2}$$

and find for the Fourier-transform in space and imaginary time the equation (dropping the index σ)

$$(\omega_l - \varepsilon_k)G(k\omega_l) = 1 + iVH(k\omega_l) \tag{3}$$

and

$$H(kt) \equiv \sum_p{}' H(pkt) \equiv -\sum_p{}' \langle T\{B_p(t)a_{-k\downarrow}^+(t)a_{k\uparrow}^+(0)\}\rangle. \tag{4}$$

The usual first order decoupling consists in writing

$$iVH(kt) \simeq \Delta\bar{F}(kt) \tag{5}$$

where

$$\Delta = -iV\sum{}' \langle B_p(t)\rangle. \tag{6}$$

We wish to carry the decoupling scheme one step further, and calculate the equation of motion for $H(pkt)$. This calculation is trivial and yields the equations

$$(\omega_l - \varepsilon_k)G(k\omega_l) = 1 + iVH(k\omega_l) \tag{7}$$

$$(\omega_l + \varepsilon_k)\bar{F}(k\omega_l) = iV\bar{I}(k\omega_l) \tag{8}$$

$$\begin{aligned}(\omega_l + \varepsilon_k - 2\varepsilon_p)H(pk\omega_l) &= (n_{-k\downarrow} - 1)\,\delta_{kp}\\ &+ V\sum_q{}' \langle T\{(n_{p\uparrow}(t) - \bar{n}_{-p\downarrow}(t))B_q(t)a_{-k\downarrow}(t)a_{k\uparrow}(0)\}\rangle\\ &- \sum_q{}' \langle T\{B_q^+(t)B_p(t)a_{k\uparrow}(t)a_{k\uparrow}(0)\}\rangle\end{aligned} \tag{9}$$

$$\begin{aligned}(\omega_l - \varepsilon_k + 2\varepsilon_p)\bar{I}(pk\omega_l) &= i\langle B_p^+\rangle\\ &+ V\sum_q{}' \langle T\{B_q^+(t)(\bar{n}_{-p\downarrow}(t) - n_{p\uparrow}(t))a_{k\uparrow}(t)a_{k\uparrow}^+(0)\}\rangle\\ &- V\sum_q{}' \langle T\{B_p^+(t)a_{-k\downarrow}^+(t)B_q(t)a_{k\uparrow}^+(0)\}\rangle\end{aligned} \tag{10}$$

where

$$\bar{n}_{p\uparrow} = 1 - n_{p\uparrow} \tag{11}$$

$$\bar{I}(pkt) \equiv -\langle T\{B_p^+(t)a_{k\uparrow}(t)a_{k\uparrow}^+(0)\}\rangle. \tag{12}$$

Since $\bar{I}(pk\omega_l)$ and $H(pk\omega_l)$ are to be summed over p over a shell around the Fermi surface, we introduce the approximation $\varepsilon_p \simeq \mu$ and we set $\mu = 0$.

Moreover the inhomogeneous term in the equation for H will lead to a contribution of the order $1/N'$ compared to the others, where N' is the number of terms in the sum $\sum'$. We will also drop it. These two approximations allow to write directly equations of motion for $H(k\omega_l) = \sum_p{}' H(pk\omega_l)$ and $\bar{I}(k\omega_l) = \sum_p{}' \bar{I}(pk\omega_l)$. To simplify the notations, we shall write

$$(\omega_l \pm \varepsilon_k) \equiv g_\pm^{-1} \tag{13}$$

and we get the four equations

$$g_-^{-1}G = 1 + iVH \qquad (14)$$
$$g_+^{-1}G = iV\bar{I}$$

$$g_+^{-1}H = V\sum_{qp}{}' \langle T\{(n_{p\uparrow}(t) - \bar{n}_{-p\downarrow}(t))B_q(t)a_{k\downarrow}(t)a_{k\uparrow}(0)\}\rangle - V\sum_{qp}{}' \langle T\{B_q^+(t)B_p(t)a_{k\uparrow}(t)a_{k\uparrow}(0)\}\rangle$$
$$g_-^{-1}\bar{I} = i\sum_p{}' \langle B_p^+\rangle + V\sum_{qp}{}' \langle T\{B_q^+(t)(\bar{n}_{-p\downarrow}(t) - n_{p\uparrow}(t))a_{k\uparrow}(t)a_{k\uparrow}^+(0)\}\rangle - V\sum_{qp}{}' \langle T\{B_p^+(t)a_{-k\downarrow}^+(t)B_q(t)a_{k\uparrow}^+(0)\}\rangle. \qquad (15)$$

The whole problem is to decouple the Green's functions appearing on the right-hand side of the two last equations in a manner to produce the BCS results.

III. Decoupling procedure

The decoupling procedure presented in Reference 2 is very simple. Given a correlation function of the type (say)

$$\langle T\{A(t)B(t)C(0)\}\rangle$$

one decouples it in the form

$$\langle T\{A(t)B(t)C(0)\}\rangle = \alpha\langle A\rangle\langle T\{B(t)C(0)\}\rangle + \beta\langle B\rangle\langle T\{A(t)C(0)\}\rangle \qquad (16)$$

where all possible lower order correlation functions appear on the right-hand side and one calculates the coefficients α and β by requiring that the two first frequency moments of the spectral function of the two sides of the equation are equal.

Practically, one writes the corresponding commutator or auticommutator

$$\langle[A(t)B(t),C(0)]_\pm\rangle = \alpha\langle A\rangle\langle[B(t),C(0)]_\pm\rangle + \beta\langle B\rangle\langle[A(t),C(0)]_\pm\rangle \qquad (17)$$

and one identifies the two sides and their first derivative for $t = 0$. The highest order of derivatives is determined, of course, by the number of constants to be calculated.

IV. Decoupling of the higher order Gorkov equations

We are now led to decouple the correlation function appearing on the right-hand side of equations (15). We have for instance

$$\sum_{pq}{}' \langle T\{(n_{p\uparrow}(t) - \bar{n}_{-p\downarrow}(t))\}B_q(t)a_{-k\downarrow}(t)a_{k\uparrow}^+(0)\}\rangle =$$
$$\alpha\sum_p{}' \langle n_{p\uparrow} - \bar{n}_{-p\downarrow}\rangle \sum_q{}' \langle T\{B_q(t)a_{-k\downarrow}(t)a_{k\uparrow}^+(0)\}\rangle + \beta\sum_q{}' \langle B_q\rangle \sum_p{}' \langle T\{(n_{p\uparrow}(t) - \bar{n}_{-p\downarrow}(t))a_{-k\downarrow}(t)a_{k\uparrow}^+(0)\}\rangle + \gamma\sum_{pq}{}' \langle(n_{p\uparrow} - \bar{n}_{-p\downarrow})B_q\rangle\langle T\{a_{-k\downarrow}(t)a_{k\uparrow}^+(0)\}\rangle. \qquad (18)$$

This leads, of course, to new correlations functions, like

$$I(kt) \equiv -\sum_q{}' \langle T\{B_q(t)a_{-k\downarrow}(t)a^+_{k\uparrow}(0)\}\rangle \tag{19}$$

for which we have to calculate equations of motion. Since these calculations are straightforward, we shall only present the results, in which we have made two approximations. Firstly, we have set

$$\sum{}' \langle n_{p\uparrow} - \bar{n}_{-p\downarrow}\rangle = \sum{}' \langle 2n\rangle - \sum{}' = 0 \tag{20}$$

which means that the shell around the Fermi surface is symmetrical: in this shell there are twice as many states as electrons. This eliminates some uninteresting terms.

On the other hand, we neglect correlations between the fluctuation of the number of particles and the other physical quantities like the order parameter.

Thus, for instance

$$\sum_p{}' \langle T\{(n_{p\uparrow}(t) - \bar{n}_{-p\downarrow}(t))a_{-k\downarrow}(t)a^+_{k\uparrow}(0)\}\rangle$$
$$\simeq \sum_p{}' \langle n_{p\uparrow} - \bar{n}_{-p\downarrow}\rangle\langle T\{a_{-k\downarrow}(t)a^+_{k\uparrow}(0)\}\rangle = 0.$$

This approximation is essential to get the BCS results with higher-order equations of motion. We now write down the resulting equations of motion which read

$$\begin{aligned}
g_-^{-1}G &= 1 + iVH\\
g_+^{-1}\bar{F} &= iV\bar{I}\\
g_-^{-1}I &= V^{-1}\Delta + 2ai\Delta H + biV^{-1}\psi\bar{F}\\
g_+^{-1}H &= -ci\Delta^*I + di\Delta\bar{I} - eiV^{-1}\tilde{\Delta}G\\
g_+^{-1}K &= -2fi\Delta^*\bar{I} + hiV^{-1}\psi^*G\\
g_-^{-1}\bar{I} &= -V^{-1}\Delta^* - ki\Delta^*H + li\Delta k - miV^{-1}\tilde{\Delta}\bar{F}.
\end{aligned} \tag{21}$$

In these equations we have

$$\begin{aligned}
H \equiv H(kt) &\equiv -\sum_p{}' \langle T\{a_{-p\downarrow}a_{p\uparrow}a^+_{-k\downarrow}a^+_{k\uparrow}\}\rangle\\
I \equiv I(kt) &\equiv -\sum_p{}' \langle T\{a_{-p\downarrow}a_{p\uparrow}a_{k\uparrow}a^+_{k\uparrow}\}\rangle\\
\bar{I} \equiv \bar{I}(kt) &\equiv -\sum_p{}' \langle T\{a^+_{p\uparrow}a^+_{-p\downarrow}a_{k\uparrow}a^+_{k\uparrow}\}\rangle\\
K \equiv K(kt) &\equiv -\sum_p{}' \langle T\{a^+_{p\uparrow}a^+_{-p\downarrow}a^+_{-k\downarrow}a^+_{k\uparrow}\}\rangle
\end{aligned} \tag{22}$$

$$\begin{aligned}
\Delta &\equiv -i\sum_p{}' V\langle a_{-p\downarrow}a_{p\uparrow}\rangle\\
\tilde{\Delta} &= \tilde{\Delta}^* \equiv V^2\sum_{pq}{}' \langle a^+_{p\uparrow}a^+_{-p\downarrow}a_{-q\downarrow}a_{q\uparrow}\rangle\\
\psi^* &= -V^2\sum_{pq}{}' \langle a^+_{p\uparrow}a^+_{-p\downarrow}a^+_{q\uparrow}a^+_{-q\downarrow}\rangle
\end{aligned} \tag{23}$$

and the coefficients a, b, etc. are to be determined by the method outlined in Section III.

The equations (21) can be solved to give

$$\left.\begin{aligned} G &= g_-(Z_2 - xZ_3Z_1)^{-1} \\ \bar{F} &= -ig_+\Delta^* Z_1 G \\ H &= -iV^{-1}(1 - Z_2 + xZ_1Z_3)g_-^{-1}G \\ K &= ig_+V^{-1}\psi^*\left(h + 2f\frac{\Delta^{*2}}{\psi^*}Z_1\right)G \end{aligned}\right\} \tag{24}$$

$$\left.\begin{aligned} Z_1 &= \frac{k + lhw^*}{1 - my - 2lfx} \\ Z_2 &= \frac{1 - 2acx - ey}{1 - 2acx + cx} \\ Z_3 &= \frac{d + bcw}{1 - 2acx + cx} \end{aligned}\right\} \tag{25}$$

$$\left.\begin{aligned} x &= g_+g_-|\Delta|^2 \\ y &= g_+g_-\tilde{\Delta} \\ w^* &= g_+g_-\psi^*\frac{\Delta}{\Delta^*}. \end{aligned}\right\} \tag{26}$$

The coefficients a, b etc., are now to be determined by the method of moments. The calculation is straightforward but lengthy. We just list the results

$$(1 - h)\psi^* = 2f\Delta^{*2} \tag{27}$$

$$h = -1 \tag{28}$$

$$(1 - e)\tilde{\Delta} = (c + d)|\Delta|^2 \tag{29}$$

$$c|\Delta|^2 = -\tilde{\Delta} \tag{30}$$

$$e = 1 \tag{31}$$

$$b\psi\Delta^* = -2a\Delta\tilde{\Delta} - iV^3 \sum_{qpm}{}' \langle B_q B_{q'}^+ B_m \rangle \tag{32}$$

$$k = 1 \tag{33}$$

$$m = -k \tag{34}$$

$$\Delta\psi^* l = iV^3 \sum_{qpm}{}' \langle B_q^+ B_p^+ B_m \rangle. \tag{35}$$

From equations (27) to (35) one gets

$$\left.\begin{aligned} h &= -1 \\ f &= \frac{\psi^*}{\Delta^{*2}} \\ e &= 1 \\ c &= -d = -\frac{\tilde{\Delta}}{|\Delta|^2} \\ m &= -k = -1. \end{aligned}\right\} \tag{36}$$

Introducing the values (36), (32) and (35) in (25) one gets

$$Z_1 = \frac{1 - ig_+g_-V^3 \sum' \langle B_q^+ B_p^+ B_m \rangle (\Delta^*)^{-1}}{1 + y - 2ig_+g_-V^3 \sum' \langle B_q^+ B_p^+ B_m \rangle (\Delta^*)^{-1}} \tag{37}$$

$$Z_2 = 1 \tag{38}$$

$$Z_3 = \frac{\tilde{\Delta}}{|\Delta|^2} \frac{1 + 2ay + ig_+g_-V^3 \sum' \langle B_q B_p^+ B_m \rangle \Delta^{-1}}{1 + (2a - 1)y}. \tag{39}$$

One notices that the values of a, b and l and therefore the values of Z_1 and Z_3 are not fully determined by the method. Let us now compare these results with the BCS results, which are

$$\begin{aligned} G &= g_-(1 - x)^{-1} \\ \bar{F} &= -ig_+\Delta^* G. \end{aligned} \tag{40}$$

From this, one sees that to get results analog to the BCS-results one has to write

$$\begin{aligned} -iV^3 \sum \langle B_q^+ B_p^+ B_m \rangle &= -\Delta^* \tilde{\Delta} \\ iV^3 \sum \langle B_q^+ B_p B_m \rangle &= -\Delta \tilde{\Delta}. \end{aligned} \tag{41}$$

The last two equations are not obtainable by the method of moments, which thus proves not to determine completely the decoupling.

One now gets

$$\begin{aligned} G &= g_-(1 - y)^{-1} \\ \bar{F} &= -ig_+\Delta^* G \\ H &= -iV^{-1} y(1 - y)^{-1} \\ K &= iV^{-1} w^*(1 - y)^{-1} \\ I &= V^{-1}\Delta G \\ \bar{I} &= -V^{-1}\Delta^* G \end{aligned} \tag{42}$$

One sees that the order parameter is now $\tilde{\Delta}$ and that the values of ψ^* and Δ are undetermined.

These results will be useful in a forthcoming calculation on a more complicated system.

REFERENCES

[1] A. Theumann and R. D. Mattuck, Arkiv. Det. Fysika seminar i Trondheim *7* (1970).
[2] R. A. Takir-Kehli and H. S. Jarrett, Phys. Rev. *180*, 544 (1969).
[3] L. M. Roth, Phys. Rev. Letters *20*, 1431 (1968).
[4] R. A. Young, Phys. Rev. *184*, 601 (1969).