BOUND STATES IN SUPERCONDUCTORS CONTAINING A MAGNETIC IMPURITY. I

By K. Bortel

Department of Theoretical Physics, Silesian University, Katowice*

(Received June 2, 1972; Revised paper received April 26, 1973)

Using the method of double-time temperature Green's functions an integral equation for the non-spin-flip scattering amplitude has been obtained and solved exactly in the limit $U \to \infty$. The position of bound states within the gap is found and their structure is examined by means of the density of states and the electronic density distribution.

1. Introduction

The problem of bound states in superconductors with a magnetic impurity has already been discussed in the works of Sato [1], Celli [2] and Zittartz [3], [4]. In Zittartz's paper the hamiltonian used was the sum of the *s-d* exchange and the linearized BCS hamiltonians.

In the present work we examine the position and structure of bound states on the basis of calculations employing a hamiltonian made up of the Anderson and linearized BCS hamiltonians. The hamiltonian chosen thus allows only states of antiferromagnetic impurities having negative energies. The resulting set of equations of Green's functions can be reduced to an integral equation for a non-spin-flip scattering amplitude, very much like the equation arrived at the case of an ordinary metal by Mamada [5].

In the second part of this work we derive the whole set of equations of Green's functions. Its solution consists in finding the integral equation for the non-spin-flip scattering amplitude. This equation is solved exactly in the limit $U \to \infty$ in Sec. 3. Furthermore, this section gives the parameters determinating the location of bound states within the gap and a related residue constant. These parameters are further considered in Sec. 4, which finally deals with the structure of the bound state. The results and their physical interpretation are given in part 5. Some additional calculations are given in the appendices.

---

* Address: Zakład Fizyki Teoretycznej, Uniwersytet Śląski, Uniwersytecka 4, 40-007 Katowice, Poland.

2. *Formulation of the problem*

Let us consider a superconductor with a magnetic impurity described by the hamiltonian

$$H = H_A - \Delta \sum_k [c_{k+}^+ c_{-k-}^+ + c_{-k-} c_{k+}] \tag{2.1}$$

where

$$H_A = \sum_{ks} \varepsilon_k c_{ks}^+ c_{ks} + E \sum_s d_s^+ d_s + \sum_{ks} [V_k c_{ks}^+ d_s + V_k^* d_s^+ c_{ks}] + \tfrac{1}{2} U \sum_s n_s n_{-s} \tag{2.2}$$

is the one-impurity Anderson hamiltonian. The energy gap of the superconductor Δ is expressed as

$$\Delta = \frac{I}{N} \sum_k \langle c_{-k-} c_{k+} \rangle \tag{2.3}$$

where N is the number of cells and I is the usual coupling constant for a superconductor. The summation in equation (2.3) over k is limited by Debye's frequency ω_D. In our considerations we overlook the changes in Δ associated with the distance from the impurity. When we take one particle temperature Green's function in Nambu notation

$$G_{kk'} = \langle c_{ks} | c_{k's} \rangle^T. \tag{2.4}$$

Here, the symbol $\langle \ldots | \ldots \rangle^T$ indicates the matrix

$$\langle A_{ks} | B_{k's} \rangle^T = \frac{1}{2} \sum_s \begin{pmatrix} \langle A_{ks} | B_{k's}^+ \rangle \ , & s \langle A_{ks} | B_{-k'-s} \rangle \\ s \langle A_{-k-s}^+ | B_{k's}^+ \rangle, & \langle A_{-k-s}^+ | B_{-k'-s} \rangle \end{pmatrix} \tag{2.5}$$

where $s = \pm 1$. Rotational invariance in spin space leads to

$$\langle c_{ks} | c_{k's}^+ \rangle = \langle c_{k-s} | c_{k'-s}^+ \rangle,$$

$$\langle c_{ks} | c_{-k'-s} \rangle = -\langle c_{k-s} | c_{-k's} \rangle. \tag{2.6}$$

Introducing the unperturbed propagator

$$G_k^0(z) = \begin{pmatrix} z - \varepsilon_k, & \Delta \\ \Delta \ , & z - \varepsilon_k \end{pmatrix}^{-1} \tag{2.7}$$

where z is complex energy, we can write $G_{kk'}$ as

$$G_{kk'} = G_{k'}^0(z) \delta_{kk'} + V_k G_k^0(z) t(z) G_{k'}^0(z) V_{k'}^*. \tag{2.8}$$

Here, $t(z)$ is the non-spin-flip scattering amplitude, which satisfies the usual hermicity condition

$$[t(z)]^+ = t(z^*). \tag{2.9}$$

Some simplifications may be made a symmetrical conduction band is assumed, that is, the density of states function $\varrho(\varepsilon)$ appearing in the equation

$$\frac{1}{N}\sum_{k} \ldots = N_0 \int_{-\infty}^{\infty} d\varepsilon \varrho(\varepsilon) \ldots \tag{2.10}$$

where N_0 is the density of states on the Fermi's surface, is symmetrical,

$$\varrho(\varepsilon) = \varrho(-\varepsilon). \tag{2.11}$$

Moreover, we can make use of the "particle-hole" symmetry of the hamiltonian (2.1); this is equivalent to the transformation

$$c_{ks} \to isc^{+}_{\bar{k}-s}, \quad \varepsilon_k \to -\varepsilon_{\bar{k}}, \quad V_k \to V^*_{-k},$$

$$d_s \to isd^{+}_{-s}, \quad E \to -E, \quad U \to U. \tag{2.12}$$

With the "particle-hole" symmetry of the model certain additional properties can be found which are connected both with components of Green's function and the non-spin-flip scattering amplitude $t(z)$. These properties has been discussed in the first paper of Zittartz [3]. From the hamiltonian (2.1), we can construct the following set of the equations of motion for Green functions:

$$\langle c_{ks}|c_{k's}\rangle^T = G^0_k(\delta_{kk'} + V_k\sigma_z\langle d_s|c_{k's}\rangle^T), \tag{2.13a}$$

$$\sigma_z\langle d_s|c_{k's}\rangle^T = G^0_d(\sum_k V^*_k\langle c_{ks}|c_{k's}\rangle^T + U\langle n_{-s}d_s|c_{k's}\rangle^T), \tag{2.13b}$$

$$\langle n_{-s}d_s|c_{k's}\rangle = -\Gamma^0_d\sum_k (V^*_k\langle d^+_{-s}d_sc_{k-s}|c_{k's}\rangle^T - V^*_k\sigma_z\langle c_{ks}n_{-s}|c_{k's}\rangle^T +$$
$$+ V_{-k}\langle c^+_{-k-s}d_{-s}d_s|c_{k's}\rangle^T), \tag{2.13c}$$

$$\langle d^+_{-s}d_sc_{k-s}|c_{k's}\rangle^T = G^0_k[-V_k\langle n_{-s}d_s|c_{k's}\rangle^T +$$
$$+\sigma_z\sum_l (V^*_l\langle d^+_{-s}c_{ls}c_{k-s}|c_{k's}\rangle^T - V_{-l}\langle c^+_{-l-s}d_sc_{k-s}|c_{k's}\rangle)], \tag{2.13d}$$

$$\sigma_z\langle c_{ks}n_{-s}|c_{k's}\rangle^T = G^0_k[\langle n\rangle\delta_{kk'} + V_k\langle n_{-s}d_s|c_{k's}\rangle^T +$$
$$+\sigma_z\sum_l V^*_l\langle c_{ks}d^+_{-s}c_{l-s}|c_{k's}\rangle^T - V_{-l}\langle c_{ks}c^+_{-l-s}d_{-s}|c_{k's}\rangle)], \tag{2.13e}$$

$$\langle c^+_{-k-s}d_{-s}d_s|c_{k's}\rangle^T = \Gamma^0_k[-V^*_k\langle n_{-s}d_s|c_{k's}\rangle^T +$$
$$+\sigma_z\sum (V^*_l\langle c^+_{-k-s}d_{-s}c_{ls}|c_{k's}\rangle^T + V^*_l\langle c^+_{-k-s}c_{l-s}d_s|c_{k's}\rangle^T)]. \tag{2.13f}$$

In equations (2.13) we use the notation

$$G_d^0(z) = \begin{pmatrix} z-E, & 0 \\ 0 & , z-E \end{pmatrix}^{-1}, \tag{2.14}$$

$$\Gamma_d^0(z) = \begin{pmatrix} z-E-U, & 0 \\ 0 & , z-E-U \end{pmatrix}^{-1}, \tag{2.15}$$

$$\Gamma_k^0(z) = \begin{pmatrix} z-2E-U+\varepsilon_k, & \Delta \\ \Delta & z+2E+U-\varepsilon_k \end{pmatrix}^{-1} \tag{2.16}$$

and

$$\langle n \rangle = \mathscr{F}_n\{\langle d_s | d_s \rangle^T\}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.17}$$

In order to close the above equations, we adopt the usual approximation of the decoupling for the terms on the right-hand side of equations (2.13d)–(2.13f). For example, we can write the terms on the right-hand side of equation (2.13d) as follows:

$$\langle c_{-l-s}^{+} d_s c_{k-s} | c_{k's}^{+} \rangle = \langle d_s c_{k-s} \rangle \langle c_{-l-s}^{+} | c_{k's}^{+} \rangle - \langle c_{-l-s}^{+} c_{k-s} \rangle \langle d_s | c_{k's}^{+} \rangle$$

$$\langle d_{-s}^{+} c_{ls} c_{k-s} | c_{k's}^{+} \rangle = \langle c_{ls} c_{k-s} \rangle \langle d_{-s}^{+} | c_{k's}^{+} \rangle - \langle d_{-s}^{+} c_{k-s} \rangle \langle c_{ls} | c_{k's}^{+} \rangle. \tag{2.18}$$

Then, equation (2.13d) becomes

$$\langle d_{-s}^{+} d_s c_{k-s} | c_{k's} \rangle^T = G_k^0 (-V_k \langle n_{-s} d_s | c_{k's} \rangle^T +$$

$$+ \sigma_z \langle d_s | c_{k's} \rangle^T \sum_l V_{-l} n_{kl} - n_{dk} \sum_l V_l^* \langle c_{ls} | c_{k's} \rangle^T),$$

where

$$n_{kl} = \mathscr{F}_n\{\langle c_{ks} | c_{k's} \rangle^T\}, \tag{2.19}$$

$$n_{dk} = \mathscr{F}_n\{\langle d_s | c_{ks} \rangle^T\}. \tag{2.20}$$

Making the same approximation in equations (2.13e) and (2.13f), and substituting these results into equation (2.13c), we obtain a closed set of equations of motion for Green functions $\langle c_{ks} | c_{k's} \rangle^T$, $\sigma_z \langle d_s | c_{k's} \rangle^T$ and $\langle n_{-s} d_s | c_{k's} \rangle^T$.

A similar set of equations of Green's function may be obtained by starting out with the equation for the function

$$\sigma_z \langle d_s | d_s \rangle^T = \frac{1}{2} \begin{pmatrix} 1, & 0 \\ 0, & -1 \end{pmatrix} \sum_s \begin{pmatrix} \langle d_s | d_s^{+} \rangle, & s \langle d_s | d_{-s} \rangle \\ s \langle d_{-s}^{+} | d_s \rangle, & \langle d_{-s}^{+} | d_{-s} \rangle \end{pmatrix}. \tag{2.21}$$

The solutions of the set of equations (2.13) and the similar set obtained with the function $\sigma_z \langle d_s|d_s\rangle^T$ can be expressed as

$$\langle c_{ks}|c_{k's}\rangle^T = G_{kk'} = G_k^0\delta_{kk'} + V_k G_k^0 t(z) G_{k'}^0 V_{k'}^*, \tag{2.22}$$

$$\sigma_z\langle d_s|c_{k's}\rangle^T = t(z)G_{k'}^0 V_{k'}^*, \quad \langle c_{ks}|d_s\rangle^T = V_k G_k^0 t(z) \tag{2.23}$$

and

$$\sigma_z\langle d_s|d_s\rangle^T = t(z) = \frac{N(z)}{\Phi(z)}. \tag{2.24}$$

Defining the matrix functions

$$F(z) = \sum_k |V_k|^2 G_k^0(z) \text{ and } F(z-2E-U) = \sum_k |V_k|^2 \Gamma_k^0(z-2E-U) \tag{2.25}$$

we may write the numerator and denominator of equation (2.24) as

$$N(z) = z-E-U-2F(z)-F(z-2E-U)+U\langle n\rangle + U(L_1(z)-F(z)\,L_0(z))+$$
$$+U(L_1(z-2E-U)-F(z-2E-U)\,L_0(z-2E-U)) \tag{2.26}$$

and

$$\Phi(z) = (z-E-F(z))\,(z-E-U-2F(z)-F(z-2E-U))+$$
$$+U(R_1(z)-F(z)\,R_0(z)+L_2(z)-2F(z)\,L_1(z)+F^2(z)\,L_0(z))-$$
$$-U[R_1(z-2E-U)-F(z-2E-U)-R_0(z-2E-U)+L_2(z-2E-U)+$$
$$+(F(z)-F(z-2E-U))\,L_1(z-2E-U)-F(z)\,F(z-2E-U)\,L_0(z-2E-U)]. \tag{2.27}$$

Here, we use the notation

$$R_\alpha(z) = \mathscr{F}_n\left\{\frac{F^\alpha(i\omega_n)}{z-i\omega_n}\right\}, \quad L_\alpha(z) = \mathscr{F}_n\left\{\frac{F^\alpha(i\omega_n)t(i\omega_n)}{z-i\omega_n}\right\}. \tag{2.28}$$

In the $U \to \infty$ limit the numerator and denominator of equation (2.24) are reduced to

$$N(z) = -1+\langle n\rangle - F(z)\,L_0(z)-L_1(z) \tag{2.29}$$

and

$$\Phi(z) = -(z-E-F(z))+R_1(z)-F(z)R_0(z)+L_2(z)-2F(z)\,L_1(z)+F^2(z)\,L_0(z). \tag{2.30}$$

Equations (2.22) to (2.24) clearly show that the problem of solving either the first or the second sets of equations can be reduced to solving an integral equation for $t(z)$. Note that equation (2.24) for $t(z)$ is the same as in the case of a normal metal except that the matrix functions $F(z)$ and $F(z-2E-U)$ are expressed differently; they transform into the common form when $\Delta = 0$.

3. *Solution of the integral equation in the limit $U \to \infty$*

Before we proceed to solve the integral equation (2.24), let us make certain assumptions regarding the density of states function, $\varrho(z)$. Let us assume that singularities of $\varrho(z)$ are behind the large circle of a radius D (where D is the band width of the conduction band), $\varrho(z)$ is analytic in some neighbourhood of the real axis, and

$$\int_{-\infty}^{\infty} \varrho(\varepsilon) d\varepsilon = \text{finite}.$$

These properties are characteristic of a density of states function in the parabolical form

$$\varrho(\omega) = \begin{cases} \sqrt{1-\dfrac{\omega^2}{D^2}} & |\omega| \leqslant D \\ 0 & |\omega| > D \end{cases} \tag{3.1}$$

Let us analyse the properties of the function $F(z)$ defined in (2.25) with the density of states function as given above,

$$F(z) = -\lambda \frac{z+\Delta}{\sqrt{z^2-\Delta^2}} \int_{-\infty}^{\infty} \frac{d\varepsilon \varrho(\varepsilon)}{\varepsilon-\sqrt{z^2-\Delta^2}} \quad \text{where } \lambda = N_0 \langle |V|^2 \rangle, \tag{3.2}$$

limiting ourselves only to the upper half-plane, which means assuming that

$$\operatorname{Im} \sqrt{z^2-\Delta^2} > 0 \quad \text{for any } z.$$

$F(z)$ is an ambiguous. If we want it to be single-valued we must cut the plane from $-\sqrt{\Delta^2+D^2}$ to $-\Delta$ and from Δ to $\sqrt{\Delta^2+D^2}$ and choose a single-valued branch. We do this by assuming that $\sqrt{z^2-\Delta^2} = i\sqrt{\Delta^2-z^2}$ for z real numbers of the range $-\Delta \leqslant z \leqslant \Delta$.

In the plane thus defined $F(z)$ is an analytical function which jumps when passing from the upper half-plane into the lower one

$$F(\omega+i\delta)-F(\omega-i\delta) = -2\pi i\lambda \frac{\omega+\Delta}{\sqrt{\omega^2-\Delta^2}} \varrho(\sqrt{\omega^2-\Delta^2}). \tag{3.3}$$

Then, near the real axis $F(z)$ can be continued analytically with account taken of the values of the jump expressed by equation (3.3)

$$F(z)-\overline{F}(z) = -2\pi i\lambda \frac{z+\Delta}{\sqrt{z^2-\Delta^2}} \varrho(\sqrt{z^2-\Delta^2}). \tag{3.4}$$

Let us introduce into our considerations the auxiliary function

$$X(z) = -(z-E-F(z))+R_1(z)-F(z)\,R_0(z)+(F(z)-\overline{F}(z))\,(\langle n\rangle-1)+\chi(z) \tag{3.5}$$

where

$$\chi(z) = L_2(z)-(F+\overline{F})\,L_1(z)+F\overline{F}L_0(z). \tag{3.6}$$

Function $\chi(z)$ may be determined by its singularities (Cauchy's integral formula) because it disappears at infinity, so

$$\chi(z) = \frac{\lambda \Delta a}{z-\Delta} + \chi_p(z) \tag{3.7}$$

where

$$a = \operatorname*{Res}_{z=\Delta} \frac{\chi(z)}{\lambda \Delta} = 2\pi^2 \lambda L_0(\Delta) \tag{3.8}$$

and

$$\chi_p(z) = \frac{1}{2\pi i} \oint_c \frac{dz'}{z'-z} \chi(z') \leqslant O(\lambda^2). \tag{3.9}$$

In the last equation $|z'| \sim D \gg |z|$, which consequently gives $\chi_p(z) \leqslant O(\lambda^2)$, so $\chi_p(z)$ can in practice be omitted in the following calculations. Making use of the introduced auxiliary function $X(z)$ the equation (2.24) for $t(z)$ may be rewritten as follows:

$$t(z) = -(F-\bar{F})^{-1}\left(1 - \frac{X(z)}{\Phi(z)}\right). \tag{3.10}$$

Solution of the above equation is simplified by calculating the equation for $\Phi(z)$ in terms of $X(z)$. Then we form the difference $\Phi\bar{\Phi} - X\bar{X}$. The algebra is simple and we obtain

$$\Phi\bar{\Phi} - X\bar{X} = (F-\bar{F})^2 H(z) \tag{3.11}$$

where $\bar{\Phi}(z)$ and $\Phi(z)$ are functions received by replacing $F(z)$ by $\bar{F}(z)$ in equations (2.30) for $\Phi(z)$, (3.5) for $X(z)$, and

$$H(z) = (1-\langle n\rangle)(R_0 - \langle n\rangle) + L_0(z)\,[-(z-E)+R_1+L_2] + L_1(1-R_0-L_1). \tag{3.12}$$

The last function is analytic except for simple poles and double poles at the set $z_n = i\omega_n$ along the imaginary axis. Then, the value of the $H(z)$ function is determined by its value at infinity,

$$\lim_{z\to\Delta} H(z) = \langle n\rangle^2 - 2\langle n\rangle = H(z). \tag{3.13}$$

Disregarding bandstructure effects ($D \to \infty$), we see that the difference $\Phi\bar{\Phi} - X\bar{X}$ expressed by equation (3.13) is finite when $z \to \infty$ and is thereby determined by its value at infinity over the whole complex plane. Using the equations (3.4), (3.13) and (3.11) we get the equation

$$\Phi\bar{\Phi} = (z-E-F(z))\,(z-E-\bar{F}(z))K(z) = X\bar{X} + 4\pi^2\lambda^2(2\langle n\rangle - \langle n\rangle^2)\frac{z+\Delta}{z-\Delta}\,\varrho(\sqrt{z^2-\Delta^2}) \tag{3.14}$$

which results in a function $\Phi(z)$ which behaves at the cutting points as

$$\frac{\Phi(\omega+i\delta)}{(\omega+i\delta-E-F(\omega))}\,\frac{\Phi(\omega-i\delta)}{(\omega-i\delta-E-F(z))} = K(\omega); \qquad |\omega| \geqslant \Delta \tag{3.15}$$

where $K(\omega)$ is positive and real. A particular solution of the relation (3.15) is

$$\psi(z) = -(z-E-F(z))\exp\left\{-\frac{\sqrt{z^2-\Delta^2}}{2\pi i}\left(\int_{\Delta}^{\infty}-\int_{-\infty}^{-\Delta}\right)\frac{d\omega}{z-\omega}\,\frac{\ln K(\omega)}{\sqrt{\omega^2-\Delta^2}}\right\} \tag{3.16}$$

as can be checked. The particular choice of $\psi(z)$ is explained by the fact that ψ already reflects the correct behaviour of Φ at the branch points $\pm\Delta$ up to a sign perhaps as is shown in Appendix A. This solution does not yet possess the properties of the function $\Phi(z)$ in the range $(-\Delta, \Delta)$, so we must supplement them by introducing the function

$$G(z) = \frac{\Phi(z)}{\psi(z)} \tag{3.17}$$

with the properties

(a) $$G(\omega+i\delta)\,G(\omega-i\delta) = 1, \qquad |\omega| \geqslant \Delta$$

(b) $$G(-\Delta) = \operatorname{sign}\Phi(-\Delta) = \operatorname{sign}X(-\Delta) = \operatorname{sign}\left(\Delta+E+\frac{\lambda}{g}-\frac{a\lambda}{2}\right)$$

(c) $$G(\Delta) = \operatorname{sign}\lambda a$$

(d) $$G(\infty) = \Phi(\infty)/\psi(\infty) = 1.$$

Property (a) stems from the equation (3.14), (b) and (c) are fully discussed in Appendix A (see Eqs (A.2) and (A.3)) and follow from expression defining $G(z)$. We can clearly see from equation (3.17) that $G(z)$ is an analytic function beyond the discontinuous points of $\Phi(z)$ because $\psi(z) \neq 0$ over the whole complex plane.

In order to find $G(z)$ we may use the function

$$f(z) = \frac{G'(z)}{G(z)}\sqrt{z^2-\Delta^2}\,. \tag{3.18}$$

This equation clearly demonstrates that the only possible singularities of the function f are simple poles at the zeroes of G or Φ, respectively, which can be present only within the gap. Using the Mittag-Leffler theorem we get

$$f(z) = \frac{G'(z)}{G(z)}\sqrt{z^2-\Delta^2} = \sum_{j=1}^{N}\frac{i\sqrt{\Delta^2-\omega_j^2}}{z-\omega_j} \tag{3.19}$$

where the number of zeroes N is finite. The solution of the equation (3.19) when we assume property (b) has the form

$$G(z) = [\text{sign } X(-\Delta)] \prod_{j=1}^{N} A_j(z) \tag{3.20}$$

where

$$A_j(z) = \frac{\Delta(z-\omega_j)}{\omega_j z - \Delta^2 - i\sqrt{z^2-\Delta^2}\sqrt{\Delta^2-\omega_j^2}} \tag{3.21}$$

and

$$A_j(\pm\Delta) = \mp 1.$$

If we know the zeroes ω_j and residue constant a, the function

$$\Phi(z) = [\text{sign } X(-\Delta)] \prod_{j=1}^{N} A_j(z)\psi(z), \tag{3.22}$$

which we obtain from equations (3.17) and (3.20) is the solution of the integral equation.

4. *Position and structure of bound states*

Let us now find the residue constant a and zeroes ω_j of the function $\Phi(z)$, which we can from the equation

$$\Phi(z)\,\overline{\Phi}(z) = (z-E-F)(z-E-\overline{F})\,K(z) = 0. \tag{4.1}$$

The product of the functions $\Phi(z)$ and $\overline{\Phi}(z)$ does not introduce any ambiguous solutions because these functions are analytical inside the gap. The explicit form of $K(z)$ is obtained from knowledge of the function $X(z)$,

$$X(z) = \lambda\Bigg[\tau + y(y+1)r(y^2) + \frac{a}{y+1} - \frac{\Delta}{\lambda} + \\ + i\pi\frac{y+1}{\sqrt{y^2-1}}\left(1+\frac{1}{2}\,\text{tgh}\,\frac{\beta\Delta y}{2} - 2\langle n\rangle\right)\Bigg], \quad y = \frac{z}{\Delta}. \tag{4.2}$$

Here, we use the relation

$$\tau = \frac{E}{\lambda} + \frac{1}{g} = \ln\frac{T_k}{T_{c0}} \tag{4.3}$$

where g is the effective superconductor coupling constant, T_{c0} the superconducting transition temperature of the pure metal, and T_k the Kondo-Suhl temperature.

In equation (4.2) we make use of the fact that

$$R_1(z) = R_1(-\Delta)+\frac{1}{\beta}\sum_n F(i\omega_n)\left(\frac{1}{z-i\omega_n}+\frac{1}{\Delta+i\omega_n}\right) = \tag{4.4}$$

$$= \frac{\lambda}{g}+\lambda y(y+1)r(y^2)$$

where

$$r(y^2) = \sum_n \frac{\pi}{\sqrt{\omega_n^2+\Delta^2}}\left(y^2+\frac{\omega_n^2}{\Delta^2}\right)^{-1}. \tag{4.5}$$

Using (4.2) and (3.14) we can express the function $K(z)$ by the equation

$$(z-E-F)(z-E-\bar{F})K(z) = \lambda^2\left\{\left[\tau^2+y(y+1)r(y^2)+\frac{a}{y+1}-\frac{\Delta}{\lambda}\right]^2+\right.$$

$$\left.+\pi^2\frac{y+1}{y-1}\left[\left(1+\frac{1}{2}\operatorname{tgh}\frac{\beta\Delta y}{2}\right)^2+4n\left(1-\frac{1}{2}\operatorname{tgh}\frac{\beta\Delta y}{2}\right)\right]\right\}, \tag{4.6}$$

the zeroes of which given by the relation

$$y_{1,2} = \frac{\tau(\tau-a)\pm\sqrt{\pi^2(1+4n)\,[\pi^2(1+4n)+a(2\tau-a)]}}{\tau^2+\pi^2(1+4n)}, \quad n = \langle n\rangle \tag{4.7}$$

when $\beta\Delta \to 0$ ($r(y^2) = \operatorname{tgh}\beta\Delta y/2 = 0$).

In order to solve (4.7) we have to impose on equation (4.6) an additional condition stemming from property (d) of function $G(z)$ which, on the other hand, allows us to find the residue constant a. The fact that zeroes y_1, y_2 occur in both the functions

$$\psi(z)|_{z=i\infty} = -(z-E-F)|_{z=i\infty}\exp\left\{-\frac{1}{2\pi i}\int_\Delta^\infty \frac{d\omega}{\sqrt{\omega^2-\Delta^2}}\ln\frac{K(\omega)}{K(-\omega)}\right\} \tag{4.8}$$

and

$$G(i\infty) = [\operatorname{sign} X(-\Delta)]\prod_{j=1}^{2} e^{i-\left(\frac{\pi}{2}-\varphi_j\right)\nu_j} \tag{4.9}$$

where

$$\varphi_j = \arcsin y_j, \quad -\frac{\pi}{2}\leqslant\varphi_j\leqslant\frac{\pi}{2} \tag{4.10}$$

let us deduce (see Appendix B, Eqs (B.4), (B.5)) that the equation (4.6) should possess one double-root

$$y_2 = \bar{y}_1 \equiv y_2, \tag{4.11}$$

which requires a definition of the sign of the expression $(\tau - a/2)$

$$\operatorname{sign}\left(\tau - \frac{a}{2}\right) = \operatorname{sign} \lambda = 1. \tag{4.12}$$

Making use of the last relations (4.11) and (4.12) we may find the constant

$$a = \tau + \sqrt{\tau^2 + \pi^2(1+4n)} \tag{4.13}$$

and

$$y_1 = \bar{y}_1 = -\frac{\tau}{\sqrt{\tau^2 + \pi^2(1+4n)}}. \tag{4.14}$$

The location of the bound states inside the energy gap can be seen in Fig. 1. We still have to analyse the behaviour of the curve in the antiferromagnetic state ($E < 0$). Considering this state we can see that for $\lambda/E < 0$ and $T_k \ll T_{c0}$ the bound state is at the edge of the

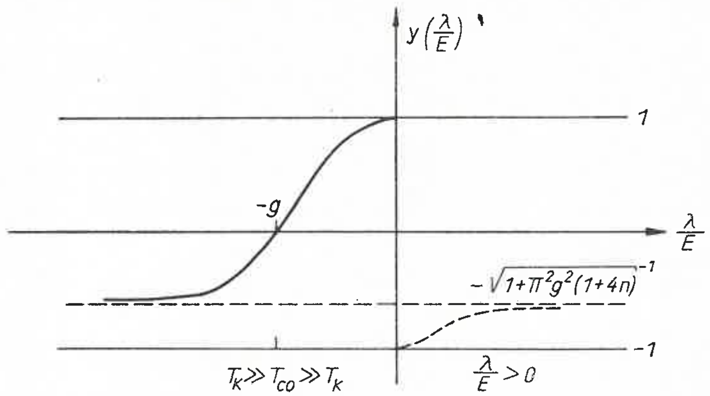

Fig. 1. Qualitative plot of the bound state location as a function of λ/E

gap $y_1 = 1$, shifting in position towards the middle. The quantity $\tau = E/\lambda + 1/g$ in this region is very large and we can expand formulas (4.13) and (4.14) in terms of $1/\tau$:

$$y_1 = 1 - \frac{\pi^2(1-4n)}{2\tau^2} \text{ and } a = -\frac{\pi^2(1+4n)}{2\tau}. \tag{4.15}$$

The corrections to (4.15) for all $T < T_{c0}$ are calculated in Appendix C with the result

$$y_1 = 1 - \frac{\pi^2}{2\left(\tau - \frac{\Delta}{\lambda}\right)^2}\left\{\sqrt{\left(\frac{1}{2}\operatorname{tgh}\frac{\beta\Delta}{2} - 1\right)^2 - 8\left[(1-n)\frac{1}{2}\operatorname{tgh}\frac{\beta\Delta}{2} + n\right]} + \right.$$
$$\left. + \frac{1}{2}\operatorname{tgh}\frac{\beta\Delta}{2} - 1\right\}^2. \tag{4.16}$$

When $\lambda/E = -g$, the bound state is right in the middle of the gap $y_1(T_k = T_{c0}) = 0$. After passing the middle of the gap the bound state tends to the asymptote

$$y_1\left(\frac{\lambda}{E} = -\infty\right) = -\sqrt{1+\pi^2 g^2(1+4n)}^{-1} \tag{4.17}$$

when $\lambda/E \to -\infty$. The location of the bound state in this region is defined by

$$y_1 = -1+\frac{\pi^2(1+4n)}{2\tau^2}, \quad a = 2\tau+\frac{\pi^2(1+4n)}{2\tau}. \tag{4.18}$$

The corrections to (4.18) for all $T > T_{c0}$ can be calculated, too, with the result

$$y_1 = -1+\frac{\pi^2}{2\left(\tau-\frac{\Delta}{\lambda}\right)^2}\left\{\sqrt{\left(\frac{1}{2}\operatorname{tgh}\frac{\beta\Delta}{2}-1\right)^2-8\left[(1-n)\frac{1}{2}\operatorname{tgh}\frac{\beta\Delta}{2}+n\right]}+\right.$$
$$\left.+\frac{1}{2}\operatorname{tgh}\frac{\beta\Delta}{2}-1\right\}^2. \tag{4.19}$$

Finally, let us examine the structure of the bound states. Information about this is provided by the density of states and electronic density distribution, which we can calculate, by using Green's function $G_{kk'}$ given by equation (2.22). Let us find the t-matrix which appears in equation (2.22) by assuming $z \approx \Delta$ ($z = \Delta y$). Then the functions $X(z)$ and $\Phi(z)$ which can be found from equation (3.10) for $t(z)$ are expressed as

$$X(y) = \lambda\left(\tau-\frac{a}{y-1}\right) \tag{4.20}$$

and

$$\Phi(y) = \frac{y-y_1}{yy_1-\sqrt{1-y^2}\sqrt{1-y_1^2}-1}\,\psi(y) \tag{4.21}$$

where y_1 given by equation (4.14) describes the location of bound states inside the energy gap and

$$\psi(y) = -(z-E-F)e^{S(y)}, \quad S(y) = \frac{\sqrt{1-y^2}}{2\pi}\int_1^\infty \frac{dx}{\sqrt{x^2-1}}\left(\frac{\ln K(x)}{x-y}+\frac{\ln K(-x)}{x+y}\right). \tag{4.22}$$

Calculation of $\psi(y)$ is possible when we know the explicit form of $K(x)$ given by equation (3.14), which under these conditions changes into

$$K(x) = \frac{\Phi_0^2(0)}{|\Delta-E-F(\Delta)|^2}\left(\frac{x-y_1}{x-1}\right)^2 \tag{4.23}$$

where

$$\Phi_0(0) = \lambda\sqrt{\tau^2+\pi^2(1+4n)} \tag{4.24}$$

is the value of $\Phi_0(z)$ of a non-superconducting metal ($\Delta = 0$) on Fermi's surface $z = 0$. Thus,

$$\psi(y) = -\Phi_0(0)\,\frac{1-yy_1+\sqrt{1-y^2}\,\sqrt{1-y_1^2}}{1-y}, \tag{4.25}$$

with the same

$$\Phi(y) = \Phi_0(0)\,\frac{y+y_1}{1-y}.$$

Upon substituting (4.20) and (4.26) into (3.10) we obtain the final form of the t-matrix

$$\lambda t(z, \Delta) = \frac{\sqrt{y^2-1}}{2\pi i}\,\frac{1-y_1}{y-y_1} \tag{4.26}$$

and of its diagonal and off-diagonal components

$$\lambda t_1(z, \Delta) = \frac{\sqrt{y^2-1}}{2\pi i}\,\frac{y(1-y_1)}{y^2-y_1^2}, \tag{4.27}$$

$$\lambda t_1(z, \Delta) = -\frac{\sqrt{y^2-1}}{2\pi i}\,\frac{y_1(1-y_1)}{y^2-y_1^2} \tag{4.28}$$

and thus of Green's function $G_{kk'}$. We can find the density of states from the first diagonal component of the Nambu matrix, *vis.*,

$$N(\omega) = -\frac{2}{\pi}\,\frac{1}{N}\,\mathrm{Im}\sum_k G_{kk}^{(11)}(\omega+i\delta). \tag{4.29}$$

Using the equations (4.28), (4.27) for the components of the t-matrix we obtain

$$N(\omega) = N_{s0}(\omega)+\tfrac{1}{2}\left[\delta(\omega-\Delta y_1)-\delta(\omega-\Delta)+\delta(\omega+\Delta y_1)-\delta(\omega+\Delta)\right] \tag{4.30}$$

where

$$N_{s0}(\omega) = 2N_0\begin{cases}\dfrac{1}{\sqrt{1-(\Delta/\omega)^2}} & |\omega| \geqslant \Delta\\[2ex] 0 & |\omega| < \Delta\end{cases} \tag{4.31}$$

From this relation we can deduce that there can occur bound states with energies $\pm\Delta y_1$ having a symmetrical superposition structure of a particle and a hole. A bound state like this structure is also confirmed by the electronic density distribution

$$\varrho(r) = -\frac{2}{\pi\Omega}\sum_{kk'} e^{i(k-k')r}\int_{-\infty}^{\infty} d\omega f(\omega)\,\mathrm{Im}\,G_{kk'}^{(11)}(\omega+i\delta) \tag{4.32}$$

where Ω is the volume of the system and $f(\omega)$ is Fermi's distribution function. From equation (4.32) we get

$$\Delta\varrho(r) = \varrho(r)-\varrho_0 = \frac{k_f N_0(1-y_1^2)}{6\pi^2 r^2} \int\limits_{-\infty}^{\infty} d\omega f(\omega) \operatorname{Re}\left[\frac{y}{(y^2-y_1^2)\sqrt{y^2-1}}\left(\cosh\frac{r}{L}+1\right)\right] \quad (4.33)$$

where $L^{-1} = \frac{4}{3} k_f N_0 \Delta \sqrt{1-y^2}$, and $\varrho_0 = \frac{k}{3\pi^2}$ is the uniform electronic density of the pure superconductor.

The formula (4.23) includes two distinct contributions to the electronic density distribution. One of them is

$$\Delta\varrho_1(r) = (8\pi r^2 l)^{-1} e^{-r/l} \quad (4.34)$$

where the characteristic length l is defined by $l^{-1} = L^{-1}(y_1)$ and describes the bound states within the gap $|\omega| < \Delta$. Such a contribution fulfills the relation

$$\int d^3r \Delta\varrho_1(r) = \tfrac{1}{2},$$

which is the expected result because only the "particle" part of the bound state should contribute to the "particle" density. We can also associate the normalized bound state wave function with the density distribution (4.34),

$$\varphi(r) = \sqrt{2\pi l^{-1}}\, \frac{e^{-r/l}}{r}. \quad (4.35)$$

This relation indicates that the bound state decreases exponentially with distance from the impurity.

The second contribution to the electronic density distribution

$$\Delta\varrho_2(r) = -\frac{e^{-r/l}}{8\pi l r^2} \quad (4.36)$$

from all the band states cancels the bound state contribution apart some uninteresting Rudermann-Kittel oscillating terms.

5. *Discussion*

In Section 4 we analysed the structure and the position of bound states inside the energy gap. The bound states have the structure of a symmetrical superposition of the "hole" state with energy $-\Delta|y_1|$ and "particle" state with energy $\Delta|y_1|$. This structure of bound states is determined by the fact that $t(-z, \Delta) = -t(z, -\Delta)$.

The density of states and the electronic density distribution are concordant with the fact the bound states have a structure exactly the same as that of Bogoliubov's quasiparticle.

The position of bound states inside the energy gap was found only in the case when an antiferromagnetic impurity alone was present ($E < 0$), because Anderson's hamiltonian can describe this state only. In this case the location of bound states inside energy gap is exactly the same as that received by Zittartz [3]. Extrapolating the plot to positive values of E, we notice that the location of bound states at the point $\lambda/E = 0$ changes jumpwise. There is a bound state at the upper edge of the gap $y_1 = 1$ when $\lambda/E \to 0^-$ ($|E| \gg \lambda, E < 0$), and at the lower edge when $\lambda/E \to 0^+$ ($|E| \gg \lambda, E > 0$). It is to be noted that at the point $\lambda/E = 0$ there is a certain energy jump from the value $-E$ to E, which shifts this bound state from one edge of the gap $y_1 = 1$, to the other, $y_1 = -1$. The author would like to thank Dr B. Kozarzewski for suggesting this topic and for many helpful discussions.

APPENDIX A

From equation (3.16) we obtain

$$\psi(\pm\Delta) = |\Phi(\pm\Delta)|, \tag{A.1}$$

which allows us to deduce the properties (b) and (c) of function $G(\pm\Delta)$. Then

$$G(-\Delta) = \frac{\Phi(-\Delta)}{\psi(-\Delta)} = \frac{X(-\Delta)}{\psi(-\Delta)} = \operatorname{sign}\left[\Delta + E + \lambda\left(\tau - \frac{a}{2}\right)\right], \tag{A.2}$$

where the fact $\Phi(-\Delta) = X(-\Delta) = \Delta + E + \lambda\left(\tau - \frac{a}{2}\right)$ is used.

In the same way we can derive property (c),

$$G(\Delta) = \frac{\Phi(\Delta)}{\psi(\Delta)} = \operatorname{sign}(\lambda a). \tag{A.3}$$

At the point $z = \Delta$ functions $\Phi(z)$ and $X(z)$ are discontinuous, so it is preferable to use the limit

$$\lim_{z\to\Delta} \frac{z-\Delta}{\Delta} X(z) = -\lim_{z\to\Delta} \frac{z-\Delta}{\Delta} \Phi(z) = \lambda a. \tag{A.4}$$

APPENDIX B

When $\beta\Delta \to 0$ the ratio $K(x)/K(-x)$ can be formulated,

$$\frac{K(x)}{K(-x)} = \frac{(x-y_1)(x-y_2)}{(x+y_1)(x+y_2)} \left(\frac{x+1}{x-1}\right)^2 \left(\frac{E+\Delta}{E-\Delta}\right)^2$$

whereby we get from the equation (3.16)

$$\psi(z)|_{z=i\infty} = -(z-E-F(z))|_{z=i\infty} e^{\frac{i}{2}(\pi-\varphi_1-\varphi_2)} \tag{B.1}$$

where $\varphi_j = \arcsin y_j$, $j = 1, 2$.

Taking into consideration the equation (4.9) and property (d) of function $G(z)$, we obtain

$$e^{-\frac{i}{2}(\pi-\varphi_1-\varphi_2)} = [\text{sign}\, X(-\Delta)] \prod_{j=1}^{2} e^{-i\left(\frac{\pi}{2}-\varphi_j\right)\nu_j}. \tag{B.2}$$

The only physically sensible solution can be obtained by assuming that $\nu_2 = 1$, $\nu_1 = 0$. Then the equation (B.2) will take the form

$$e^{\frac{i}{2}(\varphi_2-\varphi_1)} = [\text{sign}\, X(-\Delta)], \tag{B.3}$$

from which we can draw the final conclusion $\varphi_1 = \varphi_2 \equiv \bar{\varphi}_1$, which means that $y_1 = \bar{y}_1$ and sign $X(-\Delta) = \text{sign}\, \lambda\left(\tau - \frac{a}{2}\right) = 1$.

But sign $\lambda = 1$, thus

$$\text{sign}\left(\tau - \frac{a}{2}\right) = 1.$$

APPENDIX C

For $z \approx \pm\Delta$ we can calculate the zeroes of $\Phi(z)$ straight from the equation (2.30). Making use of the equations (3.12) and (3.13) we can find the value

$$L_0(y) = \frac{(n-1)\frac{1}{2}\,\text{tgh}\,\frac{\beta\Delta y}{2} - n}{-(z-E) + \frac{\lambda}{g}}, \quad y = \frac{z}{\Delta}, \tag{C.1}$$

which, in turn, can be put into the equation for $\Phi(z)$,

$$\Phi(y) = -(\Delta-E) + \frac{\lambda}{g} + \pi\lambda\sqrt{\frac{1+y}{1-y}}\left(\frac{1}{2}\,\text{tgh}\,\frac{\beta\Delta y}{2} - 1\right) +$$

$$+\pi^2\lambda^2\,\frac{1+y}{1-y}\,\frac{\frac{1}{2}(n-1)\,\text{tgh}\,\frac{\beta\Delta y}{2} - n}{-(\Delta-E) + \frac{\lambda}{g}} = 0. \tag{C.2}$$

This equation gives more precise results for y_1 in the region of large negative values of λ/E.

REFERENCES

[1] H. Sato, K. Maki, *Progr. Theor. Phys.*, **38**, 865 (1970).
[2] V. Celli, M. J. Zuckermann, *Nuovo Cimento*, **58B**, 154 (1968).
[3] J. Zittartz, E. Muller-Hartmenn, *Z. Phys.*, **232**, 11 (1970).
[4] J. Zittartz, *Z. Phys.*, **237**, 419 (1970).
[5] H. Mamada, F. Takano, *Progr. Theor. Phys.*, **43**, 1458 (1970).