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From the Laboratorium für Festkörperphysik der Eidg. Technischen Hochschule, Zürich

Superconductivity in Antiferromagnets

By

W. BALTENSPERGER and S. STRÄSSLER

With 1 Figure

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In a perfect spin up spin down antiferromagnet new B.C.S. electronpairs are being described, which are coupled by only a slightly decreased effective interaction. A repulsive interaction is added by virtual spin wave excitation. Depending on the relative strength, superconductivity may exist in such an antiferromagnet.

On a adapté la théorie de B.C.S. à un antiferromagnétique parfait caractérisé par un double réseau à spins inversés. L'interaction entre les nouveaux pairs d'électrons est légèrement plus faible que dans un corps non magnétique. Malgré l'interaction répulsive causée par les excitations virtuelles des ondes de spins, un tel modèle peut être supraconducteur pour certaines valeurs du quotient entre les deux interactions.

In einem perfekten Spin aufwärts Spin abwärts Antiferromagneten werden neue B.C.S. Elektronenpaare beschrieben, deren Kopplung gegenüber einem nichtmagnetischen Körper nur leicht vermindert ist. Durch die Anregung von virtuellen Spinwellen tritt eine abstoßende Wechselwirkung zwischen den Elektronen auf, so daß es von der relativen Größe der beiden Wechselwirkungen abhängt, ob Supraleitung möglich ist oder nicht.

1. Introduction

ANDERSON [*1*] in his theory of dirty superconductors starts with the exact one particle eigenfunctions in the perturbed crystal. To each wave $\varphi_{\boldsymbol{n},\sigma}$, there exists another eigenfunction $\mathscr{T}\varphi_{\boldsymbol{n},\sigma}$ of the same energy, where the time reversal operator $\mathscr{T}$ leads to the conjugate complex wave function with opposite spin. These pairs of functions are then used to build a B.C.S. [*2*] state. In this new representation the effective interaction between pairs is only slightly diminished.

ANDERSON's treatment does not apply when the system contains magnetic ions. Magnetic impurities have in fact a strong influence on the properties of a superconductor.

In the present work the superconductivity in an antiferromagnet is being discussed. The model used is an ideal antiferromagnet in which equal ionic spins point up and down alternatively on successive lattice positions. It describes an antiferromagnet with a sufficiently strong anisotropy energy. ANDERSON's method can be generalized in order to provide a treatment for this case. To each eigenfunction $\varphi_{\boldsymbol{n},\sigma}$ there exists an orthogonal eigenfunction $\mathscr{G}\varphi_{\boldsymbol{n},\sigma}$ of the same energy, where $\mathscr{G} = \mathscr{T}\mathscr{S}$. The operator $\mathscr{S}$ translates the space coordinates by half of a primitive translation vector of the magnetic structure.

The effective phonon induced and Coulomb interactions between these pairs are not much different from those between Bloch states in a similar non magnetic lattice, and they can therefore give rise to superconductivity.

Falk [3] and Karpenko [4] have pointed out that spinwaves contribute to the effective electron-electron interaction. This contribution is of opposite sign as compared to the phonon part. It is repulsive for scatterings in which the energy changes less than the spinwave energy. Numerically this interaction will often be weaker than the attractive interaction in good superconductors.

It is therefore possible that antiferromagnetic metals are superconductors. It may be of interest in this connection that vanadium has some antiferromagnetic properties [5].

2. The model

The Hamiltonian which describes conduction electrons in an antiferromagnet is written as

$$H = H_e + H_{ph} + H_{sp} + H_{e-ph} + H_{e-sp} + H_c \tag{1}$$

$$H_e = \sum_{\boldsymbol{k},\sigma} E(\boldsymbol{k})\, a^+_{\boldsymbol{k}\,\sigma} a_{\boldsymbol{k}\,\sigma} \tag{1a}$$

$$H_{ph} = \sum_{\boldsymbol{q}}{}' \,\omega(\boldsymbol{q})\, b^+_{\boldsymbol{q}}\, b_{\boldsymbol{q}} \tag{1b}$$

$$H_{sp} = \sum_{\boldsymbol{q}}{}' \sum_{p=1,2} w(\boldsymbol{q})\, d^{p+}_{\boldsymbol{q}}\, d^p_{\boldsymbol{q}} \tag{1c}$$

$$H_{e-ph} = \sum_{\substack{\boldsymbol{k},\boldsymbol{k}',\sigma\\ \boldsymbol{k}-\boldsymbol{k}'=\boldsymbol{q}}} g(\boldsymbol{q}) \left(\frac{\omega(\boldsymbol{q})}{2V}\right)^{\frac{1}{2}} a^+_{\boldsymbol{k}',\sigma} a_{\boldsymbol{k},\sigma}\, b^+_{\boldsymbol{q}} + adj\,. \tag{1d}$$

$$\begin{aligned} H_{e-sp} = -\frac{\Omega}{2V} \sum_{\substack{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{R}_l\\ \boldsymbol{k}'-\boldsymbol{k}=\boldsymbol{q}}} J(\boldsymbol{q})\, e^{-i\boldsymbol{q}\cdot\boldsymbol{R}_l} &\left[\{a^+_{\boldsymbol{k}'+} a_{\boldsymbol{k}+} - a^+_{\boldsymbol{k}'-} a_{\boldsymbol{k}-}\} S^z_l \right.\\ &+ a^+_{\boldsymbol{k}'+} a_{\boldsymbol{k}-} \{S^x_l - i S^y_l\} \\ &\left. + a^+_{\boldsymbol{k}'-} a_{\boldsymbol{k}+} \{S^x_l + i S^y_l\}\right] \end{aligned} \tag{1e}$$

$$H_c = \frac{1}{2V} \sum_{\boldsymbol{k}',\boldsymbol{k},\boldsymbol{q},\sigma,\sigma'} V^c(\boldsymbol{q})\, a^+_{\boldsymbol{k}'+\boldsymbol{q},\sigma'} a^+_{\boldsymbol{k}-\boldsymbol{q},\sigma} a_{\boldsymbol{k},\sigma} a_{\boldsymbol{k}',\sigma'} \tag{1f}$$

a^+, a creation and annihilation operators for Bloch electrons;

$E(\boldsymbol{k})$ Bloch energy;

b^+, b creation and annihilation operators for phonons;

$\omega(\boldsymbol{q})$ phonon energy;

$\sum'$ sum over the first Brillouin zone;

d^{p+}, d^p creation and annihilation operators for the two modes of spin waves in an antiferromagnet;

$w(\boldsymbol{q})$ spin wave energy;

$g(\boldsymbol{q})$	coupling constant between electrons and phonons;
V	volume of the system;
Ω	atomic volume;
$J(\boldsymbol{q})$	exchange coupling between the conduction electrons and an inner shell [6];
$\boldsymbol{R}_l$, $\boldsymbol{S}_l$	position and spin of the ion l;
$V^c(\boldsymbol{q})$	shielded Coulomb interaction.

We consider a magnetic structure of ionic spins with two sublattices with labels i respectively j, such that in the ground state $\langle S_i^z \rangle = S$ and $\langle S_j^z \rangle = -S$. The x- and y-components of the ionic spins are related to the spin wave operators [7].

The normal coordinates

$$\begin{aligned} Q_{1\boldsymbol{q}} &= \sqrt{\frac{2\Omega}{VS}} \sum_i e^{i\boldsymbol{q}\cdot\boldsymbol{R}_i} S_i^x \\ Q_{2\boldsymbol{q}} &= \sqrt{\frac{2\Omega}{VS}} \sum_j e^{-i\boldsymbol{q}\cdot\boldsymbol{R}_j} S_j^x \\ P_{1\boldsymbol{q}} &= \sqrt{\frac{2\Omega}{VS}} \sum_i e^{-i\boldsymbol{q}\cdot\boldsymbol{R}_i} S_i^y \\ P_{2\boldsymbol{q}} &= \sqrt{\frac{2\Omega}{VS}} \sum_j e^{i\boldsymbol{q}\cdot\boldsymbol{R}_j} S_j^y \end{aligned} \tag{2a}$$

form the following operators in an antiferromagnet

$$\begin{aligned} Q_{1,\boldsymbol{q}} &= c_{1,\boldsymbol{q}} Q'_{1,\boldsymbol{q}} + c_{2,\boldsymbol{q}} Q'_{2,-\boldsymbol{q}} \\ Q_{2,-\boldsymbol{q}} &= c_{2,\boldsymbol{q}} Q'_{1,\boldsymbol{q}} + c_{1,\boldsymbol{q}} Q'_{2,-\boldsymbol{q}} \\ P_{1,\boldsymbol{q}} &= c_{1,\boldsymbol{q}} P'_{1,\boldsymbol{q}} - c_{2,\boldsymbol{q}} P'_{2,-\boldsymbol{q}} \\ P_{2,-\boldsymbol{q}} &= -c_{2,\boldsymbol{q}} P'_{1,\boldsymbol{q}} + c_{1,\boldsymbol{q}} P'_{2,-\boldsymbol{q}} \end{aligned} \tag{2b}$$

where the coefficients $c_{p,\boldsymbol{q}}$ ($p = 1, 2$) are given by formula (92) of reference [7]

$$c_{1,\boldsymbol{q}} + c_{2,\boldsymbol{q}} = C(\boldsymbol{q}). \tag{2c}$$

The spin wave absorption and emission operators are given by

$$\begin{aligned} d_{\boldsymbol{q}}^p &= \frac{1}{\sqrt{2}} [Q'_{p,\boldsymbol{q}} + i P'_{p,-\boldsymbol{q}}], \\ d_{\boldsymbol{q}}^{p+} &= \frac{1}{\sqrt{2}} [Q'_{p,-\boldsymbol{q}} - i P'_{p,\boldsymbol{q}}]. \end{aligned} \tag{2d}$$

The electron-spin interaction by this transformation takes the following form

$$H_{e-sp} = H_{e-sp}^1 + H_{e-sp}^2 , \tag{3}$$

$$H_{e-sp}^1 = \frac{\Omega}{2V} \sum_{\substack{i,j \\ k,k' \\ k'-k=q}} J(q)\, S \{a_{k'+}^+ a_{k+} - a_{k'-}^+ a_{k-}\} \{e^{-iq\cdot R_i} - e^{-iq R_j}\}, \tag{3a}$$

$$H_{e-sp}^2 = -\frac{1}{2}\sqrt{\frac{S\Omega}{V}} \sum_{\substack{k',k \\ k'-k=q}} C(q)\, J(q) [a_{k'+}^+ a_{k-} \{d_q^{1+} + d_q^2\} + a_{k'-}^+ a_{k+} \{d_{-q}^1 + d_{-q}^{2+}\}] \tag{3b}$$

where terms of second order in creation and annihilation operators for spin deviations have been neglected.

3. Superconducting pairs in an antiferromagnet

The wave functions which satisfy

$$(H_e + H_{e-sp}^1)\, \psi_{n,\sigma} = E_{n,\sigma} \psi_{n,\sigma} \tag{4}$$

are Bloch functions

$$\psi_{n,\sigma}(r, s) = u_{n,\sigma}(r)\, e^{in\cdot r} \eta_\sigma(s) \tag{5}$$

for the magnetic period $2R$;

$$u_{n,\sigma}(r + 2R) = u_{n,\sigma}(r) \tag{6}$$

where R is a period of the crystal lattice.

The conjugate complex function $\psi_{n,\sigma}^*$ is an eigenfunction to the same energy. Furthermore $H_e + H_{e-sp}$ is invariant with respect to an operation which simultaneously reverses the electron spins and translates the coordinates from one sublattice to the other. Let $\mathscr{G}$ contain the three operations

$$\mathscr{G} = (^*, s \to -s, r \to r + R) \tag{7}$$

then

$$e^{in\cdot R} \mathscr{G}\, \psi_{n,\sigma}(r, s) \equiv \psi_{-n,-\sigma}(r, s) = u_{-n,-\sigma}(r)\, e^{-in\cdot r} \eta_{-\sigma}(s) \tag{8}$$

is an orthogonal eigenfunction to the same energy. The phase factor has been chosen so that

$$u_{-n,-\sigma}(r) = u_{n,\sigma}^*(r + R). \tag{9}$$

Let $c_{n,\sigma}^+$ and $c_{n,\sigma}$ be the creation and annihilation operators for electrons in the states $\psi_{n,\sigma}$. Since $E_{n+} = E_{-n-} \equiv E_n$ the pairs $c_{n+}^+ c_{-n-}^+$ can be used to construct the B.C.S. wave function. Superconductivity always appears when the sum of all interactions has a negative matrixelement between pair states near the Fermi surface.

4. Effective interactions

The effective interaction between the electrons in the $(\boldsymbol{n}, \sigma)$ representation has to be evaluated. The terms $H_{ph} + H_{e-ph}$ and $H_{sp} + H^2_{e-sp}$ give rise to phonon and spin wave induced interactions.

$$H_{eff} = \sum_{\boldsymbol{n}', \boldsymbol{n}} (V^{ph}_{\boldsymbol{n}', \boldsymbol{n}} + V^{sp}_{\boldsymbol{n}', \boldsymbol{n}} + V^{c}_{\boldsymbol{n}', \boldsymbol{n}})\, c^+_{\boldsymbol{n}'+}\, c_{\boldsymbol{n}+}\, c^+_{-\boldsymbol{n}'-}\, c_{-\boldsymbol{n}-}. \tag{10}$$

Here and in the following, only the interactions between the chosen pairs are retained.

To obtain $V^{ph}_{\boldsymbol{n}', \boldsymbol{n}}$ we first replace in (1 d) the operators $a_{\boldsymbol{k},\sigma}$ by the operators $c_{\boldsymbol{n},\sigma}$

$$c_{\boldsymbol{n},\sigma} = \sum_{\boldsymbol{k}} (\boldsymbol{n} \,|\, \boldsymbol{k})_\sigma\, a_{\boldsymbol{k},\sigma}, \tag{11}$$

$$H_{e-ph} = \sum_{\substack{\boldsymbol{n}, \boldsymbol{n}', \sigma \\ \boldsymbol{k}', \boldsymbol{k} \\ \boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{q}}} g(\boldsymbol{q}) \left(\frac{\omega(\boldsymbol{q})}{2V}\right)^{\frac{1}{2}} (\boldsymbol{n}' | \boldsymbol{k}')_\sigma\, (\boldsymbol{n} | \boldsymbol{k})^*{}_\sigma\, c^+_{\boldsymbol{n}',\sigma}\, c_{\boldsymbol{n},\sigma} (b^+_{\boldsymbol{q}} + b_{-\boldsymbol{q}}). \tag{12}$$

Using the relevant terms in the equation of motion we get

$$\hbar\, \dot{b}^+_{\boldsymbol{q}} = i\,\omega(\boldsymbol{q})\, b^+_{\boldsymbol{q}} + i \sum_{\substack{\boldsymbol{l}, \boldsymbol{l}' \\ \boldsymbol{l}' - \boldsymbol{l} = \boldsymbol{q}}} g(-\boldsymbol{q}) \left(\frac{\omega(\boldsymbol{q})}{2V}\right)^{\frac{1}{2}} (-\boldsymbol{n}' | \boldsymbol{l}')_{-\sigma}\, (-\boldsymbol{n} | \boldsymbol{l})^*_{-\sigma}\, c^+_{-\boldsymbol{n}',-\sigma}\, c_{-\boldsymbol{n},-\sigma}. \tag{13a}$$

In first order perturbation theory (13 a) becomes

$$\hbar\, \dot{b}^+_{\boldsymbol{q}} = i (E_{\boldsymbol{n}'} - E_{\boldsymbol{n}})\, b^+_{\boldsymbol{q}}. \tag{13b}$$

With

$$b^+_{\boldsymbol{q}} + b_{-\boldsymbol{q}} = \sum_{\substack{\boldsymbol{l}', \boldsymbol{l} \\ \boldsymbol{l}' - \boldsymbol{l} = \boldsymbol{q}}} \frac{2\,\omega(\boldsymbol{q})\, g(-\boldsymbol{q}) \left(\frac{\omega(\boldsymbol{q})}{2V}\right)^{\frac{1}{2}}}{(E_{\boldsymbol{n}'} - E_{\boldsymbol{n}})^2 - \omega(\boldsymbol{q})^2} (-\boldsymbol{n}' | \boldsymbol{l}')_{-\sigma}\, (-\boldsymbol{n} | \boldsymbol{l})^*_{-\sigma} \cdot c^+_{-\boldsymbol{n}',-\sigma}\, c_{-\boldsymbol{n},-\sigma} \tag{14}$$

the phonon operators can be eliminated.

Since in this treatment the effective interaction of the density mode $c^+_{-\boldsymbol{n},-\sigma} c_{-\boldsymbol{n},-\sigma}$ with the electron field is considered, a factor 1/2 is necessary in the Hamiltonian to avoid counting interactions twice.

$$V^{ph}_{\boldsymbol{n}', \boldsymbol{n}} = -\frac{1}{V} \sum_{\substack{\boldsymbol{k}, \boldsymbol{k}' \\ \boldsymbol{l}, \boldsymbol{l}' \\ \boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{q} = \boldsymbol{l}' - \boldsymbol{l}}} \frac{|g(\boldsymbol{q})|^2\, \omega^2(\boldsymbol{q})}{\omega^2(\boldsymbol{q}) - (E_{\boldsymbol{n}} - E_{\boldsymbol{n}'})^2} (\boldsymbol{n} | \boldsymbol{k})^*_+\, (\boldsymbol{n}' | \boldsymbol{k}')_+ (-\boldsymbol{n} | \boldsymbol{l})^*_-\, (-\boldsymbol{n}' | \boldsymbol{l}')_-. \tag{15}$$

The part H^1_{e-sp} of the electron spin interaction has been diagonalized at the beginning. The remaining part H^2_{e-sp} is an electron-spin wave-interaction, which by a similar treatment leads to

$$V^{sp}_{\boldsymbol{n}', \boldsymbol{n}} = +\frac{S\,\Omega}{2V} \sum_{\substack{\boldsymbol{k}, \boldsymbol{k}' \\ \boldsymbol{l}, \boldsymbol{l}' \\ \boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{q} = \boldsymbol{l}' - \boldsymbol{l}}} \frac{J^2(\boldsymbol{q})\, C^2(\boldsymbol{q})\, w(\boldsymbol{q})}{w^2(\boldsymbol{q}) - (E_{\boldsymbol{n}} - E_{\boldsymbol{n}'})^2} \cdot (\boldsymbol{n} | \boldsymbol{k})^*_+\, (\boldsymbol{n}' | \boldsymbol{k}')_+ (-\boldsymbol{n} | \boldsymbol{l})^*_-\, (-\boldsymbol{n}' | \boldsymbol{l}')_-. \tag{16}$$

The positive sign corresponds to a repulsive interaction for electron levels near the Fermi surface. This sign is due to the fact, that the emission and absorption of spin waves by an electron is accompanied by a spin flip. Fig. 1 shows graphically, that for the pair interaction this produces an exchange of the members of the scattered pair. The anticommutation property of the electron operators then leads to a change in sign, which does not occur in the phonon case.

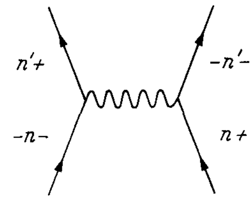

Fig. 1. Spin wave induced pair interaction

For the Coulomb interaction the transformation gives

$$V^c_{n',n} = \sum_{\substack{k,k',l,l' \\ k'-k=q=l'-l}} V^c(q)\,(n|k)^*_+\,(n'|k')_+\,(-n|l)^*_-\,(-n'|l')_- \,. \tag{17}$$

For a rough numerical comparison the parameters in (15), (16) and (17) may be replaced by suitable constants g, ω, J, w, C, and c.

$$\overline{V^{ph}_{n',n}} = \begin{cases} -\dfrac{g^2}{V}\,\overline{\alpha_{n',n}} & \text{for } |E_n - E_{n'}| < \omega \\ 0 & \text{for } |E_n - E_{n'}| > \omega \end{cases} \tag{18a}$$

$$\overline{V^{sp}_{n',n}} = \begin{cases} \dfrac{J^2 S C^2 \Omega}{V 2w}\,\overline{\alpha_{n',n}} & \text{for } |E_n - E_{n'}| < w \\ 0 & \text{for } |E_n - E_{n'}| > w \end{cases} \tag{18b}$$

$$\overline{V^c_{n',n}} = \frac{c^2}{V}\,\overline{\alpha_{n',n}} \tag{18c}$$

$$\alpha_{n',n} = \sum_{\substack{k',k,l,l' \\ k'-k=q=l'-l}} (n|k)^*_+\,(n'|k')_+\,(-n|l)^*_-\,(-n'|l')_- \tag{19}$$

As a measure of the relative strength we consider

$$(g^2 - c^2) \Big/ \left(\frac{J^2 S C^2 \Omega}{2w}\right). \tag{20}$$

Using the typical values

$$\begin{aligned} g^2 - c^2 &= 10^{-35}\,\text{erg cm}^3 & w &= 3\cdot 10^{-14}\,\text{erg} \\ J &= 1/10\,\text{eV} & \Omega &= 5\cdot 10^{-24}\,\text{cm}^3 \\ S &= 1 & C &= 1 \end{aligned} \tag{21}$$

(20) becomes 5. In this case the attractive interaction is predominant.

The effect of the ordered background on the interactions appears in the form of the factor $\alpha_{n',n}$. Of course when $J^2 S = 0$, we have $\alpha_{n',n} = 1$.

The wave functions (5) adapt themselves to the magnetic structure. In an antiferromagnet, however, the occuring increase of the kinetic energy keeps the deformation small. Therefore $\overline{\alpha_{n',n}}$ will not deviate much from 1.

To estimate $\overline{\alpha_{n',n}}$ we neglect the Bloch potential and assume a spin potential H^1_{e-sp} with simple cubic structure. The variational function

$$u_\pm(r) = \frac{1}{\sqrt{1+\frac{\beta^2}{8}}}\left\{1 \pm \beta\cdot\cos\frac{2\pi x}{L}\cdot\cos\frac{2\pi y}{L}\cdot\cos\frac{2\pi z}{L}\right\} \tag{22}$$

where L is the magnetic period, satisfies (9). The corresponding energy increase

$$E(\beta) = \frac{\pi^2 \hbar^2}{L^2 m} \cdot \frac{3}{4} \beta^2 - \frac{J S \beta}{2} \tag{23}$$

is minimized with

$$\beta = \frac{L^2 J S m}{\hbar^2 3 \pi^2} \tag{24}$$

which is of the order 10^{-1} for $L = 2R$. For small β (19) becomes

$$\overline{\alpha_{n',n}} = 1 - \frac{1}{4} \beta^2 \tag{25}$$

so that $\overline{\alpha_{n',n}}$ is practically 1. Obviously this is no more true, when the magnetic period L is large.

This model therefore suggests, that a pure and perfect antiferromagnetic metal may well be a superconductor.

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