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J. Phys.: Condens. Matter **18** (2006) 1553–1560 doi:10.1088/0953-8984/18/5/007

Bound states of Cooper pairs and electrons in the superconducting phase of MgB_2

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Received 16 September 2005, in final form 13 December 2005
Published 17 January 2006
Online at stacks.iop.org/JPhysCM/18/1553

Abstract

The two-band theory of superconductivity of MgB_2 with additional six-fermion interaction is considered. It is shown that a bound state of a spin-singlet Cooper pair of fermions from one of the bands and an individual fermion from the other one is possible. The spin-$\frac{1}{2}$ triples with zero angular momentum are made up of three spin-$\frac{1}{2}$ fermions with charge e. They are gapped Fermi excitations with the gap induced by the gaps of the single fermions. Their contribution to the thermodynamics of the MgB_2 superconductors is considered.

1. Introduction

The main goal of the present paper is to explore the bound states of spin-singlet Cooper pairs and individual electrons in the superconducting phase of MgB_2. The three-body bound states are everywhere in physics, but the study of their role in collective condensed matter behaviour is still limited. Phase transitions driven by an instability in a three-fermion channel have been explored. The anomalous three-body scattering amplitude is used as an ansatz to develop a mechanism of odd-frequency superconductivity [1]. Unlike a BCS theory, the authors involve a cooperative pairing of electrons and spins. The three-body bound state formation leads to a gap which is an odd function of frequency. The application to heavy fermion superconductors is discussed.

In the present paper the interest in this topic is inspired by the anomalous superconducting properties of MgB_2 [2]. The superconductivity in magnesium diboride is s wave, mediated by electron–phonon coupling. It differs from that of ordinary metallic superconductors in several ways. Scanning tunnelling microscopy [3] and point contact studies [4] revealed double-peaked spectra at low temperature that were interpreted as evidence for two-gap superconductivity. *Ab initio* calculations suggest that multiple gaps are a consequence of the coupling of distinct electronic bands [5, 6]. MgB_2 has a strongly anisotropic Fermi surface of four separate sheets that are grouped into two-dimensional σ bands and three-dimensional π bands. The different energy gaps are associated with the π and σ sheets. The key quantity in phonon-mediated superconductivity is the Eliashberg function $\alpha^2(\omega)F(\omega)$, where $F(\omega)$ is the phonon

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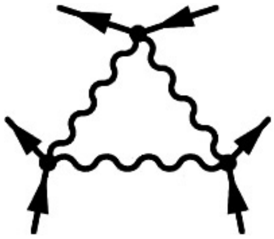

Figure 1. Triangle diagram with three phonon lines (undulating lines) which results from the two-phonon exchange.

density of states and $\alpha(\omega)$ is the electron–phonon coupling averaged over directions in k space. Electron tunnelling spectroscopy is used [7] to determine the three distinct Eliashberg functions $(\alpha^2 F)_{\pi-\pi}$, $(\alpha^2 F)_{\sigma-\sigma}$, and $(\alpha^2 F)_{\pi-\sigma}$. The authors consider the differential conductance of a tunnel junction between MgB_2 and In or Pb in superconducting state. With counter-electrodes In in the superconducting phase the curves 1, 2 and 3 (figure 1) show only a small gap, while the tiny bumps are considered as a 1% contribution of the large gap. The larger gap is well seen in the case of tunnelling in the ab plane with counter-electrodes Pb in the superconducting phase. In this case the authors do not comment on the tiny bumps at 10 mV (−10 mV) and the fact that $\mathrm{d}I/\mathrm{d}V$ increases near the 15 mV, which indicates the existence of new bump.

The double-gap structure is used to explain some of the unusual physical properties of MgB_2, such as the rapid rise of the specific heat coefficient C/T [8], tunnelling [4] and upper critical field anisotropy [9]. Quite different methods of theoretical investigation, including weak-coupling two-band BCS theory [10], the Eliashberg strong-coupling formalism [6], and strong-coupling density-functional technique with explicit account for the Coulomb repulsion [11], lead to astonishingly identical curves for the specific heat, as a function of temperature. The calculations reproduce the different slopes, above $0.5T_c$ and below $0.25T_c$, which apparently result from the existence of two gaps, but cannot explain the shoulder between them [8, 12]. Unexpected are the effects on the specific heat of Mg substitution by Al. The changes are in rather poor agreement with those predicted by taking into account changes in the electronic and phononic structure only [13].

A large B isotope effect is another argument in favour of phonon-mediated pairing [14, 15]. The isotope coefficient α is defined by the relation $T_c \propto M^{-\alpha}$, where M is the mass of the element. In BCS theory $\alpha = 0.5$, and for metals like Hg, Pb and Zn the coefficient is found experimentally to be close to 0.5. The isotope coefficient for MgB_2 is $\alpha \approx 0.32$. The density-functional calculations of the phonon spectrum and electron–phonon coupling in MgB_2 predict that, in this compound, phonon modes of boron oscillations may have relatively high frequencies, and that nonlinear coupling via two-phonon exchange is comparable to or even larger than the linear coupling [5, 16]. Both effects may contribute to the anomalous isotope effect coefficient [15], and to the significant increasing of the critical temperature $T_c = 39$ K.

Motivated by the theoretical and experimental findings I consider the theory of two-band superconductors [17, 18] with two-phonon–electron interaction. The main goal is to study the formation of coherent behaviour of Cooper pairs and electrons in the two-band superconductors MgB_2, as a result of a strong two-phonon–electron coupling. It is shown that spin-$\frac{1}{2}$ triples with zero angular momentum, made up of three spin-$\frac{1}{2}$ fermions with charge e, are possible. They are gapped Fermi excitations with the gap induced by the gaps of the single fermions. Effectively one can represent them as gapped fermions and write an effective action. This enables one to calculate the contribution of the triples to the thermodynamics of the MgB_2

superconductors. To reproduce the shoulder in the specific heat as a function of temperature, one has to choose the gaps of the triples larger than the gaps of the incipient electrons.

The paper is organized as follows. In section 2 the formation of triples and their contribution to the specific heat is explored. A summary in section 3 concludes this paper. The tunnelling experiments are debated as a most direct way to observe the triples experimentally.

2. Triples in two-band superconductors with nonlinear electron–phonon coupling

I consider the theory of two-band superconductors [17, 18] with two-phonon electron interaction. An important consequence of this interaction is the effective six-fermion interaction. One can obtain it from the triangle diagram (figure 1) with three phonon lines (undulating lines). There are two fermion species in the theory; therefore the low frequency and low momenta limit of the diagram lead to an effective local six-fermion term. The effective Hamiltonian H_{f^6} of the six-fermion interaction has the form

$$H_{f^6} = -\sum_{\ell\sigma} \lambda_\ell \int \mathrm{d}^3x\, c^\dagger_{\ell\uparrow}(\mathbf{x}) c^\dagger_{\ell\downarrow}(\mathbf{x}) c^\dagger_{-\ell\sigma}(\mathbf{x}) c_{-\ell\sigma}(\mathbf{x}) c_{\ell\downarrow}(\mathbf{x}) c_{\ell\uparrow}(\mathbf{x}) \tag{1}$$

where $c^\dagger_{\ell\sigma}(\mathbf{x})$ and $c_{\ell\sigma}(\mathbf{x})$ are creation and annihilation operators for fermions, with orbital index ℓ ($\ell = 1, 2, -\ell = 2, 1$) and spin projection σ ($\sigma = \uparrow, \downarrow$)[1].

The BCS Hamiltonian of the theory of two-band superconductivity is [17, 18]

$$H_{\mathrm{BCS}} = -\sum_{\ell} g_\ell \int \mathrm{d}^3x\, c^\dagger_{\ell\uparrow}(\mathbf{x}) c^\dagger_{\ell\downarrow}(\mathbf{x}) c_{\ell\downarrow}(\mathbf{x}) c_{\ell\uparrow}(\mathbf{x}) - g_3 \times \int \mathrm{d}^3x \sum_{\ell} c^\dagger_{\ell\uparrow}(\mathbf{x}) c^\dagger_{\ell\downarrow}(\mathbf{x}) c_{-\ell\downarrow}(\mathbf{x}) c_{-\ell\uparrow}(\mathbf{x}). \tag{2}$$

The partition function can be written as a path integral over the Grassmann functions of the Matsubara time τ $c^\dagger_{\ell\sigma}(\tau, \mathbf{x})$ and $c_{\ell\sigma}(\tau, \mathbf{x})$:

$$\mathcal{Z}(\beta) = \int \mathrm{D}\mu\left(c^\dagger c\right) \mathrm{e}^{-S}. \tag{3}$$

The action is given by the expressions

$$S = S_0 + \int_0^\beta \mathrm{d}\tau\, H_{\mathrm{int}}(\tau) \tag{4}$$

$$S_0 = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3x \sum_{\ell} c^\dagger_{\ell\sigma}(\tau, \mathbf{x}) \left[\partial_\tau + \epsilon_\ell(\nabla)\right] c_{\ell\sigma}(\tau, \mathbf{x}) \tag{5}$$

where β is the inverse temperature and $\epsilon_\ell(\nabla)$ is the dispersion of the band ℓ fermion. The Hamiltonian $H_{\mathrm{int}}(\tau)$ is a sum of the BCS Hamiltonian (2) and the six-fermion Hamiltonian (1). It is obtained from equations (1) and (2) by replacing the operators with Grassmann functions.

Let us introduce two spin-$\frac{1}{2}$ Fermi collective fields (**triples**) $\zeta_{\ell\sigma}(\tau, \mathbf{x})(\zeta^\dagger_{\ell\sigma}(\tau, \mathbf{x}))$ by means of the Hubbard–Stratanovich transformation of the six-fermion term (1):

$$\mathrm{e}^{-H_{f^6}} = \int \mathrm{D}\mu(\zeta^\dagger\zeta) \exp\Big\{-\int \mathrm{d}^4x \sum_{\ell} \lambda_\ell \Big[\zeta^\dagger_{\ell\sigma}(x)\zeta_{\ell\sigma}(x) + c^\dagger_{\ell\uparrow}(x) c^\dagger_{\ell\downarrow}(x) c^\dagger_{-\ell\sigma}(x)\zeta_{\ell\sigma}(x) + \zeta^\dagger_{\ell\sigma}(x) c_{-\ell\sigma}(x) c_{\ell\downarrow}(x) c_{\ell\uparrow}(x)\Big]\Big\} \tag{6}$$

where $x = (\tau, \mathbf{x})$ and $\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3x = \int \mathrm{d}^4x$.

[1] After some algebra the term can be rewritten in the form $\sum_\ell \int \mathrm{d}^3x\, n_\ell(\mathbf{x}) n_\ell(\mathbf{x}) n_{-\ell}(\mathbf{x})$ where $n_\ell(\mathbf{x}) = \sum_\sigma c^\dagger_{\ell\sigma}(\mathbf{x}) c_{\ell\sigma}(\mathbf{x})$.

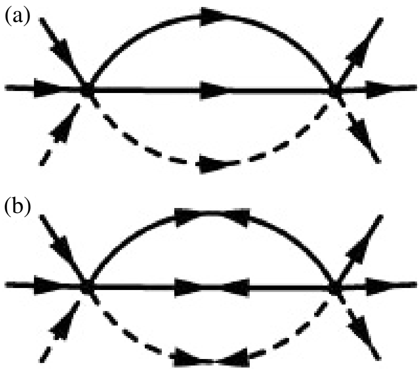

Figure 2. Two loop diagrams which represent the leading order of: (a) $\Pi^{\ell\ell}_{\sigma\sigma'}$, (b) $\Sigma^{\ell\ell}_{\sigma\sigma'}$ and $\overline{\Sigma}^{\ell\ell}_{\sigma\sigma'}$.

The effective action of the triples is defined by the equality

$$\mathrm{e}^{-S_{\mathrm{eff}}(\zeta^\dagger,\zeta)} = \exp\left\{-\int \mathrm{d}^4x \sum_{\ell\sigma} \lambda_\ell \zeta^\dagger_{\ell\sigma}(x)\zeta_{\ell\sigma}(x)\right\}$$
$$\times\left\langle \exp\left\{-\int \mathrm{d}^4x \sum_{\ell\sigma} \lambda_\ell\left[c^\dagger_{\ell\uparrow}(x)c^\dagger_{\ell\downarrow}(x)c^\dagger_{-\ell\sigma}(x)\zeta_{\ell\sigma}(x)\right.\right.\right.$$
$$\left.\left.\left. + \zeta^\dagger_{\ell\sigma}(x)c_{-\ell\sigma}(x)c_{\ell\downarrow}(x)c_{\ell\uparrow}(x)\right]\right\}\right\rangle \tag{7}$$

with

$$\langle Q\rangle = \int \mathrm{D}\mu\,(c^\dagger, c)Q\mathrm{e}^{-S_0-H_{\mathrm{BCS}}}. \tag{8}$$

The quadratic part of the effective action $S_{\mathrm{eff}}(\zeta^\dagger,\zeta)$ has the form

$$S_{\mathrm{eff}} = \int \mathrm{d}^4x\,\mathrm{d}^4y\left[\zeta^\dagger_{\ell\sigma}(x)\Pi^{\ell\ell'}_{\sigma\sigma'}(x-y)\zeta_{\ell'\sigma'}(y) + \zeta^\dagger_{\ell\sigma}(x)\Sigma^{\ell\ell'}_{\sigma\sigma'}(x-y)\zeta^\dagger_{\ell'\sigma'}(y)\right.$$
$$\left. + \zeta_{\ell\sigma}(x)\overline{\Sigma}^{\ell\ell'}_{\sigma\sigma'}(x-y)\zeta_{\ell'\sigma'}(y)\right] \tag{9}$$

where

$$\Pi^{\ell\ell'}_{\sigma\sigma'}(x-y) = \delta_{\ell,\ell'}\delta_{\sigma\sigma'}\lambda_\ell\delta^4(x-y) - \lambda_\ell\lambda_{\ell'}\langle c_{-\ell\sigma}(x)c_{\ell\downarrow}(x)c_{\ell\uparrow}(x)c^\dagger_{\ell'\uparrow}(y)c^\dagger_{\ell'\downarrow}(y)c^\dagger_{-\ell'\sigma'}(y)\rangle \tag{10}$$

$$\Sigma^{\ell\ell'}_{\sigma\sigma'}(x-y) = \frac{\lambda_\ell\lambda_{\ell'}}{2}\langle c_{-\ell\sigma}(x)c_{\ell\downarrow}(x)c_{\ell\uparrow}(x)c_{-\ell'\sigma'}(y)c_{\ell'\downarrow}(y)c_{\ell'\uparrow}(y)\rangle \tag{11}$$

$$\overline{\Sigma}^{\ell\ell'}_{\sigma\sigma'}(x-y) = \frac{\lambda_\ell\lambda_{\ell'}}{2}\langle c^\dagger_{\ell\uparrow}(x)c^\dagger_{\ell\downarrow}(x)c^\dagger_{-\ell\sigma}(x)c^\dagger_{\ell'\uparrow}(y)c^\dagger_{\ell'\downarrow}(y)c^\dagger_{-\ell'\sigma'}(y)\rangle. \tag{12}$$

In theory, with the Hamiltonian H_{BCS} (2) the off-diagonal elements are zero: $\Pi^{\ell\ell'}_{\sigma\sigma'} = 0$, $\Sigma^{\ell\ell'}_{\sigma\sigma'} = 0$ and $\overline{\Sigma}^{\ell\ell'}_{\sigma\sigma'} = 0$ if $\ell \neq \ell'$. The diagonal functions are calculated in leading order represented by the diagrams (figure 2). In the case of $\Pi^{\ell\ell}_{\sigma\sigma'}$ (figure 2(a)), two lines of the diagram (solid lines) correspond to the normal Green function of fermions with one and just the same band-index, while the third line (dashed line) corresponds to the normal Green function of a fermion with different band-index. The diagrams for $\Sigma^{\ell\ell}_{\sigma\sigma'}$ and $\overline{\Sigma}^{\ell\ell}_{\sigma\sigma'}$ (figure 2(b)) have two lines (solid lines) corresponding to the anomalous Green functions of fermions with equal band-index and one line (dashed line) which corresponds to the anomalous Green function of a fermion with different band-index.

The system of gap equations in the theory of two-band superconductivity has the form [17, 18]

$$\begin{aligned} \Delta_1 &= \frac{g_1}{2}\int \mathrm{d}^3p\,\frac{\tanh(\frac{\beta}{2}E_{1\mathbf{p}})}{E_{1\mathbf{p}}}\Delta_1 + \frac{g_3}{2}\int \mathrm{d}^3p\,\frac{\tanh(\frac{\beta}{2}E_{2\mathbf{p}})}{E_{2\mathbf{p}}}\Delta_2 \\ \Delta_2 &= \frac{g_3}{2}\int \mathrm{d}^3p\,\frac{\tanh(\frac{\beta}{2}E_{1\mathbf{p}})}{E_{1\mathbf{p}}}\Delta_1 + \frac{g_2}{2}\int \mathrm{d}^3p\,\frac{\tanh(\frac{\beta}{2}E_{2\mathbf{p}})}{E_{2\mathbf{p}}}\Delta_2 \end{aligned} \tag{13}$$

with $E_{\ell\mathbf{p}} = \sqrt{\varepsilon_{\ell\mathbf{p}}^2 + |\Delta_\ell^2|}$, where $\varepsilon_{\ell\mathbf{p}}$ is the ℓ-band fermion dispersion. The system of gap equations shows that the gaps Δ_ℓ can be chosen real. Then the normal and anomalous Green functions in two-band theory, calculated in the standard way, have the form [19]

$$S^{\ell}_{\uparrow\uparrow}(\omega,\mathbf{p}) = S^{\ell}_{\downarrow\downarrow}(\omega,\mathbf{p}) = -\frac{\mathrm{i}\omega + \varepsilon_{\ell\mathbf{p}}}{\omega^2 + \varepsilon_{\ell\mathbf{p}}^2 + \Delta_\ell^2} \tag{14}$$

$$F_\ell(\omega,\mathbf{p}) = F_\ell^\dagger(\omega,\mathbf{p}) = \frac{\Delta_\ell}{\omega^2 + \varepsilon_{\ell\mathbf{p}}^2 + \Delta_\ell^2}. \tag{15}$$

I calculate the diagrams in the low-frequency limit:

$$\Pi^{\ell\ell}_{\sigma\sigma'}(\omega,\mathbf{p}) = \delta_{\sigma\sigma'}\left[-\mathrm{i}\omega Z_\ell^{-1}(\mathbf{p}) + \hat{\varepsilon}_\ell(\mathbf{p})\right] \tag{16}$$

$$\Sigma^{\ell\ell}_{\downarrow\uparrow}(0,\mathbf{p}) = \overline{\Sigma}^{\ell\ell}_{\uparrow\downarrow}(0,\mathbf{p}) = \Sigma_\ell(\mathbf{p}). \tag{17}$$

The result is

$$\begin{aligned} Z_\ell^{-1}(\mathbf{p}) = \int \prod_{i=1}^{3} \frac{\mathrm{d}^3p_i}{(2\pi)^3} & \frac{(2\pi)^3\delta^3(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3-\mathbf{p})}{4E_{-\ell\mathbf{p}_1}E_{\ell\mathbf{p}_2}E_{\ell\mathbf{p}_3}(E_{-\ell\mathbf{p}_1}+E_{\ell\mathbf{p}_2}+E_{\ell\mathbf{p}_3})} \\ & \times \left[E_{-\ell\mathbf{p}_1}E_{\ell\mathbf{p}_2}E_{\ell\mathbf{p}_3} + E_{-\ell\mathbf{p}_1}\varepsilon_{\ell\mathbf{p}_2}\varepsilon_{\ell\mathbf{p}_3} + \varepsilon_{-\ell\mathbf{p}_1}E_{\ell\mathbf{p}_2}\varepsilon_{\ell\mathbf{p}_3} + \varepsilon_{-\ell\mathbf{p}_1}\varepsilon_{\ell\mathbf{p}_2}E_{\ell\mathbf{p}_3}\right] \end{aligned} \tag{18}$$

$$\begin{aligned} \hat{\varepsilon}_\ell(\mathbf{p}) = \frac{1}{\lambda_\ell} + \int \prod_{i=1}^{3} \frac{\mathrm{d}^3p_i}{(2\pi)^3} & \frac{(2\pi)^3\delta^3(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3-\mathbf{p})}{4E_{-\ell\mathbf{p}_1}E_{\ell\mathbf{p}_2}E_{\ell\mathbf{p}_3}(E_{-\ell\mathbf{p}_1}+E_{\ell\mathbf{p}_2}+E_{\ell\mathbf{p}_3})} \\ & \times \left[\varepsilon_{-\ell\mathbf{p}_1}\varepsilon_{\ell\mathbf{p}_2}\varepsilon_{\ell\mathbf{p}_3} + \varepsilon_{-\ell\mathbf{p}_1}E_{\ell\mathbf{p}_2}E_{\ell\mathbf{p}_3} + E_{-\ell\mathbf{p}_1}\varepsilon_{\ell\mathbf{p}_2}E_{\ell\mathbf{p}_3} + E_{-\ell\mathbf{p}_1}E_{\ell\mathbf{p}_2}\varepsilon_{\ell\mathbf{p}_3}\right] \end{aligned} \tag{19}$$

$$\Sigma_\ell(\mathbf{p}) = \frac{1}{2}\int \prod_{i=1}^{3} \frac{\mathrm{d}^3p_i}{(2\pi)^3} \frac{\Delta_\ell^2\Delta_{-\ell}(2\pi)^3\delta^3(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3-\mathbf{p})}{4E_{-\ell\mathbf{p}_1}E_{\ell\mathbf{p}_2}E_{\ell\mathbf{p}_3}(E_{-\ell\mathbf{p}_1}+E_{\ell\mathbf{p}_2}+E_{\ell\mathbf{p}_3})}. \tag{20}$$

The equations

$$\hat{\varepsilon}_\ell(\tilde{p}_{f\ell}) = 0 \tag{21}$$

define the Fermi surface of the triples. Using the approximate expressions for $Z_\ell(\mathbf{p})$ and $\Sigma_\ell(\mathbf{p})$

$$Z_\ell(\mathbf{p}) \simeq Z_\ell(p_{f\ell}) = Z_\ell, \qquad \Sigma_\ell(\mathbf{p}) \simeq \Sigma_\ell(p_{f\ell}), \tag{22}$$

and rescaling the triples' fields

$$Z^{-\frac{1}{2}}\zeta^\dagger_{\ell\sigma}(\omega,\mathbf{p}) \to \zeta^\dagger_{\ell\sigma}(\omega,\mathbf{p}), \tag{23}$$

$$Z^{-\frac{1}{2}}\zeta_{\ell\sigma}(\omega,\mathbf{p}) \to \zeta_{\ell\sigma}(\omega,\mathbf{p}) \tag{24}$$

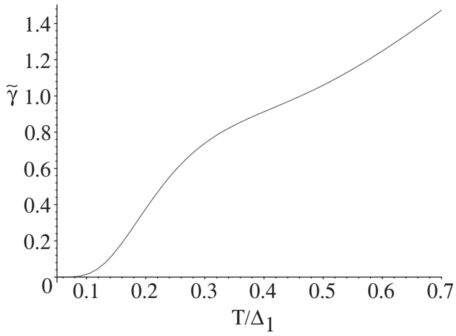

Figure 3. The heat capacity coefficient $\frac{\pi^2}{m_1 p_{f1}\sqrt{2\pi}}\frac{C}{T} = \tilde{\gamma}$ as a function of $\frac{T}{\Delta_1}$ for $\frac{\Delta_2}{\Delta_1} = 3$, $\frac{\varrho_1}{\Delta_1} = 4$, $\frac{\varrho_2}{\Delta_1} = 5$ and $m_1 p_{f1} \simeq m_2 p_{f2} \simeq \tilde{m}_1 \tilde{p}_{f1} \simeq \tilde{m}_2 \tilde{p}_{f2}$.

one obtains the effective action of the triples

$$S_{\text{eff}} = \int_0^\beta \mathrm{d}\tau \sum_p \big\{\zeta^\dagger_{\ell\sigma}(\tau, \mathbf{p})\,(\partial_\tau + \tilde{\varepsilon}_\ell(\mathbf{p}))\,\zeta_{\ell\sigma}(\tau, \mathbf{p}) + \varrho_\ell\big[\zeta^\dagger_{\ell\uparrow}(\tau, \mathbf{p})\zeta^\dagger_{\ell\downarrow}(\tau, -\mathbf{p}) + \zeta_{\ell\downarrow}(\tau, -\mathbf{p})\zeta_{\ell\uparrow}(\tau, \mathbf{p})\big]\big\} \tag{25}$$

with $\tilde{\varepsilon}_\ell(\mathbf{p}) = Z_\ell \hat{\varepsilon}_\ell(\mathbf{p})$ and $\varrho_\ell = Z_\ell \Sigma_\ell(\mathbf{p}_{f\ell})$. Near the Fermi surface $\tilde{\varepsilon}_\ell(\mathbf{p}) \simeq \frac{\tilde{p}_{f\ell}}{\tilde{m}_\ell}(p - p_{f\ell})$, where $\tilde{m}_\ell$ are the triples' masses.

The effective action (25) shows that the triples are spin-$\frac{1}{2}$ Fermi excitations with gap ϱ_ℓ induced by the gaps of the single fermion excitations (20). Next one diagonalizes the effective Hamiltonian using a Bogoliubov transformation, and rewrites it in terms of Bogoliubov excitations with dispersion $\tilde{E}_\ell(p) = \sqrt{\tilde{\varepsilon}^2_\ell(p) + \varrho^2_\ell}$. This enables us to calculate the contribution of triples to the thermodynamics of superconductors. In particular the low temperature behaviour of the heat capacity is

$$C_s = \sum_\ell \left[\frac{m_\ell p_{f\ell}}{\pi^2}\sqrt{\frac{2\pi\Delta^5_\ell}{T^3}}\mathrm{e}^{-\frac{\Delta_\ell}{T}} + \frac{\tilde{m}_\ell \tilde{p}_{f\ell}}{\pi^2}\sqrt{\frac{2\pi\rho^5_\ell}{T^3}}\mathrm{e}^{-\frac{\rho_\ell}{T}}\right] \tag{26}$$

where the first terms come from the single fermion contribution, while the other terms are the triples' contributions. Recent experiments, including photoemission [20] and tunnelling experiments [3, 21], show that the ratio of the single fermions' gaps is $2.6 \leqslant \Delta_2/\Delta_1 \leqslant 3.5$. The low temperature behaviour of the heat capacity coefficient $\frac{\pi^2}{m_1 p_{f1}\sqrt{2\pi}}\frac{C}{T} = \tilde{\gamma}$ is depicted as a function of $\frac{T}{\Delta_1}$ in figure 3 for $\frac{\Delta_2}{\Delta_1} = 3$, $\frac{\varrho_1}{\Delta_1} = 4$, $\frac{\varrho_2}{\Delta_1} = 5$ and $m_1 p_{f1} \simeq m_2 p_{f2} \simeq \tilde{m}_1 \tilde{p}_{f1} \simeq \tilde{m}_2 \tilde{p}_{f2}$. The curve is in a good agreement with the experimental one for MgB_2 [8, 12, 13].

3. Summary

In summary, new types of excitations, triples—made up of three spin-$\frac{1}{2}$ fermions, are predicted in the theory of two-band superconductivity with additional six-fermion interaction. They can be thought of as a bound-state of an s-type Cooper pair of fermions from one of the bands and a fermion from the other one with zero angular momentum. The triples are gapped excitations with the gap induced by the single fermion gaps. It is important to emphasize that the triples result from the nonlinear two-phonon–electron interaction.

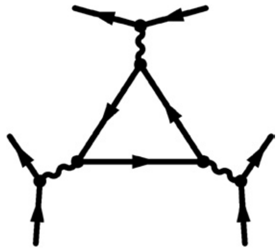

Figure 4. Six-fermion interaction obtained from the linear phonon–electron coupling.

Commonly the bound-state problem is studied by means of Bethe–Salpeter equations. In the present case, these are equations for the six-fermion Green functions $\langle cccc^\dagger c^\dagger c^\dagger \rangle$, $\langle cccccc \rangle$ and $\langle c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger \rangle$ with kernels given by diagrams in figure 1. The path integral calculations used in the paper are equivalent to the so-called ladder approximation for the Bethe–Salpeter equations. Since the kernels are in a local approximation, the ladder diagrams look like sausages with elements the diagrams given in figure 2. The solution of the Bethe–Salpeter equations is the sum over the infinite many ladder diagrams. I solve the problem by means of the path integral and Hubbard–Stratanovich transformation. It is important to stress that the anomalous Green functions $\langle cccccc \rangle$ and $\langle c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger \rangle$ are non-zero in the superconducting phase only. The normal Green functions $\langle cccc^\dagger c^\dagger c^\dagger \rangle$ are non-zero even in the normal phase but the pole structure exists in the superconducting phase. One can specify this from equation (18) by setting the gaps equal to zero. Then $Z_\ell^{-1} = \infty$; hence the residues of the poles Z_ℓ are zero. This means that triples exist only in the superconducting phase. This is why the triples are thought of as bound states of Cooper pairs and single electrons.

One can consider excitations made up of more than three spin-$\frac{1}{2}$ fermions while studying diagrams with more than three vertices. Due to the Pauli principle these excitations have non-zero angular momentum. The specific form of the fermion interactions determines the symmetry of these excitations. They in turn result from the nonlinear two-phonon–fermion interaction. Therefore knowledge of the nonlinear phonon interaction is crucial for the development of a theory of excitations made up of more than three fermions. The excitations with non-zero angular momentum have nodes, which lead to the anomalous temperature dependence of the specific heat. This anomaly is not observed and I do not consider these excitations.

The same is true for triples made up of fermions from one band. They have non-zero angular momentum too, and the symmetry of the triples results from the nonlinear two-phonon–fermion interaction.

The six-fermion interaction (1) can be alternatively obtained from the linear phonon–electron coupling. The leading order diagram is depicted in figure 4. Since my investigation is based on the assumption that nonlinear coupling via two-phonon exchange is comparable to or even larger than the linear coupling [5, 16], the contribution of the linear phonon–electron coupling (figure 4) is a small perturbation to the contribution of the nonlinear phonon–electron interaction and one can drop it.

It is easy to see from the formula for the heat capacity (26) that the contribution of the triples is decisive in explaining the shoulder-like part of the curve.

The most promising way to observe the triples in MgB_2 is by tunnelling experiments. It is evident that the contribution of the triples to the tunnelling current is with much smaller weight than those of the single electrons. Therefore, we can observe the triples only at very low temperature. If one considers the differential conductance of a tunnel junction with counter-electrodes in the superconducting state, for example In, or Pb as in [7], two new peaks should emerge when the temperature decreases. Tunnelling experiments achieved below 1 K can answer the question about the existence or non-existence of the triples.

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