Three-Body Collective Excitations in the Superconducting Phase of $MgB_2$

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It is shown that coherent behavior of Cooper’s pairs and electrons in the two-band superconductors $MgB_2$ is possible as a result of a strong two-phonon-electron coupling. The spin-1/2 triples with zero angular momentum are made up of three spin-1/2 fermions with charge $e$. They are gapped Fermi excitations with gap induced by the gaps of the single fermions. Their contribution to the thermodynamics of the $MgB_2$ superconductors is considered.

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I INTRODUCTION

The three-body bound states are everywhere in the physics, but the study of their role in collective condensed matter behavior 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 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 ordinary metallic superconductors in several ways. Scanning tunneling 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 strongly anisotropic Fermi surface of four separate sheets that are grouped into two-dimensional $\sigma$ bands and three-dimensional $\pi$ bands. The different energy gaps are associated with the $\pi$ and $\sigma$ sheets. The key quantity in phonon-mediated superconductivity is the Eliashberg function $\alpha^2(\omega)F(\omega)$, where $F(\omega)$ is phonon density of states and $\alpha(\omega)$ is the electron-phonon coupling averaged over directions in $k$ space. The electron tunneling spectroscopy is used [7] to determine the three distinct Eliashberg functions $(\alpha^2F)_{\pi-\pi}, (\alpha^2F)_{\sigma-\sigma},$ and $(\alpha^2F)_{\pi-\sigma}.$

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], tunneling [4] and upper critical field anisotropy [9]. Quite different methods of theoretical investigation, including weak-coupling two-band BCS theory [10], 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 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 can not explain the shoulder between them [5, 12]. Unexpected are the effects of $Mg$ substitution by $Al$ on the specific heat. The changes are in rather poor agreement with those predicted by taking into account changes in the electronic and photonic structure only [13].

A large $B$ isotope effect is another argument in favor of phonon-mediated pairing [14, 15]. The isotope coefficient $\alpha$ 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 [3, 16]. Both effects may contribute to the anomalous isotope effect coefficient [15], and to the significant increasing of the critical temperature $T_c = 39K$. It is thought that $T_c$ of $MgB_2$ probably represents the upper limit of the phonon mediated superconductivity.

Motivated by the theoretical and experimental findings I consider theory of two-band superconductors [17, 18] with two-phonon electron interaction. The main goal is to study the formation of coherent behavior of Cooper’s 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-$1/2$ triples with zero angular momentum, made up of three spin-$1/2$ fermions with charge $e$, are possible. They are gapped Fermi excitations with gap induced by the gaps of the single fermions. Effectively one can represent them as gapped fermions and to write an effective action. This enable 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 Sec. II the formation of triples and their contribution to the specific
heat is explored. A summary in Sec. IV concludes this paper. The tunneling experiments are debated as a most direct way to observe the triples experimentally.

II TRIPLES IN TWO-BAND SUPERCONDUCTORS WITH NONLINEAR ELECTRON-PHONON COUPLING

I consider theory of two-band superconductors 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 (Fig.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 leads to an effective local six-fermion term. The effective Hamiltonian $H_{\text{eff}}$ of the six-fermion interaction has the form

$$H_{\text{eff}} = -\sum_{\ell\sigma} \lambda_{\ell} \int d^{3}x \left( c^{\dagger}_{\ell\sigma} (x) c^{\dagger}_{\ell\sigma} (x) c_{-\ell\sigma} (x) c_{\ell\sigma} (x) \right)$$

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

The BCS Hamiltonian of the theory of two-band superconductivity is

$$H_{\text{BCS}} = \sum_{\ell} g_{\ell} \int d^{3}x \left( c^{\dagger}_{\ell\uparrow} (x) c_{\ell\downarrow} (x) c_{\ell\downarrow} (x) c^{\dagger}_{\ell\uparrow} (x) \right)$$

The partition function can be written as a path integral over the Grassmann functions of the Matsubara time $\tau$

$$Z(\beta) = \int D\mu \ (c^{\dagger} c) e^{-S}.$$  \hspace{1cm} (3)

The action is given by the expressions

$$S = S_{0} + \int d\tau H_{\text{int}} (\tau)$$

$$S_{0} = \int d\tau \int d^{3}x \sum_{\ell} \partial_{\tau} c^{\dagger}_{\ell\sigma} (\tau, x) \left[ \partial_{\tau} + \epsilon_{\ell}(\nabla) \right] c_{\ell\sigma} (\tau, x)$$

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

Let us introduce two spin-$1/2$ fermi collective fields (triples) $\zeta_{\ell\sigma} (\tau, x)$ ($\zeta^{\dagger}_{\ell\sigma} (\tau, x)$) by means of the Hubbard-Stratanovich transformation of the six-fermion term $H_{\text{eff}}$.

$$e^{-H_{\text{eff}}} = \int D\mu (\zeta^{\dagger}, \zeta) \exp \left\{ - \int d^{3}x \sum_{\ell\sigma} \lambda_{\ell} \left[ \zeta^{\dagger}_{\ell\sigma} (x) \zeta_{\ell\sigma} (x) + c^{\dagger}_{\ell\uparrow} (x) c_{-\ell\downarrow} (x) \zeta_{\ell\sigma} (x) + \zeta_{\ell\sigma} (x) c_{-\ell\sigma} (x) c_{\ell\downarrow} (x) c^{\dagger}_{\ell\uparrow} (x) \right] \right\}$$

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

The effective action of the triples is defined by the equality

$$e^{-S_{\text{eff}} (\zeta^{\dagger}, \zeta)} = \exp \left\{ - \int d^{3}x \sum_{\ell\sigma} \lambda_{\ell} \left[ c^{\dagger}_{\ell\uparrow} (x) c_{\ell\downarrow} (x) c^{\dagger}_{\ell\sigma} (x) \zeta_{\ell\sigma} (x) + \zeta_{\ell\sigma} (x) c_{-\ell\sigma} (x) c_{\ell\downarrow} (x) c^{\dagger}_{\ell\uparrow} (x) \right] \right\}$$

with

$$< Q > = \int D\mu (c^{\dagger}, c) Q e^{-S_{\text{eff}}}$$

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

$$S_{\text{eff}} = \int d^{4}x d^{4}y \left[ \zeta^{\dagger}_{\ell\sigma} (x) \Pi^{\ell\sigma'}_{\sigma\sigma'} (x-y) \zeta_{\ell\sigma'} (y) + (9) \right]$$

where

$$\Pi^{\ell\sigma'}_{\sigma\sigma'} (x-y) = \delta_{\ell,\ell'} \delta_{\sigma\sigma'} \lambda_{\ell} \delta^{4}(x-y) - \lambda_{\ell} \lambda_{\ell'} < c_{-\ell\sigma} (x) c_{\ell\tau} (x) c^{\dagger}_{\ell\tau'} (y) c^{\dagger}_{\ell\sigma'} (y) >$$

$$\sum_{\sigma\sigma'} \sigma' (x-y)$$

$$\frac{\lambda_{\ell} \lambda_{\ell'}}{2} < c_{-\ell\sigma} (x) c_{\ell\tau} (x) c^{\dagger}_{\ell\tau'} (y) c^{\dagger}_{\ell\sigma'} (y) >$$

In theory with Hamiltonian $H_{\text{BCS}}$, the off-diagonal elements are zero: $\Pi^{\ell\sigma'}_{\sigma\sigma'} = 0$, $\Sigma^{\ell\sigma'}_{\sigma\sigma'} = 0$ and $\sum_{\sigma\sigma'} \sigma' = 0$ if $\ell \neq \ell'$. The diagonal functions are calculated in leading order represented by the diagrams (Fig.2). In the case of $\Pi_{\sigma\sigma'}^{\ell\ell'}$ (Fig.2a), 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 fermion with different band-index. The system of gaps’ equations shows that anomalous Green functions in two-band theory, calculated in the standard way, have the form

\[ \Delta = \frac{g_1}{2} \int d^3p \frac{\tanh(\frac{\beta}{2}E_1p)}{E_1p} \Delta_1 + \frac{g_2}{2} \int d^3p \frac{\tanh(\frac{\beta}{2}E_2p)}{E_2p} \Delta_2 \]

with \( E_\ell = \sqrt{\epsilon_\ell p + |\Delta_\ell|^2} \), where \( \epsilon_\ell p \) is \( \ell \)-band fermion dispersion. The system of gaps’ equations shows that the gaps \( \Delta_\ell \) can be chosen real. Then the normal and anomalous Green functions in two-band theory, 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 fermion with different band-index.

\[ S_{\ell\ell}(\omega, p) = S_{\ell\ell}(\omega, p) = -\frac{i\omega + \epsilon_\ell p}{\omega^2 + \epsilon_\ell^2 p + \Delta_\ell^2} \]

\[ F(\omega, p) = F(\omega, p) = \frac{\Delta_\ell}{\omega^2 + \epsilon_\ell^2 p + \Delta_\ell^2} \]

I calculate the diagrams in low-frequency limit

\[ \Pi_{\ell\ell}(\omega, p) = \delta_{\ell\ell} \left[ -i\omega Z_\ell^{-1}(p) + \xi_\ell(p) \right] \]

The result is

\[ \Sigma_{\ell\ell}(0, p) = \Sigma_{\ell\ell}(0, p) = \Sigma_{\ell}(p). \]

The equations define the Fermi surface of the triples. Using the approximate expressions for \( Z_\ell(p) \) and \( \Sigma_\ell(p) \)

\[ Z_\ell(p) \simeq Z_\ell(p_{\rm f\ell}) = Z_\ell, \quad \Sigma_\ell(p) \simeq \Sigma_\ell(p_{\rm f\ell}), \]

and re-scaling the triples’ fields

\[ Z^{-\frac{1}{2}} \xi_{\ell\sigma}(\omega, p) \to \xi_{\ell\sigma}(\omega, p), \quad \xi_{\ell(\sigma)}(\omega, p) \to \xi_{\ell(\sigma)}(\omega, p) \]

one obtains the effective action of the triples

\[ S_{\ell\ell}^{\rm eff} = \int d\tau \sum_p \{ \xi_{\ell\sigma}(\tau, p) (\partial_\tau + \dot{\xi}_\ell(p)) \xi_{\ell\sigma}(\tau, p) + \dot{\xi}_\ell \left[ \xi_{\ell\sigma}(\tau, p) \xi_{\ell\sigma}(\tau, -p) + \xi_{\ell\sigma}(\tau, -p) \xi_{\ell\sigma}(\tau, p) \right] \}

with \( \xi_\ell(p) = Z_\ell \xi_\ell(p) \) and \( \dot{g}_\ell = Z_\ell \Sigma_\ell(p_{\rm f\ell}) \). Near the Fermi surface \( \xi_\ell(p) \simeq \frac{m_\ell}{\hbar^2}(p - p_{\rm f\ell}) \), where \( m_\ell \) are triples’ masses.

The effective action \[ m_\ell \] shows that triples are spin-1/2 fermi excitations with gap \( g_\ell \) induced by the gaps of the single fermion excitations \[ m_\ell \]. Next one diagonalizes the effective Hamiltonian using a Bogoliubov transformation, and rewrites it in terms of Bogoliubov excitations with...
FIG. 3: The heat capacity coefficient \( \pi \) function of \( T/\Delta_1 \) for dispersion \( \tilde{E}(p) = \sqrt{\tilde{\epsilon}_1^2(p) + \tilde{q}_f^2} \). This enables to calculate the contribution of triples to the thermodynamics of superconductors. In particular the low temperature behavior of the heat capacity is

\[
C_s = \sum_\ell \left[ \frac{m_1 p_{f1}}{\pi^2} \sqrt{\frac{2\pi \Delta_1^3}{T^3}} e^{-\frac{\tilde{m}_1 p_{f1}}{\pi^2} \sqrt{\frac{2\pi \Delta_1^3}{T^3}} e^{-\frac{\tilde{q}_f^2}{\pi^2}}} \right] \tag{26}
\]

where the first terms come from the single fermion contribution, while the other terms are triples’ contribution. Recent experiments, including photoemission [21] and tunneling experiments [3, 22], show that the ratio of the single fermions’ gaps is \( 2.6 \leq \Delta_2/\Delta_1 \leq 3.5 \). The low temperature behavior of the heat capacity coefficient \( \frac{m_1 p_{f1} \sqrt{2\pi}}{\Delta_1} \) is depicted as a function of \( T/\Delta_1 \) in Fig.3 for \( \frac{\Delta_2}{\Delta_1} = 3, \frac{\Delta_1}{\Delta_1} = 4, \frac{\Delta_1}{\Delta_1} = 5 \) and \( m_1 p_{f1} \approx m_2 p_{f2} \approx m_1 p_{f1} \approx m_2 p_{f2} \). The curve is in a good agreement with the experimental one for \( MgB_2 \) [8, 12, 13].

![FIG. 3: The heat capacity coefficient as a function of \( T/\Delta_1 \) for \( \Delta_2/\Delta_1 = 3, \Delta_1/\Delta_1 = 4, \Delta_1/\Delta_1 = 5 \) and \( m_1 p_{f1} \approx m_2 p_{f2} \approx m_1 p_{f1} \approx m_2 p_{f2} \).](image)

### III SUMMARY

In summary, new type of excitations, triples- made up of three spin-\( \frac{1}{2} \) fermions, are predicted in theory of two-band superconductivity with non-linear two-phonon-fermion interaction. They can be thought of as a bound-state of s-type Cooper pair of fermions from one of the bands and fermion from the other one with zero angular momentum. The triples are gapped excitations with gap induced by the single fermion gaps. It is important to underline that the triples result from the nonlinear two-phonon-electron interaction. One can consider excitations made up of more than three spin-\( \frac{1}{2} \) fermions while studying diagrams with more than three vertexes. Due to the Pauli principle these excitations have non-zero angular momentum. The specific form of the fermion interactions determine the symmetry of these excitations. They in turn result from the non-linear two-phonon-fermion interaction. Therefore the knowledge of the non-linear phonon interaction is crucial for the development of a theory of excitations made up of more than three fermions. 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 non-linear two-phonon-fermion interaction.

The six-fermion interaction can be alternatively obtained from the linear phonon-electron coupling. The leading order diagram is depicted in Fig4. 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 in [3, 10], the contribution of the linear phonon-electron coupling (Fig4) is 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 that the contribution of the triples is decisive to explain the shoulder like part of the curve.

The most promising way to observe the triples in \( MgB_2 \) is by tunneling experiments. It is evident that the contribution of the triples to the tunneling 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 tunnel junction with counter-electrodes in superconducting state, for example \( In \) or \( Pb \) as in [7], two new peaks should emerge when the temperature decreases. Tunneling experiments achieved below 1K can answer the question about the existence or nonexistence of the triples.

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[1] P. Coleman, E. Miranda and A. Tsvelik, Phys. Rev. Lett.,
[2] J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani and J. Akimitsu, Nature (London) 410, 63 (2001).

[3] F. Giubileo, D. Roditchev, W. Sacks, R. Lamy, D. X. Thanh, J. Klein, S. Miraglia, D. Fruchart, J. Marcus, and Ph. Monod, Phys. Rev. Lett., 87, 177008 (2001).

[4] P. Szabó, P. Samuely, J. Kačmarčík, T. Klein, J. Marcus, D. Fruchart, S. Miraglia, C. Marcenat, and A. G. M. Jansen, Phys. Rev. Lett., 87 137005 (2001).

[5] A. Y. Liu, I. I. Mazin, and J. Kortus, Phys. Rev. Lett., 87 087005 (2001).

[6] H. J. Choi, D. Roundy, H. Sun, and M. Cohen, Nature (London) 418, 758 (2002).

[7] J. Geerk, R. Schneider, G. Linker, A. G. Zaitsev, R. Heid, K. -P. Bohnen, and H. v. Löheysen, Phys. Rev. Lett., 94 227005 (2005).

[8] F. Bouquet, R. A. Fisher, N. E. Phillips, D. G. Hinks, and J. D. Jorgensen, Phys. Rev. Lett., 87 047001 (2001).

[9] M. Angst, R. Puzniak, A. Wisniewski, J. Jun, S. M. Kazakov, J. Karpinski, J. Roos, and H. Keller, Phys. Rev. Lett., 88 167004 (2002).

[10] T. M. Mishonov, V. L. Pokrovsky, and H. Wei, Phys. Rev B 71 012514 (2005).

[11] A. Floris, G. Profeta, N. N. Lathiotakis, M. Lüders, M. A. L. Marques, C. Franchini, E. K. U. Gross, A. Continenza, and S. Massida, Phys. Rev. Lett., 94 037004 (2005).

[12] H. D. Yang, J.-Y. Lin, H. H. Li, F. H. Hsu, C. J. Liu, S.-C. Li, R.-C. Yu, and C.-Q. Jin, Phys. Rev. Lett., 87 167003 (2001).

[13] M. Putti, M. Affronte, P. Manfrinetti, and A. Palenzona, Phys. Rev B 68 094514 (2003).

[14] S. L. Bud’ko, G. Lapertot, C. Petrovic, C. E. Cunningham, N. Anderson, and P.C. Canfield, Phys. Rev. Lett., 86 1877 (2001).