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SUPERCONDUCTING PROPERTIES OF MgB_2 IN A SCENARIO WITH INTRA- AND INTERBAND PAIRING CHANNELS

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IV. Kristoffel, N.; Örd, T.; Rägo, K. (2003). *A description of* MgB_2 *superconductivity including* $\sigma - \pi$ *bands coupling.* Journal of Superconductivity, **16** (3), 517 - 519.

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3. Kristoffel, N.; Örd, T.; Rägo, K. (2003). *Superconductivity of* MgB_2 *in a two-band model.* In: International Conference on Dynamic Inhomogeneities in complex oxides, Bled, Slovenia:, 2003.

4. Örd, T.; Rägo, K. (2004). *Anisotropy of* MgB_2 *superconductivity in a two-band model.* In: International Conference on Nanoscale Heterogeneity & Quantum Phenomena in Complex Matter, Roma, Italy:, 2004.

5. Örd, T.; Kristoffel, N.; Rägo, K. (2005). *Free energy functional and critical magnetic fields of a two-gap superconductor with intra- and interband interactions.* In: International Conference on Vortex Matter in Nanostructured Superconductors, Crete, Greece:, 2005.

6. Kristoffel, N.; Örd, T.; Rägo, K. (2006). *Free energy functional and critical magnetic fields anisotropy in magnesium diboride.* In: NATO Advanced Research Workshop on Electron Correlation in New Materials and Nanosystems, Yalta, Ukraina:, 2006.

7. Rägo, K.; Örd, T.; Kristoffel, N. (2006). *Gap equations and magnetic anisotropies in a two-band model of magnesium diboride.* In: International School of Solid-State Physics 37th Course "Twenty years from discovery of High T_c Superconductivity", Erice, Italy:, 2006.

Author's contribution:

Author's research has given an essential contribution to all these publications. She participated in the analytical calculations reflected in articles I – IV, and in the analysis of the results. The author is entirely responsible for the development of the theoretical schemes of papers V and VI, and for all numerical calculations.

1 Introduction

The phenomenon called superconductivity entered the research area of condensed matter physics since 1911 by the discovery of H. Kammerlingh Onnes. He found that at temperature 4.12 K the electrical resistance of mercury suddenly disappeared and remained equal to zero at further downturn of temperature [1]. Following investigations have shown the appearance of the superconductivity in other metals and also in some alloys. The superconductivity remained for long years a phenomenon of low temperature physics of unknown origin. Macroscopic descriptions have been elaborated, however the first microscopic theory of superconductivity has been formulated by Bardeen, Cooper and Schiffer (BCS) only in 1957. It is known as conventional BSC approach [2]. The central concept of BCS theory is the pairing of electrons (build up of Cooper pairs) by attractive potential exerted by the electron-phonon interaction. BCS theory is essentially an one-band theory (intraband coupling) and has been mainly proved for simple metals. Numerous experimental attempts to find superconductors with higher transition temperatures (T_c) in complex compounds have been made exploiting various theoretical elaborations and suggestions. The success has been moderate with the record of $T_c = 23$ K in the case of Nb_3Ge. However, a number of novel classes of superconductors exibiting unconventional properties has been discovered. First of all the heavy-fermion compounds and low-dimensional organic system should be mentioned.

The investigation of high-temperature superconductivity began in 1986 with the discovery of Müller and Bednorz [3] in the cuprate $La_{2-x}Sr_xCuO_4$ with $T_c = 32$ K. Figure 1 shows the superconducting critical temperature of several cuprates as a function of the year of discovery, as well as T_c of some

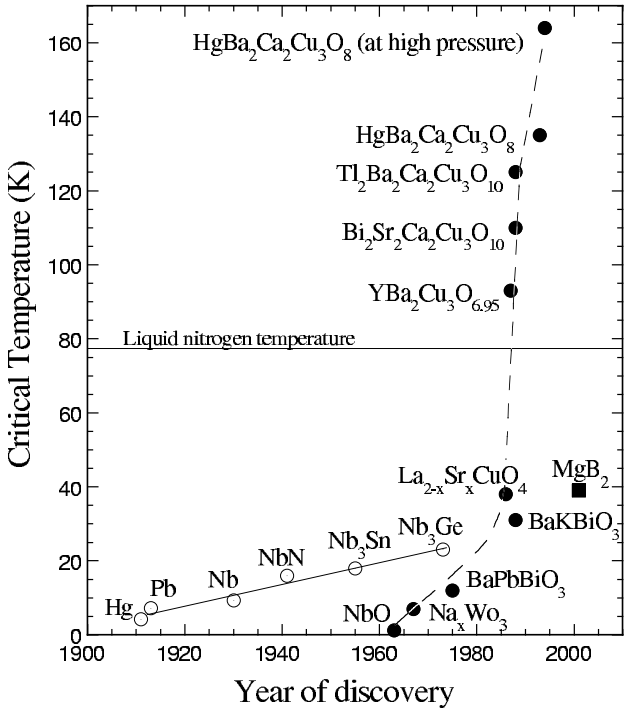

Figure 1: The time evolution of superconducting critical temperature since the discovery of superconductivity in 1911 [4].

metallic superconductors. New physics of these materials have stimulated novel theoretical attempts and reanimation of earlier unconventional ones. An essential generalization of the theory of superconductivity has been suggested by Suhl, Matthias and Walker [5], and independently by Moskalenko in 1959 [6]. These authors have investigated interacting multiband systems of complex nature with overlapping electron bands, keeping in mind transition metal compounds. So, the multiband superconductivity incorporating the interband pairing channel is known for a long time. This framework contains numerous peculiarities, novel properties and manifestations as compared with the BCS scheme. The understanding of superconductivity ex-

tends to materials with complex inner structure and varied multicomponent electronic spectra. The conditions for the appearance of superconductivity become extended by functioning of nonconvenient interaction channels. Simultaneously the strength of the pairing can be expected to be amplified.

At the present time the nomenclature of the classes of superconducting materials under interest is wide. Cuprate perovskites [7],[8],[9] with all the relative metal oxides, the MgB_2 family, heavy fermion [10],[11],[12] and A15 type compounds[13],[14], fullerides [15],[16],[17], carbon nanotubes [18],[19],[20], etc. can be mentioned. One deals here with complex materials for which a multiband electron spectrum near the Fermi energy has been found or expected. Analogous conditions of quantum resonance can be reached also by special impacts, i.e. by doping treatments, external pressure, or nanoarchitectural constructions. Accordingly the applications of multiband superconductivity schemes to more or less exotic superconductors has been recently become popular. At the same time the features which can be simply interpreted using the multiband superconductivity approaches seem to be not well and largely known.

The multicomponent order parameter describes interfering superconducting condensates with own supercarrier densities and phases. Supercarrier densities and the corresponding superconducting gaps of the band components are considerably determined by the effectiveness of the interband pairing. The change of the corresponding conditions (by doping, pressure, etc.) can lead to the variation of the characteristics of multiband superconducting systems.

The present thesis concern the elaboration of a theoretical model for explanation the MgB_2 superconductivity mechanism and description its basic superconductivity characteristics. According to the two-gap nature of the

MgB_2 superconductivity, an approach with two effective bands incorporating essentially the interband interaction has been used. Three interaction channels contribute to the pairing: $\sigma - \pi$ interband repulsion, σ-intraband attraction of electron-phonon nature and σ-intraband repulsive interaction. Anisotropic Ginzburg-Landau scheme for the corresponding two-band superconductivity model has been developed. The free energy functional has been derived and the corresponding superconducting gap equations have been obtained. Temperature dependencies of gaps as well as various thermodynamic characteristics (heat capacity, coherence lengths, critical fields) have been calculated for MgB_2 using a plausible parameter set. The influence of doping on phase transition temperature and superconducting gaps has been studied in the framework of the present model. The results obtained are in general agreement with the experimental data.

2 Overview: MgB_2 and two-band superconductivity

2.1 Superconductor MgB_2

The present work is devoted to the investigation of the mechanism of MgB_2 superconductivity. The discovery of superconductivity in MgB_2 [21] revived a search for this phenomena in non-oxides, especially in related boron compounds [22], [23]. Its high critical temperature $T_c = 39$K hold out hope for obtaining even higher T_c's for simple compounds.

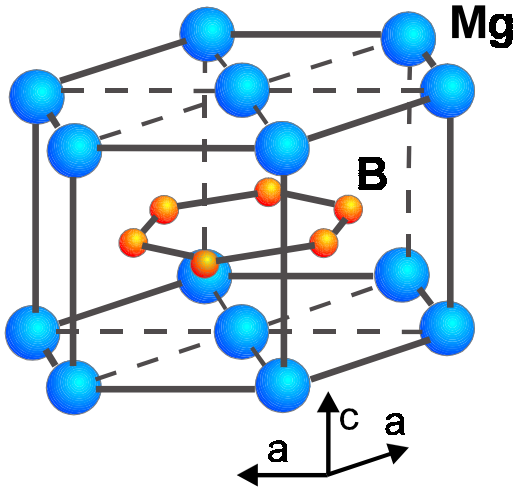

Figure 2: The structure of MgB_2 containing graphite-type B layers separated by hexagonal close-packed layers of Mg [24].

MgB_2 is an "old" material, has been known since early 1950's, but only recently discovered to be superconducting [21]. It has a simple hexagonal structure (Fig. 2).

Understanding the electronic properties of MgB_2 is crucial in order to address the promise of everyday applications and to search for materials with possibly higher T_c. Several electronic structure calculations have already been carried out, and all agree in predicting a dominant contribution of boron states near the Fermi level, while the Mg atoms act as electron reservoir donating their s-electrons to the boron-derived bands [25]-[32]. The in-plane B σ-bands retain a localized covalent bonding character, but should exhibit metallic hole-type conductivity, as opposed to the non-bonding π-bands possessing a typical delocalized character and an electron-type conductivity [25]. The bands are plotted in figure 3.

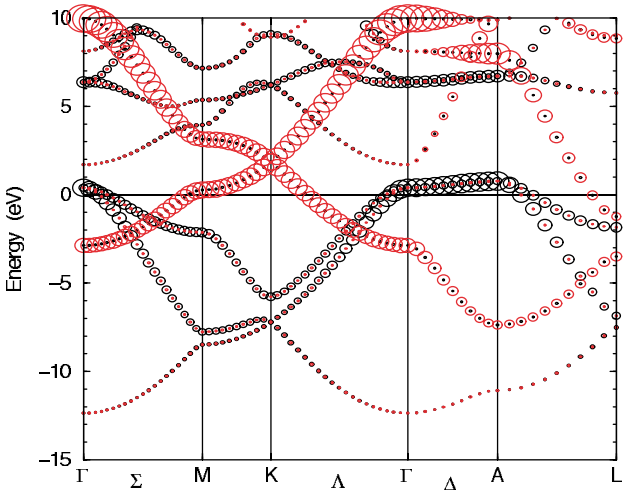

Figure 3: Band structure of MgB_2 [28].

Due to their two-dimensional character the σ-bands should give the highest

contribution to the density of states near the Fermi level [25]-[32]. In addition, because of the small dispersion of the sigma-bands, electron correlation effects should play an important role [25]-[29]. Finally, it has been argued that the boron planes are akin to the Cu-O planes in high-T_c cuprates [29]. The doping of the MgB_2 bands with holes and/or electrons (for example by intercalation of alkali metals or halogen atoms) should mirror the behaviour of underdoped and/or overdoped high-T_c cuprates [29].

Why such a large interest in MgB_2 from the physics community one may ask? One important reason is the cost high-T_c superconducting wires are 70% silver[33], therefore expensive. Unlike the cuprates, MgB_2 has a lower anisotropy, larger coherence lengths, transparency of the grain boundaries to current flow, which makes it a good candidate for applications. MgB_2 promises a higher operating temperature and higher device speed than the present electronics based on Nb. Moreover, high critical current densities, J_c, can be achieved in magnetic fields by oxygen alloying [34], and irradiation shows an increase of J_c values [35].

Since 2001, the properties of the MgB_2 have been investigated thoroughly. In particular, it has been established that the characteristics of this compound are stable in magnetic fields and under irradiation. The critical transport currents in MgB_2 are large in magnitude and relatively insensitive to contact with inter crystalline boundaries. These properties and a number of other superconductivity characteristics of MgB_2 are very attractive for practical applications (see reviews [36]-[38]).

Theoretical results [28],[39],[40] showed that boron sublattice conduction band is responsible for superconductivity in the simple compound MgB_2. From a fundamental point of view the central issue is whether the super-

conductivity in this system can be understood within the framework of a conventional electron-phonon mechanism, or a more exotic mechanism is responsible for the superconductivity. The presence of an isotope effect is a strong indicator of phonon mediation of superconducting coupling.

The large boron isotope effect, α_{B} of 0.26 [39], 0.3 [41] shows that phonons associated with B vibrations play a significant role in MgB_2 superconductivity. On the other hand, the magnesium isotope effect, α_{Mg} is very small, 0.02 [39]. Accordingly the value of the total isotope effect is $\alpha_T = \alpha_{\mathrm{B}} + \alpha_{\mathrm{Mg}} \approx 0.3$ in MgB_2. It is now evident that this compound is an electron-phonon-mediated superconductor.

Extended approaches [42]-[54] have been developed to reconcile the numerous transport, optical, microwave and thermodynamic experimental data, and the almost obvious s-wave and phonon-driven character of superconductivity in MgB_2. The idea of the multiple-gap nature of the MgB_2 superconductivity with the gap diversity on the different sheets of the Fermi surface (i.e. in the momentum $\mathbf{k}$ space) has found essential support. This is an extension of the well-known two-band (or many-band) superconductivity concept [55]-[57], which, in its turn, approximates the complex anisotropy of the electron spectrum in MgB_2[27],[28],[45],[58]-[61]. Two Fermi surface sheets are supposed to originate from nearly two-dimensional boron σ-bands and predominantly three dimensional π-bands. The coexistence of two kinds of current carriers (electron- and hole-like) discovered in Hall measurements [62] is compatible with the complex electron spectrum, although by no means directly implies the two-gap picture.

Measurements on electron- or hole-doped MgB_2 are of interest as they may help to understanding the electronic density of states and the Fermi surface

dependence on doping. The substitutions on Mg or B positions represent one of the possibilities to introduce such defects. Many experiments have attacked the central question of how superconductivity transition temperature changes upon doping by substituting Al or C for Mg or B respectively. This leads to filling of the hole states with electrons. For MgB_2 partial substitutions with many elements have been proved. The general conclusion has been that dopants destroy superconductivity [63]-[67], i.e. MgB_2 is in same sense optimally doped. The transition temperature decreased significantly for the substitutions mentioned [64],[68]-[77]. This effect has been explained by different mechanisms ranging from simple band filling effect [78],[79] (merging superconducting gaps [80]) to the influence of increased interband scattering or decrease of the electron-phonon coupling strength [81].

The coexistence of two gaps [82],[83] with different anisotropies in MgB_2 gives rise to very peculiar physical properties [44], [84]-[86]. The anisotropy of a type II superconductor is described either by $\gamma_\lambda = \lambda_c/\lambda_{ab}$, where λ is the magnetic penetration depth, or by $\gamma_{H_{C2}} = H_{C2,ab}/H_{C2,c} = \xi_{ab}/\xi_c$, with ξ being the coherence length. Traditionally these two anisotropies have been considered to be identical, but in materials with anisotropic gaps this is generally not the case [84]-[87]. Magnesium diboride represents an extreme case where $\gamma_\lambda \neq \gamma_{H_{C2}}$. The strong temperature dependence of the anisotropy of the upper critical field $\gamma_{H_{c2}}$ is now well established [88]-[92]. However, the anisotropy of the lower critical field needs to be explained. Caplin et al. [93] suggested that $\gamma_{H_{C1}} = H_{C1,c}/H_{c1,ab} \sim 2$, independent of temperature, but found temperature independent $\gamma_{H_{c2}}$ value in striking contrast with other measurements [88]-[92]. On the other hand, Zehetmayer et. al. [94] found that $\gamma_{H_{C1}}$ decreased with temperature assuming, however, that $\gamma_\lambda = \gamma_{H_{c2}}$.

Through theoretical advances, a fairly unified picture has emerged with predictions that can be experimentally substantiated [44],[47],[50],[53],[63],[85]-[87],[95]-[97]. One of the salient predictions associated with a pronounced two-band effect is a difference between the coherence length aniostropy [85], [86], [95] and the penetration depth anisotropy [84],[96] both of which become temperature dependent with opposite tendencies.

2.2 The two band model

Because the theoretical framework of the present thesis belongs to multiband superconductivity, a brief overview of this type approaches will be present in the following.

The interest to multiband superconductivity has grown particularly in connection with the difficulties in explaining the pairing mechanism in cuprate superconductors. Various connected aspects and diverse model realizations have been investigated, e.g. [98]-[104]. The first widely accepted successful application of the two-band model to a real system has been done for the mentioned two-band superconductor MgB_2 [21],[44],[54],[105],[106],[107]-[111].

The theory of two band superconductivity, including the configuration interaction of pairs of oppositive spin and momentum in the a-band and b- band, was developed on the basis of the Bogoljubov transformations [112]-[114] where the many body wave function [115] is given by

$$|\Psi_{Kondo}\rangle = \prod_k (u_k + \nu_k a^+_{k\uparrow} a^+_{-k\downarrow}) \prod_k (x_k + y_k b^+_{k\uparrow} b^+_{-k\downarrow})|0\rangle. \qquad (2.1)$$

The element corresponding to the transfer of a pair from the a-band to the b-band or vice versa appears with the negative sign in the expression of

the energy of the superconductor. This gain of energy is the origin of the increase of the transition temperature driven by interband pairing. The two band superconductivity has been proposed for metallic elements and alloys [5],[6],[113]-[116], for doped cuprate perovskites [117]-[122], for magnesium diboride [21],[44],[54],[105],[106],[107]-[111] and for few other materials as Nb doped $SrTio_3$ [123] $SrRu0_4$ [124]-[126] YNi_2B_2C, $LuNi_2B_2C$ [127] and $NbSe_2$ [128].

The multiband superconductivity shows up only in the "clean limit", where the single electron mean free path for the interband impurity scattering satisfies the condition $l > hv_F/\Delta_a$ where v_F is the Fermi velocity and Δ_a is the average superconducting gap in band a [129]-[132].

The criterium that the mean free path should be larger than the superconducting coherence length must be fulfilled. This very strict condition implies also that the impurity interband scattering rate γ_{ab} should be very small $\gamma_{ab} << (1/2)(k_B/\hbar)T_c$. Therefore most of the metals are in the "dirty limit" where the interband impurity scattering mixes the electron wave functions of electrons on different spots on bare Fermi surfaces and it reduces the system to an effective single Fermi surface. The interband pairing that transfers a pair from the "a"-band to the "b"-band and viceversa in the multiband superconductivity theory is expressed by the operators

$$\sum_{k,k'} J(k,k')(a^+_{k\uparrow}a^+_{-k\downarrow}b_{-k\downarrow}b_{k\uparrow}), \tag{2.2}$$

where a^+ and b^+ are creation operators of electrons in the a and b band respectively and $J(k,k')$ is an exchange-like integral. This interband pairing interaction may be repulsive as it was first noticed by Kondo [115]. Therefore it is a non-BCS pairing process since in the BCS theory an attractive inter-

action is required for the formation of Cooper pairs. The BCS is essentially a one band theory.

MgB_2 provides the simplest high-T_c superconductor. It could play a key role for understanding high-T_c superconductivity as atomic hydrogen for quantum mechanics. There is now growing evidence that MgB_2 is a practical realization of the proposed T_c amplification process driven by Feshbach shape resonances in interband pairing [107], [111] representing the case of a superlattice of quantum wells.

The "shape resonances" have been described by Feshbach in elastic scattering cross-section for the processes of neutron capture and nuclear fission [133] in the cloudy crystal ball model of nuclear reactions. This scattering theory is dealing with configuration interaction in multichannel processes involving states with different spatial locations. The process for increase of T_c by a Feshbach "shape resonance" was first proposed by Blatt and Thompson [116],[134],[135] in 1963 for a superconducting thin film. At the electronic topological transition [136] a small Fermi surface of a second subband disappears while the large $2D$ Fermi surface of a first subband shows minor variations. In the "clean limit" the single electrons cannot be scattered from the n-th to the $(n-l)$-th subband and vice versa, but configuration interaction between pairs in different bands is possible in an energy window. Therefore the Feshbach shape resonance occurs by tuning the Lifshitz parameter. In the Blatt proposal it is tuned by changing the film thickness. The prediction of Blatt and Thompson of the oscillatory behavior of T_c as a function of film thickness has been recently confirmed experimentally for a superconducting film [137] although phase fluctuations due to the electron confinement in the two dimension is expected to reduce the critical temperature.

Two-band model developments have further been stimulated after some approaches were proposed assuming the interaction of two groups of electrons. An original idea was offered by Little in 1964. Here the quasi one-dimensional organic superconductor was proposed with one conducting band where electron get paired with effective interaction mediated by the electronic excitations of bound electrons in a dielectric type subsystem (see [138]). The idea was based on the fact that instead of limiting electronic excitations by narrow phonon channel within the Debye layer as in BCS theory, energies of magnitude $\hbar\omega \simeq 1$ eV can be achieved if interaction arises from interband excitations. A similar model was proposed by Ginzburg in 1965 for sandwich-like structures of metallic and dielectric layers. Also some other models of this type have been discussed [139].

During many years Ginzburg has emphasized that there are no restrictions which do not allow high-T_c superconductivity even with T_c's reaching room temperatures [140],[141]. The outstanding discovery [142], [143] of real high-T_c system $La_{2-x}M_xCuO_4$ (M = Sr, Ba) by Bendorz and Müller has opened a channel for producing new high-T_c superconductors. Bendorz and Müller have pointed to the presence of a strong electron-phonon interaction in structurally deformable systems [144] when looking for suitable materials for finding high-T_c's [145].

The low-energy excitation spectrum of a multiband superconductor can manifest superconducting gaps and pseudogaps. The latter appear naturally as minimal quasiparticle excitation energies of band components not intersected by the chemical potential μ [102],[103]. Then the pseudogap energy is given by the expression $\sqrt{(\epsilon_\alpha - \mu)^2_{min} + \Delta^2_\alpha}$ and this gap survives in the normal state as $|\epsilon_\alpha - \mu|_{min}$. Such "extrinsic" source of the pseudogap does not man-

ifest itself in the supercarrier density because the interband pairing channel can induce the superconductivity also for the gapped bands. On the phase diagram, when an external impact (e.g. doping) reorganizes the spectral relations so that $\epsilon_\alpha = \mu$ is reached, the pseudogap transforms into a superconducting gap.

3 A two-band model of MgB_2 superconductivity

3.1 Superconductivity mechanism with intraband and interband couplings

We consider the following Hamiltonian to describe the MgB_2 multiband superconductivity

$$H = \sum_{\alpha \mathbf{k}s} \widetilde{\varepsilon}(\mathbf{k}) a^+_{\alpha \mathbf{k}s} a_{\alpha \mathbf{k}s} + \\ +2 \sum_{\alpha\alpha'} \sum_{\mathbf{k}\mathbf{k}'} W_{\alpha\alpha'}(\mathbf{k}, \mathbf{k}') a^+_{\alpha \mathbf{k}\uparrow} a^+_{\alpha -\mathbf{k}\downarrow} a_{\alpha' -\mathbf{k}'\downarrow} a_{\alpha' \mathbf{k}'\uparrow}. \tag{3.1}$$

Here $\widetilde{\varepsilon}_\alpha(\mathbf{k}) = \varepsilon_\alpha(\mathbf{k}) - \mu$; $\varepsilon_\alpha(\mathbf{k})$ are the energies of electrons in the bands ($\alpha = 1$ for σ and $\alpha = 2$ for π); μ is the chemical potential; $\mathbf{k}$ is the wave-vector; $s = \uparrow, \downarrow$ are spin projections; a^+ and a are the creation and annihilation operators of electrons; $W_{\alpha\alpha'}$ are the intraband ($\alpha = \alpha'$) and interband ($\alpha \neq \alpha'$) interaction constants.

Such description of MgB_2 superconductivity will incorporate electron-phonon and Coulomb interactions in the effective bands, and $\sigma - \pi$ scattering of intraband pairs. The linearized Hamiltonian corresponding to (3.1) has the form

$$H_{\text{eff}} = \sum_{\alpha \mathbf{k}s} \widetilde{\varepsilon}_\alpha(\mathbf{k}) a^+_{\alpha \mathbf{k}s} a_{\alpha \mathbf{k}s} - \sum_{\alpha \mathbf{k}} \Delta_{\alpha \mathbf{k}} < a^+_{\alpha \mathbf{k}\uparrow} a^+_{\alpha -\mathbf{k}\downarrow} > + \\ + \sum_{\mathbf{k}} [\Delta_{\alpha \mathbf{k}} a^+_{\alpha \mathbf{k}\uparrow} a^+_{\alpha -\mathbf{k}\downarrow} + \Delta^*_{\alpha \mathbf{k}} a_{\alpha -\mathbf{k}\downarrow} a_{\alpha \mathbf{k}\uparrow}] \tag{3.2}$$

where the superconductivity order parameters are determined by the anomalous operator averages (spike brackets) characterizing the pairing

$$\Delta_{\alpha\mathbf{k}} = 2\sum_{\beta\mathbf{k}} W_{\alpha\beta}(\mathbf{k},\mathbf{k}') < a_{\beta-\mathbf{k}'\downarrow} a_{\beta\mathbf{k}'\uparrow} > . \tag{3.3}$$

The statistical averages in (3.2) and (3.3) are defined as

$$< ... >= Z^{-1}\mathrm{Sp}(...\exp(-H_{\mathrm{eff}}/k_BT)) \tag{3.4}$$

where

$$Z = \mathrm{Sp}\left[\exp(-H_{\mathrm{eff}}/k_BT)\right] \tag{3.5}$$

is the partition function. Following Bogoljubov [146], to diagonalize (3.2) we introduce new operators A_α by the transformations

$$\begin{aligned} a_{\alpha\mathbf{k}\uparrow} &= u_{\alpha\mathbf{k}} A_{\alpha\mathbf{k}\uparrow} + \nu^*_{\alpha\mathbf{k}} A^+_{\alpha-\mathbf{k}\downarrow}, \\ a_{\alpha-\mathbf{k}\downarrow} &= u_{\alpha\mathbf{k}} A_{\alpha-\mathbf{k}\downarrow} - \nu^*_{\alpha\mathbf{k}} A^+_{\alpha\mathbf{k}\uparrow}, \end{aligned} \tag{3.6}$$

where

$$\begin{aligned} u_{\alpha\mathbf{k}} = u_{\alpha-\mathbf{k}},\ \nu_{\alpha\mathbf{k}} &= -\nu_{\alpha-\mathbf{k}} \\ u^2_{\alpha\mathbf{k}} &= -\frac{1}{2}\left(1 + \widetilde{\varepsilon}_\alpha(\mathbf{k}) E^{-1}_\alpha(\mathbf{k})\right) \\ |\nu_{\alpha\mathbf{k}}|^2 &= \frac{1}{2}\left(1 - \widetilde{\varepsilon}_\alpha(\mathbf{k}) E^{-1}_\alpha(\mathbf{k})\right) \\ u_{\alpha\mathbf{k}}\nu^*_{\alpha\mathbf{k}} &= \frac{1}{2}\Delta_{\alpha\mathbf{k}} E^{-1}_\alpha(\mathbf{k}), \end{aligned} \tag{3.7}$$

and $E_\alpha(\mathbf{k})$ are the energies of elementary excitations

$$E_\alpha(\mathbf{k}) = \sqrt{\widetilde{\varepsilon}^2_\alpha(\mathbf{k}) + |\Delta_{\alpha\mathbf{k}}|^2}. \tag{3.8}$$

Having in mind also (3.3), the Hamiltonian (3.2) takes the diagonal form

$$H_{\mathrm{eff}} = \sum_{\alpha\mathbf{k}} D_{\alpha\mathbf{k}} + \sum_{\alpha\mathbf{k}s} E_\alpha(\mathbf{k}) A^+_{\alpha\mathbf{k}s} A_{\alpha\mathbf{k}s} \tag{3.9}$$

where

$$D_{\alpha\mathbf{k}} = \widetilde{\varepsilon}_{\alpha}(\mathbf{k}) - E_{\alpha}(\mathbf{k}) - \Delta_{\alpha\mathbf{k}} < a^{+}_{\alpha\mathbf{k}\uparrow} a^{+}_{\alpha-\mathbf{k}\downarrow} > . \tag{3.10}$$

Further we will assume, that the superconducting gaps are real quantities.

Now on the basis of equations (3.4), (3.5) and (3.9) and using the transformation (3.6), we get

$$< a_{\alpha-\mathbf{k}'\downarrow} a_{\alpha\mathbf{k}'\uparrow} >= -\frac{1}{2}\Delta_{\alpha\mathbf{k}}\xi_{\alpha\mathbf{k}}, \tag{3.11}$$

$$\xi_{\alpha\mathbf{k}} = E^{-1}_{\alpha}(\mathbf{k})\ \mathrm{th}\left(\frac{E_{\alpha}(\mathbf{k})}{2k_BT}\right), \tag{3.12}$$

$$Z = \prod_{\alpha\mathbf{k}} \left\{ \exp(-D_{\alpha\mathbf{k}}/k_BT)[1+\exp(-E_{\alpha}(\mathbf{k})/k_BT)]^2 \right\}, \tag{3.13}$$

$$D_{\alpha\mathbf{k}} = \widetilde{\varepsilon}_{\alpha}(\mathbf{k}) - E_{\alpha}(\mathbf{k}) + \frac{1}{2}\Delta^2_{\alpha\mathbf{k}}\xi_{\alpha\mathbf{k}}. \tag{3.14}$$

Substituting the statistical average (3.11) into the expressions (3.3) for the gaps, we find self-consistence system of equations:

$$\Delta_{\alpha\mathbf{k}} = -\sum_{\alpha'\mathbf{k}'} W_{\alpha\alpha'}\Delta_{\alpha'\mathbf{k}'}\xi_{\alpha'\mathbf{k}'}. \tag{3.15}$$

Having in mind the s-wave nature the MgB_2 superconductivity, the intraband coupling constant $W_{\alpha\alpha} = V_{\alpha}+U_{\alpha}$ is supposed to contain a Coulomb part $U_{\alpha} > 0$ besides the electron-phonon attraction $V_{\alpha} \leq 0$ in Debye-layer defined by $\hbar\omega_D = 0.06$ eV [28],[147]. The repulsive interband coupling is characterized by the constant $W \geq 0$. Interactions U_{α} and W cover the energy interval from E_c to zero, which coincides with the top of the σ-band. The cut-off energy E_c is chosen to characterize the bands overlap region. In the nominally undoped hole conducting MgB_2 the chemical potential lies then at $\mu = -0.6$ eV. The effective σ- and π-bands will be characterized by constant densities of states.

With the interaction channels chosen the system of equations for the gaps (3.15) gets the following form

$$\Delta_\alpha = -(U_\alpha + V_\alpha)\rho_\alpha \Delta_\alpha \eta_\alpha^{(1)}(T, \Delta_\alpha) - U_\alpha \rho_\alpha \widetilde{\Delta}_\alpha \eta_\alpha^{(2)}(T, \widetilde{\Delta}_\alpha) - \\ -W\rho_{\alpha'}\Delta_{\alpha'}\eta_{\alpha'}^{(1)}(T, \Delta_{\alpha'}) - W\rho_{\alpha'}\widetilde{\Delta}_{\alpha'}\eta_{\alpha'}^{(2)}(T, \widetilde{\Delta}_{\alpha'}), \tag{3.16}$$

$$\widetilde{\Delta}_\alpha = -U_\alpha \rho_\alpha \Delta_\alpha \eta_\alpha^{(1)}(T, \Delta_\alpha) - U_\alpha \rho_\alpha \widetilde{\Delta}_\alpha \eta_\alpha^{(2)}(T, \widetilde{\Delta}_\alpha) - \\ -W\rho_{\alpha'}\Delta_{\alpha'}\eta_{\alpha'}^{(1)}(T, \Delta_{\alpha'}) - W\rho_{\alpha'}\widetilde{\Delta}_{\alpha'}\eta_{\alpha'}^{(2)}(T, \widetilde{\Delta}_{\alpha'}), \tag{3.17}$$

where $\alpha \neq \alpha'$, Δ_α are the gaps in the Debye-layer and $\widetilde{\Delta}_\alpha$ the gaps (order parameters) out of this layer,

$$\eta_\alpha^{(1)}(T, \Delta_\alpha) = \int_{-\hbar\omega_D}^{\hbar\omega_D} \xi_{\alpha\mathbf{k}}\, d\widetilde{\varepsilon}_\alpha \tag{3.18}$$

$$\eta_\alpha^{(2)}(T, \Delta_\alpha) = \int_{E_c-\mu}^{-\hbar\omega_D} \xi_{\alpha\mathbf{k}}\, d\widetilde{\varepsilon}_\alpha + \int_{\hbar\omega_D}^{-\mu} \xi_{\alpha\mathbf{k}}\, d\widetilde{\varepsilon}_\alpha. \tag{3.19}$$

In the case of interest when k_BT, $|\widetilde{\Delta}_\alpha| << \hbar\omega_D$, $E_c - \mu$, $-\mu$

$$\eta_\alpha^{(2)} \approx \ln\left(\frac{-\mu(\mu - E_c)}{(\hbar\omega_D)^2}\right) \equiv G. \tag{3.20}$$

From the equations (3.16) and (3.17) follows the relation

$$\widetilde{\Delta}_\alpha = \Delta_\alpha[1 + \rho_\alpha V_\alpha \eta_\alpha^{(1)}(T, \Delta_\alpha)], \tag{3.21}$$

i.e. the dependence of superconducting order parameters is taken approximately into account through the different values on momentum in the **k**-space windows near and far from the Fermi surface. The substitution of (3.21) into (3.16) leaves one with the system for Δ_α.

The parameter set of [148] will be used where $V_1 = -1.01$ eV, $U_1 = 1$ eV; $W = 0.53$ eV, $U_2 = V_2 = 0$ eV; the densities of states per one cell and spin $\rho_1 = 0.25$ eV^{-1}, $\rho_2 = 0.11$ eV^{-1}; $E_c = -2$ eV for the pure MgB_2.

3.2 Superconductivity transition temperature

The superconductivity transition temperature T_c is determined by the simultaneous vanishing of the gaps $\Delta_{1,2} \to 0$. In this limit the gap equations linearize with

$$\eta_\alpha^{(1)} \approx 2 \ln \left(\frac{1.13 \hbar \omega_D}{k_B T_c} \right) \equiv g \tag{3.22}$$

since $k_B T_c << \hbar \omega_D$. Now the system for Δ_α can be written as

$$\begin{aligned} \Delta_1 q_1 + \Delta_2 Q_2 = 0, \\ \Delta_1 Q_1 + \Delta_2 q_2 = 0, \end{aligned} \tag{3.23}$$

where

$$\begin{aligned} q_\alpha = a_\alpha g + b_\alpha, \\ Q_\alpha = A_\alpha g + B_\alpha, \end{aligned} \tag{3.24}$$

with

$$a_\alpha = \rho_\alpha (V_\alpha + U_\alpha + \rho_\alpha V_\alpha U_\alpha G), \qquad b_\alpha = 1 + \rho_\alpha U_\alpha G, \tag{3.25}$$

$$A_\alpha = \rho_\alpha W (1 + \rho_\alpha U_\alpha G), \qquad B_\alpha = \rho_\alpha W G. \tag{3.26}$$

The condition for existence of nontrivial solutions of (3.23) yields the equation

$$Q_1 Q_2 = q_1 q_2 \tag{3.27}$$

for transition temperature T_c. The solution of the latter gives

$$k_B T_c^{\pm} = 1.13 \hbar \omega_D \exp(\Lambda_\pm) \tag{3.28}$$

with

$$\Lambda_{\pm} = \frac{2P}{R \pm \sqrt{R^2 - 4SP}} \quad . \tag{3.29}$$

Here

$$P = b_1 b_2 - B_1 B_2, \qquad S = 4(a_1 a_2 - A_1 A_2),$$
$$R = 2(a_1 b_2 + a_2 b_1 - A_1 B_2 - A_2 B_1) \; . \tag{3.30}$$

One uses $T = T_c^-$ if

$$0 > \Lambda_- > \Lambda_+ \quad \text{or} \quad \Lambda_- < 0, \; \Lambda_+ > 0,$$

and $T = T_c^+$ if

$$0 > \Lambda_+ > \Lambda_- \quad \text{or} \quad \Lambda_+ < 0, \; \Lambda_- > 0.$$

In this work in case of parameters used $T_c = T_c^-$ for MgB_2.

3.3 The superconducting gaps

The superconductivity gaps for both bands in Debye-layer can be find with the help of (3.16), (3.21) and (3.20) from the system of equations ($\alpha \neq \alpha'$)

$$\Delta_\alpha = \rho_\alpha \Delta_\alpha \left\{ -(U_\alpha + V_\alpha)\eta_\alpha^{(1)}(T, \Delta_\alpha) - U_\alpha(1 + \rho_\alpha V_\alpha \eta_\alpha^{(1)}(T, \Delta_\alpha))\, G \right\} +$$
$$+ \rho_{\alpha'} \Delta_{\alpha'} \left\{ -W \eta_{\alpha'}^{(1)}(T, \Delta_{\alpha'}) - W(1 + \rho_{\alpha'} V_{\alpha'} \eta_{\alpha'}^{(1)}(T, \Delta_{\alpha'}))\, G \right\} . \tag{3.31}$$

These equations must be solved numerically and the temperature dependencies of the gaps $\Delta_\alpha = \Delta_\alpha(T)$ can be obtained.

At zero temperature ($T = 0$) one can find the analytical expression for the integral (3.18)

$$\eta_\alpha^{(1)}(0, \Delta_\alpha) = 2 \ln \left(\frac{2\hbar\omega_D}{|\Delta_\alpha(0)|} \right) . \tag{3.32}$$

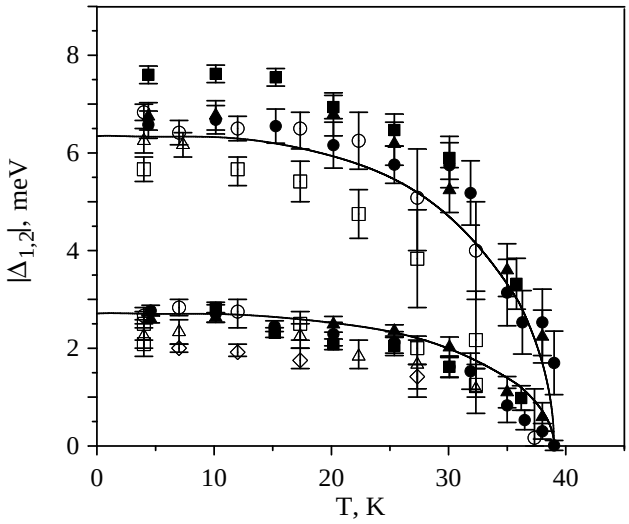

Figure 4: The calculated MgB_2 superconducting gaps vs. temperature. Solid line - theory. Filled and open symbols represent the experimental data [82],[149].

Here it is assumed, that $|\Delta_\alpha(0)| << \hbar\omega_D$. Then the system for the gaps $\Delta_\alpha(0)$ takes the form:

$$|\Delta_1(0)| = 2\hbar\omega_D \exp\left(\frac{\delta^{-1}(a_2 \ln\delta^2 + b_2) + B_1}{2(a_2\delta^{-1} + A_1)}\right),$$
$$|\Delta_2(0)| = 2\hbar\omega_D \exp\left(\frac{\delta^{-1}(a_1 \ln\delta^{-2} + b_1) + B_2}{2(a_1\delta + A_2)}\right), \qquad (3.33)$$

where $\delta = \Delta_1(0)/\Delta_2(0)$.

It has been shown that the stability of superconducting state is guaranteed if the phase difference between the gaps is properly fixed in accordance with the sign of the interband interaction constant [57]. The stable superconducting gaps are in-phase if the resulting interaction between the bands is attractive. On the other hand, the stable gaps exist in opposite phase if the net interaction between bands appears to be repulsive.

Having in mind the system of parameters chosen, follows from equations (3.33) that ratios $2|\Delta_1(0)|/k_BT_c = 3.8$ and $2|\Delta_2(0)|/k_BT_c = 1.6$ are close to the experimental findings [83],[82],[150], respectively 3.7 and 1.6 [150].

In the vincity of T_c one can find the solutions of (3.31) analytically. The functions $\eta_\alpha^{(1)}$ we expand into series of powers Δ_α and $\frac{T-T_c}{T_c}$ near $T = T_c$:

$$\rho_\alpha \eta_\alpha^{(1)} \approx \rho_\alpha g + \beta_\alpha \left(1 - \frac{T}{T_c}\right) + \nu_\alpha \Delta_\alpha^2 \tag{3.34}$$

with

$$\begin{aligned} \beta_\alpha &= 2\rho_\alpha \\ \nu_\alpha = \frac{7\rho_\alpha \zeta(3)}{4\pi^2 (k_B T_c)^2} &\approx \frac{2\rho_\alpha}{(3.06 k_B T_c)^2} \end{aligned} \tag{3.35}$$

and $\zeta(3) \approx 1.2$. Then for the system of gaps follows in agreement with [148]

$$|\Delta_{1,2}(T)| = 3.06 k_B T_c \Gamma_{1,2} \left(1 - \frac{T}{T_c}\right), \tag{3.36}$$

$$\Gamma_{1,2} = \left[\frac{Q_{2,1} q_{2,1} (Q_1 A_2 + Q_2 A_1 - q_1 a_2 - q_2 a_1)}{Q_1^2 q_1 A_2 + Q_2^2 q_2 A_1 - Q_1 q_1^2 a_2 - Q_2 q_2^2 a_1}\right]^{1/2}. \tag{3.37}$$

For the independent superconductivity transitions in the bands at $W = 0$, one has $\Gamma_{1,2} = 1$.

The temperature dependencies of the superconductivity gaps found from (3.31) for MgB_2 are shown in Fig.(4) and agree well with the measured ones [82],[149].

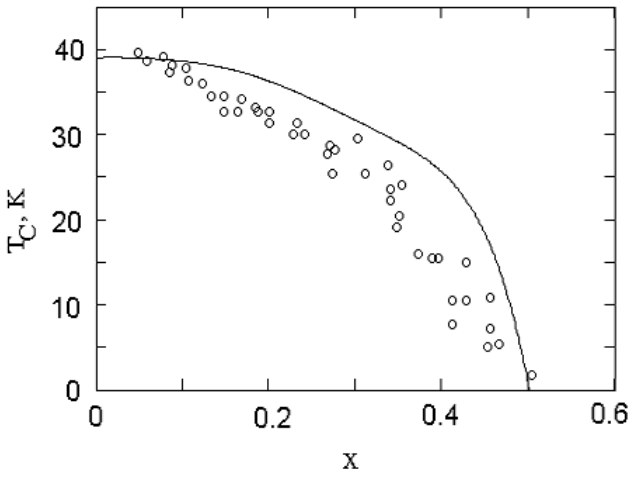

Figure 5: The influence of doping on transition temperature in $Mg_{1-x}Al_xB_2$. Solid line: theory. Points represent the experimental data of [64]

3.4 Influence of doping on transition temperature and superconducting gaps in $Mg_{1-x}Al_xB_2$

The Al substitution of Mg acts as an electron doping. Precise band-structure calculations on the effect of Al doping have been proposed [151] and these still need to be supported by experimental results. The progressive loss of superconductivity with increasing Al doping is discussed in literature in terms of the σ-band filling [72],[73], and the stiffening of the E_{2_g} mode, which decreases the electron-phonon coupling [64],[152].

The dependencies of the transition temperature and of the superconductivity gaps on the chemical potential positions are given by equations (3.28) and (3.31) containing the function G. By that in (3.28) on has to choose $T_c = T_c^-$.

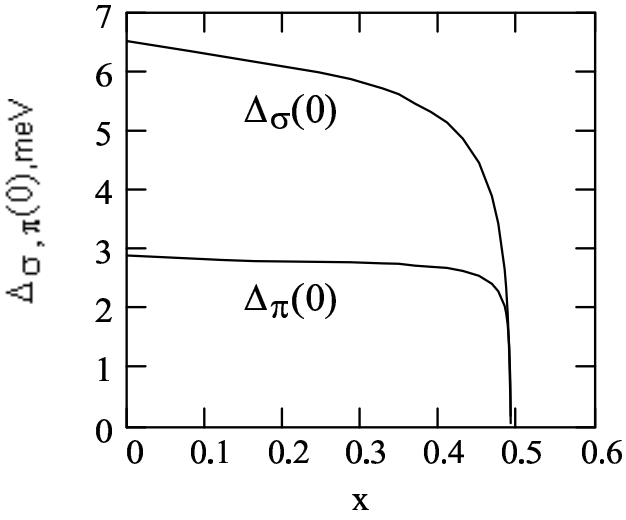

Figure 6: The σ- and π-band superconducting zero temperature gaps vs Al content in$Mg_{1-x}Al_xB_2$.

The calculated influence of electron-doping ($Mg_{1-x}Al_xB_2$) on the superconductivity transition of MgB_2 is illustrated in figures 5 and 6.

At this we take into account the changes of the band densities of states in the Debye layer near the Fermi level moving with doping by using the results of [28]. We replace the equations (3.25a) and (3.26a) into (3.28) and (3.31) with the following expressions

$$a_0 = \rho_\alpha^0(V_\alpha + U_\alpha + \rho_\alpha V_\alpha U_\alpha G), \tag{3.38}$$

$$A_\alpha = \rho_\alpha^0 W(1 + \rho_\alpha U_\alpha G), \tag{3.39}$$

where ρ_α^0 are the variable band densities of states at the Fermi level.

The linear relation between μ and x has been taken with $\mu = -0.6$ eV for $x = 0$ and $\mu = 0$ eV for $x = 0.5$

3.5 Free energy and thermodynamic critical magnetic field

The free energy is given by the expression

$$F = -k_B T \ln Z, \tag{3.40}$$

where Z is the partition function (3.5). Then the free energy of the system is

$$F = \sum_{\alpha\mathbf{k}} \left\{ \widetilde{\varepsilon}_\alpha(\mathbf{k}) - 2k_B T \ln \left(2 \operatorname{ch} \frac{E_\alpha(\mathbf{k})}{2k_B T} \right) + \frac{1}{2} \Delta^2_{\alpha\mathbf{k}} \xi_{\alpha\mathbf{k}} \right\}. \tag{3.41}$$

The free energy for the normal phase equals

$$F_n = \sum_{\alpha\mathbf{k}} \left\{ \widetilde{\varepsilon}_\alpha(\mathbf{k}) - 2k_B T \ln \left(2 \operatorname{ch} \frac{|\widetilde{\varepsilon}_\alpha(\mathbf{k})|}{2k_B T} \right) \right\}, \tag{3.42}$$

and the energy difference between the superconducting and normal phases of the system takes the form

$$\begin{aligned} F - F_n &= 2k_B T \sum_{\alpha\mathbf{k}} \ln \left(2 \operatorname{ch} \frac{|\widetilde{\varepsilon}_\alpha(\mathbf{k})|}{2k_B T} \right) - \\ &- 2k_B T \sum_{\alpha\mathbf{k}} \ln \left(2 \operatorname{ch} \frac{E_\alpha(\mathbf{k})}{2k_B T} \right) + \sum_{\alpha\mathbf{k}} \frac{1}{2} \Delta^2_{\alpha\mathbf{k}} \xi_{\alpha\mathbf{k}}. \end{aligned} \tag{3.43}$$

Now, having in mind assumptions for interaction channels in the present model, the expression (3.43) can be written as if $k_B T, |\Delta_\alpha| << \hbar\omega_D, E_c - \mu, -\mu$

$$F - F_n = \sum_\alpha \rho_\alpha \left(\zeta_\alpha(T,0) - \zeta_\alpha(T,\Delta_\alpha) + \frac{1}{2} \Delta^2_\alpha \eta^{(1)}_\alpha(T,\Delta_\alpha) \right), \tag{3.44}$$

where

$$\zeta_\alpha = 2k_B T \int_{-\hbar\omega_D}^{\hbar\omega_D} \ln \left(2 \operatorname{ch} \frac{E_\alpha(\mathbf{k})}{2k_B T} \right) d\widetilde{\varepsilon}_\alpha. \tag{3.45}$$

Therefore only the gaps Δ_α on the Fermi level enter the expression of the free energy in a good approximation.

In the limit $T \to T_c$ we can expand the free energy (3.44) into series of powers Δ_α. One finds

$$\rho_\alpha \zeta_\alpha(T, \Delta_\alpha) \approx \rho_\alpha \zeta_\alpha(T, 0) + \frac{1}{2}\rho_\alpha \Delta_\alpha^2 \eta_\alpha^{(1)}(T, \Delta_\alpha) + \frac{1}{4}\nu_\alpha \Delta_\alpha^4,$$

$$\rho_\alpha \eta_\alpha^{(1)}(T, \Delta_\alpha) \approx \rho_\alpha \eta_\alpha^{(1)}(T, 0) + \nu_\alpha \Delta_\alpha^2.$$

Respectively

$$F = F_n - \frac{1}{4}\sum_\alpha \nu_\alpha \Delta_\alpha^4. \tag{3.46}$$

Substituting here ν_α and Δ_α from equations (3.35) and (3.36), we obtain for the free energy expression in the vicinity of T_c

$$F = F_n - \frac{1}{2}\left(3.06 k_B T_c\right)^2 \left(1 - \frac{T}{T_c}\right)(\rho_1 \Gamma_1^4 + \rho_2 \Gamma_2^4). \tag{3.47}$$

The free energy at $T = 0$ K gives the ground-state energy E_g. Having in mind that $|\Delta(0)| << \hbar\omega_D$, we get by using (3.44)

$$E_g - E_{gn} = -\frac{1}{2}\sum_\alpha \rho_\alpha \Delta_\alpha^2(0), \tag{3.48}$$

where E_{gn} is the ground-state energy of the normal state ($\Delta_\alpha = 0$). For MgB_2 our calculation gives $E_g - E_{gn} \approx -540$ mJ/mol.

The thermodynamic critical magnetic field H_C is defined as

$$H_C = \sqrt{8\pi(F_n - F)}. \tag{3.49}$$

For the present moment it is clear that MgB_2 is of anisotropic nature [88]-[92] and in the next chapter we will give special attention to anisotropy. However we will find fitting for $H_{C2}(T)$ and compare the result with the experiment.

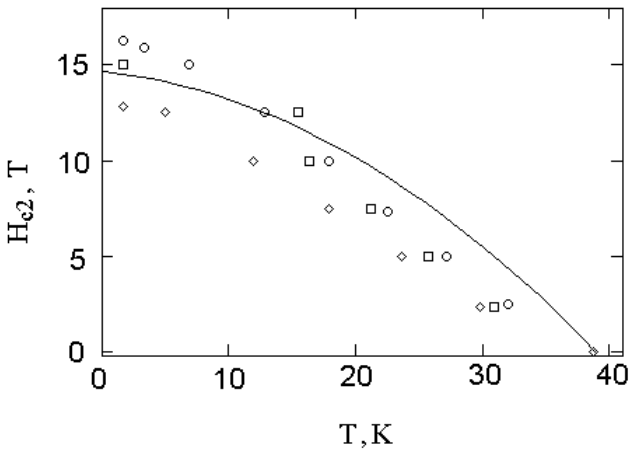

Figure 7: The critical magnetic field H_{C2} of the MgB_2 wire vs. temperature. Solid line: theory. Points represent the experimental data of [153].

Beginning from a certain value of the field one starts to register a finite induction in type II superconductor. This is called the lower critical field H_{C1}. With further increase of the external filed, the induction rises until the average field in the superconductor becomes equal to the external field and the superconductor goes into the normal state. This will happen at the upper critical field H_{C2}.

The MgB_2 is a type II superconductor, which has the large Ginzburg-Landau parameter κ (from experiments $\kappa = 26$ [154] and $\kappa = 38$ [155]). In our calculation we have supposed that Ginzburg-Landau parameter in [155]) answers to the case, where the anisotropy is smeared out by powder nature of MgB_2. Thus we can calculate the upper critical field $H_{C2}(T)$ by using the expression $H_{C2} = \kappa\sqrt{2}H_C$.

In Figure 7, the theoretical dependence of the upper critical magnetic field

H_{C2} on temperature describes the experimental data of [153] satisfactorily. We have used here the Ginzburg-Landau parameter $\kappa = 38$ [155].

3.6 Entropy and heat capacity

We proceed the examination of thermodynamic properties of MgB_2 and next calculate the entropy

$$S = -\frac{\partial F}{\partial T} \tag{3.50}$$

of a two-band superconductor. One can find with the help of the system (3.31) for the free energy (3.41) the form

$$F = \sum_{\alpha\mathbf{k}} \left\{ \widetilde{\varepsilon}_\alpha(\mathbf{k}) - 2k_B T \ln\left(2\ \mathrm{ch}\frac{E_\alpha(\mathbf{k})}{2k_B T}\right)\right\} + \\ + \sum_{\alpha\mathbf{k}} \Delta^2_{\alpha\mathbf{k}}\xi_{\alpha\mathbf{k}} + \frac{1}{2}\sum_{\alpha\mathbf{k}}\sum_{\alpha'\mathbf{k}'} W_{\alpha\alpha'}(\mathbf{k},\mathbf{k}')\Delta_{\alpha\mathbf{k}}\xi_{\alpha\mathbf{k}}\Delta_{\alpha'\mathbf{k}'}\xi_{\alpha'\mathbf{k}'}. \tag{3.51}$$

The derivative of the free energy can be expressed as

$$\frac{\partial F}{\partial T} = \left(\frac{\partial F}{\partial T}\right)_\Delta + \sum_{\alpha\mathbf{k}} \left(\frac{\partial F}{\partial \Delta_{\alpha\mathbf{k}}}\right)_T \frac{\partial \Delta_{\alpha\mathbf{k}}}{\partial T}. \tag{3.52}$$

From (3.31) it follows that

$$\left(\frac{\partial F}{\partial \Delta_{\alpha\mathbf{k}}}\right)_T = 0 \tag{3.53}$$

and then

$$\frac{\partial F}{\partial T} = \left(\frac{\partial F}{\partial T}\right)_\Delta. \tag{3.54}$$

Now, on the basis of equations (3.50), (3.51), (3.53) and (3.54) we get the entropy

$$S = \sum_{\alpha\mathbf{k}} \left(2k_B \ln\left(2\mathrm{ch}\frac{E_\alpha(\mathbf{k})}{2k_B T}\right) - \frac{E_\alpha(\mathbf{k})}{T}\mathrm{th}\frac{E_\alpha(\mathbf{k})}{2k_B T}\right). \tag{3.55}$$

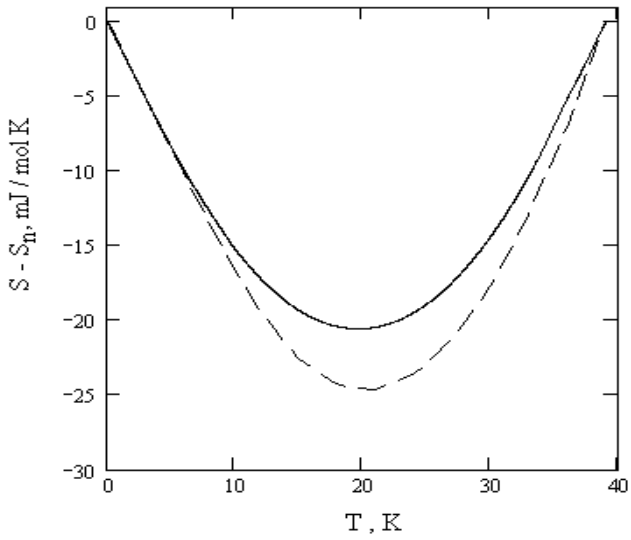

Figure 8: The MgB_2 entropy vs temperature. Dotted line: the case of a single band.

One can find the entropy for the normal state from equation (3.55), by taking $\Delta_{\alpha\mathbf{k}} = 0$:

$$S = \sum_{\alpha\mathbf{k}} \left(2k_B \ln\left(2\mathrm{ch}\frac{\widetilde{\varepsilon}_\alpha(\mathbf{k})}{2k_BT} \right) - \frac{\widetilde{\varepsilon}_\alpha(\mathbf{k})}{T}\mathrm{th}\frac{\widetilde{\varepsilon}_\alpha(\mathbf{k})}{2k_BT} \right). \tag{3.56}$$

In the case of a degenerate electron gas the equation (3.56) gives

$$S_n = \gamma_s T, \tag{3.57}$$

where

$$\gamma_s = \frac{2\pi^2 k_B^2}{3}(\rho_1 + \rho_2)$$

is the Sommerfeld constant. For MgB_2 we get with the band densities of states used $\gamma_s = 1.7$ mJ/mol K^2. The heat capacity will be calculated using thermodynamic relation

$$C = T\frac{\partial S}{\partial T} = -T\frac{\partial^2 F}{\partial T^2}. \tag{3.58}$$

In the normal state we have

$$C_n = \gamma_s T. \tag{3.59}$$

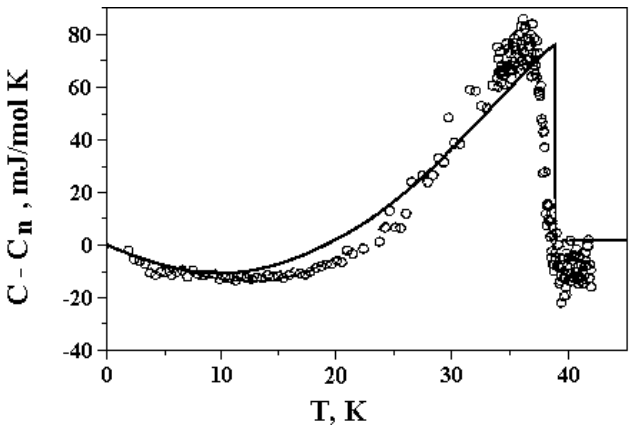

Figure 9: The MgB_2 specific heat vs temperature. Solid line: theory. Points represent the experimental data of [156].

The jump of heat capacity at the superconductivity transition point equals

$$\Delta C = T_c(3.06k_B)^2(\rho_1\Gamma_1^4 + \rho_2\Gamma_2^4). \tag{3.60}$$

With the help of the system for gaps (3.16) and the relation (3.21) we obtain the dependence of the entropy difference $S - S_n$ on temperature, as is seen in Figure 8.

The dotted line corresponds to the limiting case of a single band ($W = 0,\ \rho = \rho_1 + \rho_2$). At this the parameters $U_1,\ V_1$ have been chosen so $T_c = 39$ K that in this special case.

Now we use these calculated values of entropy to find the theoretical curve of the specific heat vs. temperature. In Figure 9 this dependence is compared with the experimental result of paper [156]. The agreement is good.

4 Free energy functional and critical magnetic fields anisotropy in MgB_2

4.1 Hamiltonian and transformations

We start from the two-band Hamiltonian which allows the pairing fluctuations

$$H = H_0 + H_{int}, \tag{4.1}$$

$$H_0 = \sum_{l,\mathbf{k}} \widetilde{\epsilon}_l(\mathbf{k})[a^+_{l\mathbf{k}\uparrow} a_{l\mathbf{k}\uparrow} + a^+_{l-\mathbf{k}\downarrow} a_{l-\mathbf{k}\downarrow}], \tag{4.2}$$

$$H_{int} = \sum_{l,l'} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{q}} 2W_{ll'}(\mathbf{k}, -\mathbf{k}+\mathbf{q}, -\mathbf{k}'+\mathbf{q}, \mathbf{k}') a^+_{l\mathbf{k}\uparrow} a^+_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l'-\mathbf{k}'+\mathbf{q}\downarrow} a_{l'\mathbf{k}'\uparrow}. \tag{4.3}$$

Here $\widetilde{\epsilon}_l(\mathbf{k}) = \epsilon_l(\mathbf{k}) - \mu$, μ is the chemical potential and $\epsilon_l(\mathbf{k})$ stands for the energy of an electron in the band counted by $l = 1, 2$ which correspond to the effective σ and π bands of MgB_2, s is the spin index. $W_{ll'}$ are the pair-transfer interaction constants which describe the corresponding intra- ($l = l'$) and interband ($l \neq l'$) scattering processes. The nonzero electron pair total momentum $\mathbf{q}$ has been introduced in the order parameters for treating spatial inhomogeneity effects.

Further we will consider a superconducting phase transition in the mean field approximation and represent H as follows:

$$H = H_1 + H_2, \tag{4.4}$$

$$H_1 = H_0 + H_\delta, \tag{4.5}$$

$$H_2 = -H_\delta + H_{int}, \tag{4.6}$$

with

$$H_\delta = \sum_l \sum_{\mathbf{k}} \sum_{\mathbf{q}} a^+_{l\mathbf{k}\uparrow} a^+_{l-\mathbf{k}+\mathbf{q}\downarrow} \delta_{l\mathbf{kq}} + a_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l\mathbf{k}\uparrow} \delta^*_{l\mathbf{kq}}. \tag{4.7}$$

where $\delta_{l\mathbf{kq}}$ are the non-equilibrium order parameters. Bogoljubov theorem [157], [158] allows us to determine the model free energy as

$$F = -k_B T \ln Z(H_1) + < H_2 >_{H_1}, \tag{4.8}$$

where the partition function

$$Z(H_1) = \mathtt{Sp} \exp\left(\frac{-H_1}{k_B T}\right), \tag{4.9}$$

and the statistical average of H_2 reads

$$< H_2 >_{H_1} = Z^{-1} \mathtt{Sp}\left[H_2 \exp\left(\frac{-H_1}{k_B T}\right)\right]. \tag{4.10}$$

Next we will derive the free energy functional as an expansion in powers of order parameters $\delta_{l\mathbf{kq}}$ near the phase transition temperature:

$$F \approx F_0 + F_2 + F_4, \tag{4.11}$$

where $F_0 = -k_B T \ln Z(H_0)$, $F_2 \sim \delta^2_{l\mathbf{kq}}$, $F_4 \sim \delta^4_{l\mathbf{kq}}$. We make now an Ansatz that free energy (4.11) will be exploited in long-wave approximation i.e. in the vicinity of $\mathbf{q} = 0$. This allows one to consider the $\mathbf{q}$-dependence in F_2 taking $\mathbf{q} = 0$ in the higher order terms. To calculate F_2 we make use of an unitary transformation for our hamiltonian H_1:

$$\widetilde{H}_1 = U^{-1} H_1 U,\ U = \exp(iS); \tag{4.12}$$

$$\begin{aligned}\widetilde{H}_1 &= \exp(-iS)(H_0+H_\delta)\exp(iS) = \\ &= H_0+H_\delta+i[H_0,S]+i[H_\delta,S]+ \\ &+ \frac{i^2}{2}[[H_0,S],S]+\frac{i^2}{2}[[H_\delta,S],S]+\ldots,\end{aligned} \tag{4.13}$$

where we demand S to be such that all terms being linear in δ in the expansion (4.13) vanish. For S, chosen to be linear in δ, the following expression in the second-order approximation must hold

$$H_\delta + i[H_0,S] = 0. \tag{4.14}$$

The last condition can be satisfied if

$$S = \sum_{l,\mathbf{k},\mathbf{q}} \vartheta_l(\mathbf{k},\mathbf{k}-\mathbf{q}) a^+_{l\mathbf{k}\uparrow} a^+_{l-\mathbf{k}+\mathbf{q}\downarrow}\delta_{l\mathbf{k}\mathbf{q}} + a_{l-\mathbf{k}+\mathbf{q}\downarrow}a_{l\mathbf{k}\uparrow}\delta^*_{l\mathbf{k}\mathbf{q}}\vartheta^*_l(\mathbf{k},\mathbf{k}-\mathbf{q}), \tag{4.15}$$

$$\vartheta_l(\mathbf{k},\mathbf{k}-\mathbf{q}) = \frac{i}{\widetilde{\epsilon}_l(\mathbf{k})-\widetilde{\epsilon}_l(\mathbf{k}-\mathbf{q})}. \tag{4.16}$$

Then for $\widetilde{H}_1$ we get in the second order approximation

$$\widetilde{H}_1 \approx H_0 + \frac{i}{2}[H_\delta, S]. \tag{4.17}$$

For an arbitrary unitary operator $U = \exp(iS)$ the equality

$$Z(H_1) = Z(U^{-1}H_1U) \tag{4.18}$$

holds and, therefore, in accordance with (4.17) we have

$$Z(\widetilde{H}_1) \approx Z(H_0 + \frac{i}{2}[H_\delta, S]). \tag{4.19}$$

The commutator in equation (4.19) equals to

$$\begin{aligned}
[H_\delta, S] &= \sum_{l,\mathbf{k},\mathbf{q}} \{|\delta_{l\mathbf{kq}}|^2(\vartheta_l(\mathbf{k},\mathbf{k}-\mathbf{q}) - \vartheta_l^*(\mathbf{k},\mathbf{k}-\mathbf{q})) + \\
&+ \sum_{\mathbf{q}'} a^+_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l-\mathbf{k}+\mathbf{q}'\downarrow} \delta^*_{l\mathbf{kq}'} \delta_{l\mathbf{kq}} \vartheta_l^*(\mathbf{k},\mathbf{k}-\mathbf{q}') - \\
&- a^+_{l-\mathbf{k}+\mathbf{q}'\downarrow} a_{l-\mathbf{k}+\mathbf{q}\downarrow} \delta^*_{l\mathbf{kq}} \delta_{l\mathbf{kq}'} \vartheta_l(\mathbf{k},\mathbf{k}-\mathbf{q}') + \\
&+ \sum_{\mathbf{q}'} a^+_{l\mathbf{k}\uparrow} a_{l\mathbf{k}+\mathbf{q}'-\mathbf{q}\uparrow} \delta^*_{l\mathbf{kq}'} \delta_{l\mathbf{kq}} \vartheta_l^*(\mathbf{k}+\mathbf{q}'-\mathbf{q},\mathbf{k}-\mathbf{q}) - \\
&- a^+_{l\mathbf{k}+\mathbf{q}'-\mathbf{q}\uparrow} a_{l\mathbf{k}\uparrow} \delta^*_{l\mathbf{kq}} \delta_{l\mathbf{kq}'} \vartheta_l(\mathbf{k}+\mathbf{q}'-\mathbf{q},\mathbf{k}-\mathbf{q})\}. \qquad (4.20)
\end{aligned}$$

In the representation of occupation numbers we diagonalize (4.20) using the random phase approximation taking $\mathbf{q}' = \mathbf{q}$. Now, by expanding the partition function (4.19) into series of powers of order parameters up to the terms proportional $\delta^2_{l\mathbf{kq}}$ we get with the help of (4.20), (4.19) and (4.16) that

$$Z(\widetilde{H}_1) = Z(H_0)\left[1 + \frac{1}{k_B T}\sum_{l,\mathbf{k},\mathbf{q}} |\delta_{l\mathbf{kq}}|^2 \eta_{l\mathbf{kq}}\right], \qquad (4.21)$$

where

$$\eta_{l\mathbf{kq}} = \frac{1}{\widetilde{\epsilon}_l(\mathbf{k}) - \widetilde{\epsilon}_l(\mathbf{k}-\mathbf{q})}\left(\mathrm{th}\left(\frac{\widetilde{\epsilon}_l(\mathbf{k})}{2k_B T}\right) + \mathrm{th}\left(\frac{\widetilde{\epsilon}_l(\mathbf{k}-\mathbf{q})}{2k_B T}\right)\right). \qquad (4.22)$$

Further we need the average

$$\begin{aligned}
< H_2 >_{H_1} &= -\sum_{l,\mathbf{k},\mathbf{q}} < a^+_{l\mathbf{k}\uparrow} a^+_{l-\mathbf{k}+\mathbf{q}\downarrow} >_{H_1} \delta_{l\mathbf{kq}} + < a_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l\mathbf{k}\uparrow} >_{H_1} \delta^*_{l\mathbf{kq}} + \\
&+ \sum_{l,l'} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{q}} 2W_{ll'}(\mathbf{k}, -\mathbf{k}+\mathbf{q}, -\mathbf{k}'+\mathbf{q}, \mathbf{k}') \times \\
&\times < a^+_{l\mathbf{k}\uparrow} a^+_{l-\mathbf{k}+\mathbf{q}\downarrow} >_{H_1} < a_{l'-\mathbf{k}'+\mathbf{q}\downarrow} a_{l'\mathbf{k}'\uparrow} >_{H_1} . \qquad (4.23)
\end{aligned}$$

By means of the unitary transformation (4.15) one can find that for a dynamic operator A the following equality holds

$< A >_{H_1} = < \widetilde{A} >_{\widetilde{H}_1} \approx < A >_{\widetilde{H}_1} + < \mathrm{i}[A, S] >_{\widetilde{H}_1}$. Therefore

$$< a_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l\mathbf{k}\uparrow} >_{H_1} \approx < a_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l\mathbf{k}\uparrow} >_{\widetilde{H}_1} + \mathrm{i} < [a_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l\mathbf{k}\uparrow}, S] >_{\widetilde{H}_1} . \quad (4.24)$$

By retaining only the contribution proportional to $\delta_{l\mathbf{kq}}$ on the right side of (4.24) we obtain

$$< a_{l-\mathbf{k}+\mathbf{q}\downarrow} a_{l\mathbf{k}\uparrow} >_{H_1} \approx -\frac{\delta_{l\mathbf{kq}}}{\widetilde{\epsilon}_l(\mathbf{k}) - \widetilde{\epsilon}_l(\mathbf{k}-\mathbf{q})} \left(\mathrm{th}\left(\frac{\widetilde{\epsilon}_l(\mathbf{k})}{2k_B T} \right) + \mathrm{th}\left(\frac{\widetilde{\epsilon}_l(\mathbf{k}-\mathbf{q})}{2k_B T} \right) \right) \quad (4.25)$$

Thus, collecting together the expressions (4.21), (4.23) and (4.25) we have found the second-order contribution into the mean-field free energy (4.11) in for the space-inhomogeneous case

$$F_2 = \sum_{l,\mathbf{k},\mathbf{q}} \left[\frac{1}{2} \eta_{l\mathbf{kq}} |\delta_{l\mathbf{kq}}|^2 + \frac{1}{2} \eta_{l\mathbf{kq}} \delta^*_{l\mathbf{kq}} \sum_{l'\mathbf{k}'} W_{ll'}(\mathbf{k}, \mathbf{k}') \eta_{l'\mathbf{k}'\mathbf{q}} \delta_{l'\mathbf{k}'\mathbf{q}} \right]. \quad (4.26)$$

4.2 Free energy expansion coefficients

In order to continue with the analytical approach we expand the quantities $\eta_{l\mathbf{kq}}$ into series of powers of $T - T_c$ and $\mathbf{q}$ near $(T - T_c)/T_c$ and $\mathbf{q} = 0$ correspondingly and limit us with linear terms only.

$$\eta_{l\mathbf{kq}}(T) \approx \eta_{l\mathbf{k}0}(T_c) - \alpha_{l\mathbf{kq}}, \quad (4.27)$$

$$\alpha_{l\mathbf{kq}} = C_{l\mathbf{k}} \theta + \sum_{ij} D_{l\mathbf{k}ij} q_i q_j, \quad (4.28)$$

with $\theta = (T - T_c)/T_c$,

$$C_{l\mathbf{k}} = -T_c \left[\frac{\partial \eta_{l\mathbf{k}0}(T)}{\partial T} \right]_{T=T_c}, \quad (4.29)$$

$$D_{l\mathbf{k}ij} = -\frac{1}{2} \left[\frac{\partial^2 \eta_{l\mathbf{kq}}}{\partial q_i \partial q_j} \right]_{\mathbf{q}=0}. \quad (4.30)$$

For the actual spectrum it is assumed that

$$\widetilde{\epsilon}_l(\mathbf{k}) = E_{0l} \pm \sum_{i=1}^{d_l} \frac{\hbar^2 k_i^2}{2m_{li}} - \mu \ , \tag{4.31}$$

where d_l is the dimension of the corresponding band, the sign + corresponds to an electron band and the sign − to a hole band. m_{li} are the bare masses of carriers and $E_{0l} - \mu$ determines the Fermi energy. The summation over $\mathbf{k}$ is implemented analogously as an integration in subsection 3.1 . The results of integration in $\mathbf{k}$-space are summarized in the table 1.

the summation over $\mathbf{k}$	the corresponding result of integration
$\sum_{\mathbf{k}} \eta_{l\mathbf{k}0}(T_c)$ in Debye-layer	$\rho_l g$, $g = 2\ln\left(\frac{1.13\hbar\omega_D}{k_B T_c}\right)$
$\sum_{\mathbf{k}} \eta_{l\mathbf{k}0}(T_c)$ out of Debye-layer	$\rho_l G$, $G = \ln\left(\frac{-\mu(\mu - E_c)}{(\hbar\omega_D)^2}\right)$
$\sum_{\mathbf{k}} C_{l\mathbf{k}}$	$2\rho_l$
$\sum_{\mathbf{k}} \sum_{i,j} D_{l\mathbf{kij}} q_i q_j$	$\rho_l \sum_{i=1}^{d_l} \beta_{li} q_i^2$, $\beta_{li} = \frac{14\zeta(3)\hbar^2 < v_{Fli}^2 >}{(4\pi k_B T_c)^2}$

Table 1: The results of integration

In the Table 1 the squared average Fermi velocities $< v_{Fli}^2 >$ are introduced, as

$$< v_{Fli}^2 > = \frac{2|E_{0l} - \mu|}{d_l m_{li}} \ . \tag{4.32}$$

Now, on the basis of Table 1 and equations (4.26), (4.27-4.30) the contribu-

tion F_2 takes the form

$$\begin{aligned} F_2 &= \frac{1}{2}\sum_{l\mathbf{q}} \rho_l R_{l\mathbf{q}}\{|\delta_{l\mathbf{q}}|^2(1+(U_l+V_l)\rho_l R_{l\mathbf{q}}) + \rho_l G U_l(\delta^*_{l\mathbf{q}}\widetilde{\delta}_{l\mathbf{q}} + \\ &+ \delta_{l\mathbf{q}}\widetilde{\delta}^*_{l\mathbf{q}})\} + \frac{1}{2}\sum_{l\mathbf{q}}[\rho_l G|\widetilde{\delta}_{l\mathbf{q}}|^2(1+\rho_l G U_l)] + \\ &+ \frac{1}{2}\sum_{\mathbf{q}}\sum_{l\neq l'} W\{\delta_{l'\mathbf{q}}\delta^*_{l\mathbf{q}}\rho_l g(1-2\rho_{l'}g+\rho_{l'}R_{l\mathbf{q}}+\rho_{l'}R_{l'\mathbf{q}}) + \\ &+ \rho_l\rho_{l'}G(\delta^*_{l\mathbf{q}}\widetilde{\delta}_{l'\mathbf{q}}R_{l\mathbf{q}} + \delta_{l'\mathbf{q}}\widetilde{\delta}^*_{l\mathbf{q}}R_{l'\mathbf{q}} + \widetilde{\delta}_{l'\mathbf{q}}\widetilde{\delta}^*_{l\mathbf{q}}G)\} \end{aligned} \tag{4.33}$$

with

$$R_{l\mathbf{q}} = g - 2\theta - \sum_i \beta_{li} q_i^2. \tag{4.34}$$

4.3 Coherence lengths and critical fields

In this subsection we consider the coherence lengths of order parameters fluctuations in a two-band superconductivity model. In the normal phase the fluctuations of superconductivity order parameters $\delta(\delta_{l\mathbf{q}}) = \delta_{l\mathbf{q}}$ and in the Gaussian approximation $\delta F_2 = F_2$. By introducing the following Fourier transforms

$$\begin{aligned} \delta_{l\mathbf{q}} &= \frac{1}{V}\int \delta_l(\mathbf{r})\exp(-i\mathbf{q}\mathbf{r})d\mathbf{r}, \\ \delta_l(\mathbf{r}) &= \sum_{\mathbf{q}} \delta_{l\mathbf{q}}\exp(i\mathbf{q}\mathbf{r}), \end{aligned} \tag{4.35}$$

and keeping in mind that

$$\begin{aligned} V^{-1}\ \sum_{\mathbf{q}}\exp[-i\mathbf{q}(\mathbf{r}-\mathbf{r}')] &= \delta(\mathbf{r}-\mathbf{r}'), \\ \int \exp[-i\mathbf{r}(\mathbf{q}-\mathbf{q}')]d\mathbf{r} &= \delta(\mathbf{q}-\mathbf{q}'), \end{aligned}$$

the following relations can be obtained:

$$\begin{aligned}\sum_{\mathbf{q}} \delta_{l\mathbf{q}}\delta^*_{l'\mathbf{q}} &= V^{-1}\int \delta_l(\mathbf{r})\,\delta^*_{l'}(\mathbf{r})\,d\mathbf{r},\\ \sum_{\mathbf{q}}(\hbar^2\delta_{l\mathbf{q}}\delta^*_{l'\mathbf{q}}\sum_i q_i^2) &= V^{-1}\int \delta^*_{l'}(\mathbf{r})(-i\hbar\sum_i\nabla_i)^2\,\delta_l(\mathbf{r})\,d\mathbf{r}. \quad (4.36)\end{aligned}$$

Substituting the equations (4.36) into the part F_2 of the free energy (4.33) and minimizing the functional, we obtain the linearized equations of gaps $\Delta_{1,2}$ on the Fermi level, in the coordinate representation

$$\begin{aligned}&\left[q_1 - a_1(2\theta - \sum_i \beta_{li}\nabla_i^2)\right]\Delta_1 + \left[Q_2 - A_2(2\theta - \sum_i \beta_{li}\nabla_i^2)\right]\Delta_2 = 0,\\ &\left[Q_1 - A_1(2\theta - \sum_i \beta_{li}\nabla_i^2)\right]\Delta_1 + \left[q_2 - a_2(2\theta - \sum_i \beta_{li}\nabla_i^2)\right]\Delta_2 = 0. \quad (4.37)\end{aligned}$$

The transition temperature T_c is determined by the condition (3.27) which is required for the existence of the nontrivial solutions of the system (4.37) in the homogeneous case if $T \to T_c$.

An orthogonal transformation to new variables Δ_-(soft) and Δ_+(rigid)

$$\begin{aligned}\Delta_1 &= \Delta_-\cos\phi + \Delta_+\sin\phi,\\ \Delta_2 &= -\Delta_-\sin\phi + \Delta_+\cos\phi; \quad (4.38)\end{aligned}$$

with

$$\tan\phi_\pm = \frac{1}{2q_1q_2}\left[v_0 \pm s_0 + \frac{s_0 \pm v_0}{2s_0Q_1Q_2}\left(2(c_1+c_2)\theta + \sum_i (c_1\beta_{1i} + c_2\beta_{2i})q_i^2\right)\right], \quad (4.39)$$

$$\begin{aligned}v_0 &= Q_2q_2 - Q_1q_1,\\ s_0 &= Q_2q_2 + Q_1q_1,\\ c_1 &= Q_2A_1(s_0+v_0) + q_2a_1(s_0-v_0), \quad (4.40)\\ c_2 &= Q_1A_2(s_0-v_0) + q_1a_2(s_0+v_0)\end{aligned}$$

splits the system(4.37) into independent equations

$$\{2(Q_2A_1 + Q_1A_2 + q_2a_1 + q_1a_2)\theta\}\Delta_- - \\ -\sum_i\{(Q_1A_2 + q_1a_2)\beta_{1i} + (Q_2A_1 + q_2a_1)\beta_{2i}\}\nabla_i^2\Delta_- = 0, \tag{4.41}$$

$$\{(q_1 + q_2)^2 - 2(Q_2A_1 + Q_1A_2 + q_2a_2 + q_1a_1)\theta\}\Delta_+ - \\ -\sum_i\{(Q_2A_1 + q_1a_1)\beta_{1i} + (Q_1A_2 + q_2a_2)\beta_{2i}\}\nabla_i^2\Delta_+ = 0. \tag{4.42}$$

Consequently, the squared coherence lengths, associated with Δ_- and Δ_+, are given by

$$\begin{aligned} \xi_i^2 \equiv \xi_{-i}^2 &= \frac{(Q_1A_2 + q_1a_2)\beta_{1i} + (Q_2A_1 + q_2a_1)\beta_{2i}}{2(Q_2A_1 + Q_1A_2 + q_2a_1 + q_1a_2)|\theta|}, \\ \xi_{+i}^2 &= \frac{(Q_2A_1 + q_1a_1)\beta_{1i} + (Q_1A_2 + q_2a_2)\beta_{2i}}{(q_1 + q_2)^2 - 2(Q_2A_1 + Q_1A_2 + q_2a_2 + q_1a_1)\theta}\ . \end{aligned} \tag{4.43}$$

As a results the fluctuations of band order parameters are governed by two coherence lengths: ξ_- acts as Ginzburg-Landau type critical (soft) coherence length in one-band systems diverging at $T \to T_c$. The other length, ξ_+, behaves noncritically (rigidly). Being an imaginary quantity,it can be probably interpreted as a characteristic of spatial periodic coherence wave. The presence of two correlation lengths is typical for two band superconductors with two superfluids of carriers.

For the critical fields we have

$$H_{c2}^i = \frac{\Phi_0}{2\pi\xi_{i'}\xi_{i''}}\ , \tag{4.44}$$

$$H_{c1}^i = \frac{H_c \ln\kappa_i}{\sqrt{2}\kappa_i}, \tag{4.45}$$

where $i \neq i' \neq i''$ and Φ_0 is the quantum of magnetic flux. The thermodynamic critical field (3.49), $H_c = \sqrt{8\pi(F_n - F_s)}$, is determined through the

equilibrium free energies in the normal state F_n and in the superconducting state F_s. On the basis of (3.47),(3.49) , we obtain near T_c

$$H_c = 8\pi k_B T_c \left[\frac{\pi}{14\zeta(3)}\left(\rho_1\Gamma_1^4 + \rho_2\Gamma_2^4\right)\right]^{1/2} |\theta|. \tag{4.46}$$

Correspondingly, the Maki parameters

$$\kappa_i = \frac{H_{C2}^i}{\sqrt{2}H_C} \tag{4.47}$$

are independent of temperature near T_c.

The gradient expansions in the Ginzburg-Landau scheme developed are justified if the coherence lengths $\xi_i(T)$ and the scaling factors

$$\xi_{li} = \left(\frac{\beta_{li}}{2}\right)^{1/2} \tag{4.48}$$

satisfy the condition [159]

$$\xi_i(T) > \xi_{li} \ . \tag{4.49}$$

In what follows we use the notations $\xi_{ab} = \xi_x = \xi_y$ and $\xi_c = \xi_z$, and analogously also for other quantities.

In the case of MgB_2, according to [159],[160], a very strong restriction appear for the the applicability of the Ginzburg-Landau approach in connection with the lengths ξ_c and $\xi_{\pi c}$. One of the reasons of such a peculiarity lies in the strong anisotropy of the Fermi surface of the σ-band in this system which reduces $\xi_{\sigma c}$ and leads by that to the decrease of ξ_c. By using average Fermi velocities from [50] and our set of the parameters , we find $\xi_c = 8/|\theta|^{1/2}$ and $\xi_{\pi c} = 28$ nm. For these values the inequality (4.49) yields the limiting condition

$$|\theta| < 0.08 \tag{4.50}$$

which is somewhat weaker compared to the estimations of [159],[160]. In this narrow region near T_c we can apply Ginzburg-Landau scheme and calculate by means of (4.43) the anisotropies of the critical fields of MgB_2. Here the coefficients of anisotropy do not depend on temperature and are given by

$$\gamma_{H_{C2}} = \frac{H_{C2}^{ab}}{H_{C2}^{c}} = \left[\frac{(Q_1 A_2 + q_1 a_2)\beta_{1ab} + (Q_2 A_1 + q_2 a_1)\beta_{2ab}}{(Q_1 A_2 + q_1 a_2)\beta_{1c} + (Q_2 A_1 + q_2 a_1)\beta_{2c}} \right]^{1/2}, \tag{4.51}$$

$$\gamma_{H_{C1}} = \frac{H_{C1}^{c}}{H_{C1}^{ab}} = \gamma_{H_{C2}} \frac{\ln\ \kappa_c}{\ln\ \kappa_{ab}}\ . \tag{4.52}$$

For the higher critical field we obtain the value

$$\gamma(T_c)_{H_{C2}} = 2.46 \tag{4.53}$$

which is comparable with the experimental data $\gamma(T_c)_{H_{C2}} \approx 2$ [161],[162], 2.2 [163], 2.3...2.7 [90], and 1.5 ± 0.5 [164]. Our calculated lower critical field anisotropy,

$$\gamma(T_c)_{H_{C1}} = 1.94, \tag{4.54}$$

is close to the experimental findings $\gamma(T_c)_{H_{C1}} \approx 2$ of [162],[165]. The agreement with the observations is checked as satisfactory.

Summary

The present thesis are devoted to the theoretical elaboration of magnesium diboride (MgB_2) superconductivity mechanism. In accordance with wide flow of analogous investigations MgB_2 has been contemporary (see also [166]) explained as a typical two-band (multiband) superconductor. This result is essential for the theory of multiband superconductivity, and a new trend of "multiband superconductivity in novel systems" (carbon nanotubes, graphite intercalate compounds etc.) has been recently opened. Possibly also the recent approaches to high-T_c cuprates can be included here.

Our model with two effective bands incorporates the following pairing channels: the σ-intraband effective electron-phonon attraction, the σ-intraband Coulomb repulsion, and the $\sigma - \pi$ interband repulsion. The presence of the latter turns both superconducting gaps simultaneously to zero at the transition temperature, which was controlled for MgB_2 in a special experiment.

A multichannel theoretical approach corresponding to the accepted prepositions mentioned has been elaborated and general expressions for the basic superconducting characteristics of MgB_2 have been developed.

We have used a plausible parameter set to obtain quantitative results for the MgB_2 basic superconducting characteristics, including the transition temperature and the superconductivity gaps together with doping dependence of them. The pure MgB_2 appears as being effectively "self-doped". Satisfactory agreement with the diverse experimental data has been found. The free energy and other thermodynamic quantities of the system have been calculated .

The fluctuation phenomena connected with the superconducting order have

been treated using the mean-field free energy derived for the Cooper pairs of nonzero momentum. Correspondingly an anisotropic Ginzburg-Landau type scheme with the account of order parameters spatial inhomogeneity has been developed for MgB_2. Two types of coherence lengths have been found in accordance with the two-band nature of the problem. The soft coherence length behaves critically at T_c and characterizes the fluctuations of superconducting order represented by the gaps. The rigid coherence length is noncritical in nature (small and imaginary) and describes spatially periodic superconducting correlations being presumably connected with the phase difference of two superfluids. The anisotropy of the second critical field (not depending on temperature in the region under consideration)calculated in the framework of the present model is in agreement with the experimental data. The applicability criteria of the Ginzburg-Landau approach have been estimated to be weaker than stated earlier in the literature.

The main result of the dissertation consists in the elaboration of a theoretical framework including intra- and interband pairing channels for the description of the MgB_2 basic superconductivity characteristics. The result obtained agree with the experimental findings and other theoretical approaches devoted to MgB_2 superconductivity.

Summary in Estonian

MgB_2 ülijuhtomadused tsoonisiseste ja tsoonidevahelise paardumiskanalitega stsenaariumis

Käesolev doktoritöö on pühendatud magneesiumdiboriidi (MgB_2) ülijuhtivusmehhanismi teoreetilisele selgitamisele. Kooskõlas paljude analoogsete uurimustega selgus, et MgB_2 on tõestatult tüüpiline kahepiluline ülijuht ja seda esmakordselt antud ainevaldkonnas. Saadud tulemuste kompleks võimaldab sihipäraselt kujundada MgB_2 ja tema sugulasühendite uurimist ja praktilist rakendamist. Teoreetilises aspektis sai uue arengutõuke ka mitmetsoonilise ülijuhtivuse mitmekülgne arendamine. Käesoleval ajal on hakanud intensiivsemalt arenema uurimissuund mida võiks nimetada "mitmetsooniline ülijuhtivus uutes ühendites ja süsteemides".

Doktoritöös kirjeldatakse MgB_2 elektronspektri aktiivset osa kahe efektiivse boori seisunditest pärineva tsooniga. Selles süsteemis toimivad järgmised paardumiskanalid: σ-tsoonisisene efektiivne elektron-foonon päritoluga tõmbumine, σ-tsoonisisene kuloniline tõukumine ja $\sigma - \pi$ tsoonidevaheline tõukeinteraktsioon. Viimase arvestamisele on pööratud erilist tähelepanu, kuna sellise interaktsioonikanali olemasolu on printsipiaalse tähendusega. Vastava tsoonidevahelise paariülekande toimimist kontrolliti spetsiaalses eksperimendis, mis kinnitas mõlema ülijuhtivuspilu korraga nulliks saamist siirdetemperatuuril.

Arendati nimetatud lähteeldustele vastav olulisemaid interaktsioone arvestav teoreetiline üldskeem ja tuletati avaldised MgB_2 põhiliste ülijuhtivuskarakteristikute jaoks.

Toetudes relevantsetele MgB_2 kohta mõõdetud ja arvutatud omadustele on valitud usaldusväärne parameetrite süsteem ülijuhtivuse põhikarakteristikute kvantitatiivseks kirjeldamiseks. Arvutati siirdetemperatuuri ja ülijuhtivuspilude sõltuvust MgB_2 dopeerimisest, s.t. käsitleti ka MgB_2 laia sugulasühendite ringi. Näidati, et dopeerimine surub maha ülijuhtivat faasisiiret, nii et puhas MgB_2 osutub optimaalselt "isedopeerituks". Saadud sõltuvused on kooskõlas erinevate eksperimentidega.

Leiti kasutatavale mudelile vastav vabaenergia avaldis, mis võimaldas arvutada MgB_2 teise kriitilise magnetvälja, soojusmahtuvuse ja entroopia sõltuvused temperatuurist kooskõlas katseandmetega.

Ülijuhtivusliku korrastusega seotud fluktuatsioonide käsitlemiseks tuletati keskmise välja lähenduses MgB_2 vabaenergia nullist erineva Cooperi paaride impulsside jaoks. See tähendab korrastusparameetrite anisotroopiat ja ruumilist mittehomogeensust arvestava Ginzburg-Landau kirjelduse arendamist MgB_2 kontekstis. Selgus, et kooskõlas probleemi kahetsoonilise iseloomuga peavad MgB_2 ülijuhtivust kirjeldama kaks oluliselt erinevat koherentsuspikkuse komponenti. Neist esimene, kriitiline komponent käitub siirdepunktis "pehmelt" nagu ühe korrastusparameetriga formalismis tavaline Cooperi paaride koherentsuspikkus. Teine komponent osutub imaginaarseks ja kirjeldab ruumiliselt perioodilist ülijuhtivat fluktuatsiooni lainel.

Temperatuurist sõltumatu karakteristikuna arvutati teise kriitilise magnetvälja anisotroopia, mis osutus eksperimendi tulemustega heas kooskõlas olevaks. Hinnati Ginzburg-Landau formalismi rakendatavuse kriteeriumi MgB_2 jaoks, mis osutus nõrgemaks kui varasemas kirjanduses eeldati.

Käesoleva töö peamiseks tulemuseks hindame tsoonisiseseid ja tsoonidevahelist interaktsioonikanaleid hõlmava teoreetilise käsitluse arendamist mag-

neesiumdibriidi ülijuhtivusmehhanismi selgitamiseks ja vastavate põhikarakteristikute kirjeldamiseks. Saadud tulemused on kooskõlas ekperimendiga ja teiste MgB_2 teoreetiliste käsitlustega.

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