Two-band model and MgB$_2$ superconductivity

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Abstract. A simple two-band model with interband scattering of intraband pairs is applied to MgB$_2$ superconductivity. An adjustable parameters set is chosen. The calculated $T_c$ vs doping, isotope exponent and the heat capacity jump are in qualitative agreement with the observations.

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The discovery [1] of MgB$_2$ superconductivity with $T_c$=39 K has qualitatively enlarged the family of high-temperature superconductors and stimulated rapid research activity.

When asking about the pairing mechanism in this compound the presence of boron isotope effect [2], the s-wave nature of the order parameter(s) [3-5,17] and the hole-type conductivity [6,12] are of guiding significance. Doping of MgB$_2$ with electrons (Mg$_{1-x}$Al$_x$B$_2$) reduces $T_c$ [7]. The same is observed for the (enhanced) hole doping (Mg$_{1-x}$Li$_x$B$_2$) [8]. Considering the whole class of doped compounds as in cuprates with a bell-type curve of $T_c(x)$ one expects MgB$_2$ being positioned nearly in the optimal doping region of the phase diagram.

High phonon frequencies by the small boron mass and strong electron-phonon interaction have stimulated the description of the MgB$_2$ superconductivity on a BCS type way [9,10]. However seemingly a limiting ability of

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such a type mechanism is exploited at this. An original approach to MgB$_2$ superconductivity has been elaborated [11,12] using a ”hole-undressing” theory [13].

The electronic structure of MgB$_2$ is known by a number of calculations [9,10,14]. The most impressive circumstance consists here in the presence of two close genealogically boron $p_{x,y}$ bands intersecting the Fermi surface. These $\sigma$-bonding hole-conducting two-dimensional bands can be modulated by $E_{2g}$-boron stretching in plane modes with a large deformation potential.

Presence of two bands near the Fermi energy in the electron spectrum of cuprates has stimulated the application of various models with interband interactions to explain their superconductivity, for a review e.g. [15]. The physical origin of these bands has remained often unclear, however a number of provising results have been obtained. This experience stimulates the attempt to use the two-band model also to describe the MgB$_2$ superconductivity which is the aim of the present note (see also [16]). References to the nature of the MgB$_2$ electron spectrum and to the specific heat data [17] serving evidence of a multicomponent gap can be made at this.

We describe a two-band s-wave superconductor with the interband scattering of intraband pairs by the mean-field Hamiltonian

\begin{equation}
H = \sum_{\vec{k}\sigma} \left[ \epsilon_a(\vec{k}) a_{\vec{k}\sigma}^+ a_{\vec{k}\sigma} + \epsilon_b(\vec{k}) b_{\vec{k}\sigma}^+ b_{\vec{k}\sigma} \right]
+ \sum_{\vec{k}} \left[ \Delta_a \left( a_{\vec{k}\uparrow}^+ a_{-\vec{k}\downarrow} + a_{-\vec{k}\uparrow}^+ a_{\vec{k}\downarrow} \right) - \Delta_b \left( b_{\vec{k}\uparrow}^+ b_{-\vec{k}\downarrow} + b_{-\vec{k}\uparrow}^+ b_{\vec{k}\downarrow} \right) \right],
\end{equation}

where

\begin{equation}
\Delta_a = 2W \sum_{\vec{k}} \langle b_{\vec{k}\uparrow} b_{-\vec{k}\downarrow} \rangle,
\quad \Delta_b = 2W \sum_{\vec{k}} \langle a_{-\vec{k}\downarrow} a_{\vec{k}\uparrow} \rangle.
\end{equation}

Usual designations of electron operators and spins are used. The band energies read $\xi_{a,b}(\vec{k}) = \epsilon_{a,b}(\vec{k}) + \mu$, $\mu$ is the chemical potential. The interband interaction constant $W$ is supposed to contain an electronic (Coulomb) part $U$ besides an electron-phonon contribution $V \sim M^{-1}$ (both repulsive). Interband type pairs interaction is omitted at present with the usual argument of much smaller momentum volume available. The gap equations ($\Theta = k_B T$)

\begin{equation}
\Delta_a = W \Delta_b \sum_{\vec{k}} E_{b}^{-1}(\vec{k}) \frac{E_b(\vec{k})}{2\Theta}
\end{equation}

\[ \]
\[ \Delta_b = W \Delta_a \sum_{\vec{k}} E^{-1}_a(\vec{k}) \text{th} \frac{E_a(\vec{k})}{2\Theta} \]

with quasiparticle energies \( E_{a,b} = \sqrt{\epsilon_{a,b}^2(\vec{k}) + \Delta_{a,b}^2} \) determine the transition temperature \( \Theta_c \) when \( \Delta_{a,b} \) simultaneously tend to zero.

The MgB\(_2\) electron spectrum in the region of interest can be modelled by two plane parabolic hole bands with the densities of states \( \rho_a = 0.18, \rho_b = 0.07\,(eV)^{-1} \) [10]. Their common origin is taken as energy zero and the chemical potential of the undoped material is \( \mu = -0.6 \) eV. Looking on the common region of the bands according to calculations [9,10] we introduce cut-off of the interband interaction at \( D = -1.5 \) eV.

Performing the approximate integration in the equation

\[ 1 = W^2 \rho_a \rho_b \int_{D}^{0} d\xi \frac{\text{th} \left( \frac{\mu - \xi}{2\Theta_c} \right)^2}{\xi - \mu} \]

for \( \Theta_c \), one finds \((\ln \gamma = 0.577)\)

\[ \Theta_c = \frac{2\gamma}{\pi} \sqrt{\mu(D - \mu)} \exp \left\{ -\frac{1}{2W \sqrt{\rho_a \rho_b}} \right\} \].

This expression reflects the usual advantage of two-band models to work with repulsive interband interaction \( W > 0 \) (note opposite signs of order parameters at this [18]) and electronic energy scale in the prefactor of the exponent. The choice of a common \( D \) for the bands leads to symmetric \( \Theta_c(\mu) \) curve. For the characteristic \( \frac{2\Delta_{a,b}}{\epsilon_{a,b}} \) ratios the BCS universality breaking is expected. For the isotope effect exponent the simple result independent of \( \mu \) follows [21]

\[ \alpha = \frac{C_B}{2W \sqrt{\rho_a \rho_b}W} \]

where \( C_B = \frac{d\ln M}{d\ln M_B} \) (\( M_B \) is the mass of boron ion) determines the participation of the boron atoms in the vibration serving the interband electron-phonon contribution \( V \sim M^{-1} \). From (6) it is seen that factors which enhance \( T_c \) reduce its isotope effect exponent. Relatively small electron-phonon contribution to the whole \( W \) is able to cause a remarkable isotope effect.

Hydrostatic pressure must shorten also the interplane B-B distances and splits the actual bands [10]. This must lead according to the present scheme
to $T_c$ reduction as observed [19]. Then also the underdoped region will be enlarged by the $\mu$ out of the bands overlap situation. A pseudogap type excitation channel connected with the lower band can be expected in this case as in cuprates [20].

For the specific heat jump at $T_c$ on finds using [15]

$$\Delta C = 9.42 \, R k_B \Theta_c, \quad R = \rho_a \gamma_a^2 + \rho_b \gamma_b^2,$$

$$\gamma_a = \left(1 + \frac{W^2 \rho_a \rho_b A}{1 + W^4 \rho_a^3 \rho_b A^2}\right)^{1/2}, \quad \gamma_b = \frac{1 + W^2 \rho_a \rho_b A}{1 + W^4 \rho_a^3 \rho_b A^2}$$

$$A = \ln^2[\mu(D - \mu)A \gamma^2(\pi \Theta_c)^{-2}].$$

In quantitative estimations we use the value $W = 0.81$ eV to reach the measured $\Theta_c = 40$ K for $\mu = -0.6$ eV. The ionic type Mg$^{2+}$(B$^-$)$_2$ configuration can play a role in determining this scale of $W$. The observed $\alpha = 0.26$ [2] determines for $C_b = 1$ (only boron atoms vibrate) the relation $V/W = 4.7\%$ which compares with the result found for cuprates [21,22].

The $\Theta_c(x)$ curve is given in Fig.1. As seen, MgB$_2$ can be considered as belonging to optimally (auto-)doped region. A further hole doping must soon (after passing the optimal region) lead to $\Theta_c$ decrease as also the electron doping in agreement with the experiment [7,8]. The heat capacity jump vs doping curve is given in Fig.2. It resembles the $\Theta_c$ behaviour. Our result for MgB$_2$ $\Delta C \sim 50 \, \text{mJ mol}^{-1} \text{K}^{-1}$ can be compared with the measured [23] value $\sim 86 \, \text{mJ mol}^{-1} \text{K}^{-1}$, and $\Delta C/T_c = 1.3 \, \text{mJ mol}^{-1} \text{K}^{-2}$ with the experimental result $2 \, \text{mJ mol}^{-1} \text{K}^{-2}$. The heat capacity characteristics do not contain further free parameters and serve as a proof of the applicability of the present theoretical scheme with the parameters set used.

A slight increase of $\rho_a \rho_b$ can significantly improve the agreement with the measured heat capacity data without notable modifications of other aspects. We note also that $\rho_{a,b}$ values appropriate for the full band widths (5.6 and 14 eV [10]) have been used and the boron $p_z$-type band has remained out of play.

We find that multiband-type models remain of interest for the explanation of doped MgB$_2$-family superconductivity.

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Figure captions

Fig. 1. Dependence of \( T_c \) on chemical potential position.

Fig. 2. Dependence of specific heat jump at \( T = T_c \) on chemical potential position.
