Properties of MgB$_2$ in a two-gap superconductivity model

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Abstract

For MgB$_2$ where coexist two coupled superconductivity gaps a two-band scheme has been developed. Three interaction channels have been taken into account: a pair-transfer type $\sigma - \pi$-interband repulsion, a $\sigma$-intraband effective attraction of electron-phonon nature, and a $\sigma$-intraband Coulomb interaction. The calculated temperature dependencies of gaps, heat capacity and $H_c2$ agree with the experimental findings. The theoretical curve of $T_c$ vs $x$ for Mg$_{1-x}$Al$_x$B$_2$ follows the experimental data.

Key words:
MgB$_2$; two-band model; superconductivity and thermodynamic characteristics

A number of experiments point to the two-gap nature of the MgB$_2$ superconductivity [1-6]. The electron structure calculations [7,8] also support this conclusion by revealing the Fermi level intersection by boron $\sigma$- and $\pi$-bands. At the same time, there is no doubt in the presence of strong $\sigma$-intraband pairing interaction in MgB$_2$ [7,8], however, the mentioned circumstances suggest to introduce the interband pairing channels and the use of two-band models of superconductivity [5,9-12].

The linearized Hamiltonian of the system incorporating electron-phonon and Coulomb interactions in the effective $\sigma$-band, and the $\sigma - \pi$ scattering of intraband pairs is taken in the form

\[ H = \sum_{\alpha k} \tilde{\epsilon}_\alpha (k) a^\dagger_{\alpha k} a_{\alpha k} - \sum_{\alpha k} \Delta_{\alpha k} < a^+_\alpha k | a^{-}_\alpha k' > + \sum_{\alpha k} (\Delta_{\alpha k} a^+_\alpha k | a^{-}_\alpha k' > + \Delta^*_{\alpha k} a^+_\alpha k' | a^{-}_\alpha k >), \] (1)

where the superconductivity order parameters are defined as $\Delta_{\alpha k} = 2 \sum_{jk'} W_{\alpha \beta}(k,k') < a_{\beta - k'} | a^{+}_{\alpha - k} >$. The band energies ($\alpha = 1$ for $\sigma$ and $\alpha = 2$ for $\pi$) read $\epsilon_\alpha = \tilde{\epsilon}_\alpha + \mu$, where $\mu$ is the chemical potential.

Other common designations are used. The gap equations ($\Theta = k_B T$)

\[ \Delta_{\alpha k} = - \sum_{\beta k'} W_{\alpha \beta}(k,k') \Delta_{\beta k'} \xi_{\beta k'} \] (2)

with $\xi_{\alpha k} = E^{-1}_\alpha(k) \tanh[E_\alpha(k)/2\Theta]$ contain the quasi-particle energies $E_\alpha(k) = [\tilde{\epsilon}_\alpha(k) + \Delta^2_{\alpha k}]^{1/2}$. The gaps are taken to be real.

Describing the s-wave superconductivity of MgB$_2$ the $\sigma$-intraband coupling constant $W_{11} = V + U$ is supposed to contain a Coulombic part $U > 0$ besides the electron-phonon attraction $V < 0$ in the Debye-layer determined by $\hbar \omega_D = 0.06$ eV [13]. The repulsive interband coupling is characterized by the constant $W > 0$. Interactions $U$ and $W$ are operative in the energy interval from $E_c$ to zero ($\sigma$-band top). The cut-off energy $E_c$ determines the bands overlap region and is taken as $E_c = -2$ eV. Then the chemical potential of the undoped MgB$_2$ is $\mu = -0.6$ eV [7]. We characterize the effective $\sigma$- and $\pi$-bands by constant densities of states $\rho_1 = 0.25$ and $\rho_2 = 0.11$ (eV$^{-1}$) [7].

The necessary values of the interaction constants have been determined in [12] by simultaneous fitting of experimental data for $T_c$, the specific heat jump and the ratio of zero-temperature gaps. As a result $V_1 =$
−1.01 and $W = 0.53$ (eV) have been chosen, and according to an estimation $U \approx 1$ eV [12]. The temperature dependencies of the gaps on the Fermi level calculated from (2) agree well with the measured ones [2,14], as it is seen from Fig. 1.

On the basis of Eqs. (1),(2) one can find the thermodynamic characteristics for MgB$_2$. Theoretical curve of specific heat vs temperature in Fig.2 follows the experimental data of [15]. In Fig.3 the calculated temperature dependence of $H_{C2}$ describes satisfactorily the experimental data of [16]. At this the Ginzburg-Landau parameter value $\kappa=38$ [4] has been used.

For the calculation of $T_c (x)$ for Mg$_{1-x}$Al$_x$B$_2$ we have taken account of $\rho_{1,2}$ changes in the Debye layer near $E_F$ with doping according to[8]. The result is shown in Fig.4 together with the experimental points from [17]. In conclusion, the model of present type seems to be able to describe the properties of the two-gap superconductor MgB$_2$.

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References