MgB_2: superconductivity and pressure effects

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Abstract

The Ginzburg-Landau (GL) theory for a two-band superconductor is constructed with emphasis on MgB_2. Then the microscopic theory of superconducting MgB_2 is presented with SC order parameter of s^*-wave symmetry. The superconducting density of electronic states (DOS) and the pressure effects are discussed.

Key words: Ginzburg-Landau equation; electron correlation; density of states

The discovery of superconducting MgB_2 [1] poses fundamental questions regarding the nature of superconductivity. MgB_2 belongs to the space group $P6/mmm$ and the electronic structure is organized by the narrow energy bands with near two-fold degenerate σ-electrons and the wide-band π-electrons.

The GL free energy functional for MgB_2 is:

$$F = \int d^3r\{\frac{1}{2m_\sigma}|\Pi\psi_\sigma|^2 + \alpha_\sigma|\psi_\sigma|^2 + \beta_\sigma|\psi_\sigma|^4 + \frac{1}{2m_\pi}|\Pi\psi_\pi|^2 + \alpha_\pi|\psi_\pi|^2 + \beta_\pi|\psi_\pi|^4 + r(\psi_\sigma^*\psi_\pi + \psi_\sigma\psi_\pi^*) + \gamma_1(\Pi_x\psi_\sigma\Pi_x^*\psi_\pi^* + \Pi_y\psi_\sigma\Pi_y^*\psi_\pi^* + c.c.) + \gamma_2(\Pi_z\psi_\sigma\Pi_z^*\psi_\pi^* + c.c.) + \beta|\psi_\sigma|^2|\psi_\pi|^2 + \frac{(\nabla\times\mathbf{A})^2}{8\pi}\},$$

where $\Pi = -i\hbar\nabla - 2e/c\mathbf{A}$, $\mathbf{A}$ is the vector potential, $\alpha_{\sigma,\pi} = \alpha^0_{\sigma,\pi}(T - T^0_{c\sigma,\pi})$.

If $r = 0$ then the above Eq is the free energy without Josephson coupling between two bands. The effect of the pressure on two order parameters is to shift the T_c's. The new T_c' s can be found by solving Eqs. for $|\psi_{\sigma,\pi}|^2$ and then setting the coefficients of $|\psi_{\sigma,\pi}|^2$ to zero. To detect the $T_{c\sigma,\pi}$ splitting, the pressure must be above a certain value, depending on the experimental resolution. If $r \neq 0$ the superconductivity in one band generates the superconductivity in the other with a single T_c. From the GL minimization we get $\alpha_\pi\alpha_\sigma/2\beta_\sigma = -r^2$ at $T^0_{c\sigma} > T > T^0_{c\pi}$. with the pressure dependence

$$T_c(p) = \frac{1}{2}\left[T^0_{c\sigma} + T^0_{c\pi} - (\eta_\pi + \eta_\sigma)p\right] + \frac{1}{2}\left[(T^0_{c\sigma} - T^0_{c\pi} + (\eta_\pi - \eta_\sigma)p)^2 - a^2\right]^{1/2} \quad (1)$$

and $a^2 = 8\beta_\sigma r^2/(\alpha^0_\pi\alpha^0_\sigma)$. In experiments the deviations from a straight line at moderate pressure [2] can be attributed to the two bands.

The next effect we address is the splitting of the two σ bands at ambient pressure due to frozen E_{2g} modes. The band σ_2 below the Fermi level at ambient pressure [3] can overcome the barrier and get above the Fermi level at a certain pressure p_c , restoring the degeneracy of the two σ bands at Γ point. The energy difference between the two subbands is approximated by $(1 - n_\sigma)^2\,\Delta$, where the carrier density per boron atom in MgB_2 is $1 - n_\sigma \sim 0.03$. The p_c suppresses the deformation potential Δ and can be estimated by the expression $p_c\Omega \sim (1 - n_\sigma)\sqrt{\Delta}$ where $\Omega = 30\text{Å}^3$ is a unit cell volume of MgB_2 and $\Delta = 0.04eV^2$ for a boron displacement $u \sim 0.03$Å [4]. At these parameters the crossover pressure is $p_c \sim 15GPa$. The physics of the crossover is similar in spirit to the Lifshits transition of 5/2 kind

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[5]. The additional term which couples the order parameters with the strain tensor ϵ in the regime where $p > p_c$ is $F_{strain} = -C_1(\Gamma_1)[\delta(\epsilon_{xx} + \epsilon_{yy}) + \epsilon_{zz}]|\psi_\sigma|^2 - C_2(\Gamma_1)(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})|\psi_\pi|^2$ (δ is given in terms of the elastic constants). The expected behavior is a change of slope of T_c and an increase of the order parameter $|\psi_\sigma|$ at p_c. This anomaly can be detected directly in a penetration depth experiment under pressure.

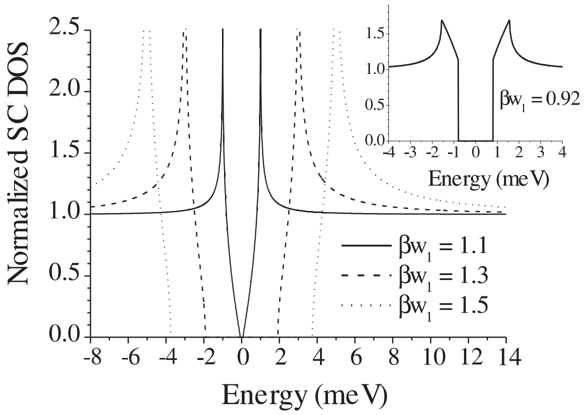

Fig. 1. The superconducting DOS, normalized with respect to the normal DOS, for the Coulomb parameter range $\beta w_1 > 1$. Inset: at $\beta w_1 = 0.92$ the result of Ref [6] is reproduced.

In the microscopic model the on-site correlations of σ-electrons are taken to be infinite. The wide π-band is shifted with respect to the σ-band by an energy r, comprising the electron-phonon interactions. The hopping between σ- and π-electrons is assumed to be negligible due to the symmetry of the orbitals. Also the nearest neighbour Coulomb repulsion V of σ-electrons is included in model. The model is mapped to X-operator basis, describing the on-site transitions of σ-electrons between the one-particle ground states (with spin projection s) and the empty polar electronic states (0) of the boron sites. The diagonal X-operators satisfy the completeness relation, $X^0 + 4X^s = 1$. Due to the orbital and spin degeneracy the σ-electrons have density $n_\sigma = 4\langle X^s\rangle$ per boron site. The correlation factor for the degenerated σ-electrons is $f = \langle X^0 + X^s\rangle = 1 - 3\langle X^s\rangle = 1 - 3n_\sigma/4$, providing the σ-band narrowing. It plays an important role in all X-operator machinery. In $Mg^{++}B^- (p^{n_\sigma} p^{n_\pi})_2$the chemical potential has to be such that the constraint $n_\sigma + n_\pi = 2$ for the electron densities is satisfied. The non-correlated π-electrons play the role of a reservoir for the σ-electrons.

The superconductivity is governed by the kinematic and Coulomb vertices: $\Gamma_0(p,q) = -2t_q + V(p-q)$, where $V(p-q) = 2\beta t_p t_q$ ($\beta = V/6t^2$) near the $\Gamma - A$ line of the Brillouin zone, t_p is the σ-energy dispersion. The equation of the anomalous self-energy for the σ-electrons defines both T_c and the gap function $\Sigma = \Sigma_0(1-\beta t_p) = b\left(1 + a\cos^2\vartheta\right)$ ($a = \beta w_1/(12(1-\beta w_1))$, $b = \Sigma_0(1-\beta w_1)$, where ϑ is the azimuthal angle) of s^*-wave symmetry and $2w_1$ is the σ-bandwidth. The MgB_2 position, $T_c = 40$ K, corresponds to $r = 0.085$ eV and a dimensionless value $\beta w_1 = 1.2$ on the bell shaped curve $T_c(r)$[7].

The near-cylindrical σ-Fermi surfaces in MgB_2 gives room to calculate the superconducting DOS. For an enhanced Coulomb repulsion $\beta w_1 > 1$ the normalized superconducting DOS (Fig. 2) is

$$\frac{\rho\left((1-|a|)b < E < b\right)}{\rho_0(E)} = \frac{1}{s}\sqrt{\frac{E}{2|a|b}}F\left(\sin^{-1}\frac{1}{q};\frac{1}{s}\right)$$

$$\frac{\rho(E > b)}{\rho_0(E)} = \sqrt{\frac{E}{2|a|b}}F\left(\sin^{-1}q;s\right). \quad (2)$$

where $q = \sqrt{(E-b)/2E}$ and $s = \sqrt{(E+b)/2E}$. Two logarithmic divergencies at $E = \pm b$ and a gap in the energy range $|E| < (1-|a|)b$ are manifested in experiments as two-gap ratio is $1/(1-|a|)$. Spectroscopic measurements [8–11] revealed the presence of two gap sizes, from which one can derive the Coulomb parameter βw_1 in the range $1.14 - 1.21$.

We have done a GL analysis of the superconductivity in MgB_2 with particular attention to pressure effects. The superconducting DOS has been analyzed in a model with the s^*-wave superconductivity driven by the kinematic interaction in the σ-band. In our approach the electron-phonon effects are hidden in the parameter r.

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