Dynamic Jahn-Teller Effect and Superconductivity in MgB_2

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Abstract

We propose a novel mechanism of superconductivity in MgB_2 based on the dynamic Jahn-Teller interactions between the doubly degenerate $p\sigma$ electronic states and the E_{2g} phonon modes. The hopping motion of holes in the $p\sigma$ states of the 2D B layers is constrained by accompanying phonons, and thereby a non-trivial superconducting state with multiple order parameters is found to arise from conventional electron-phonon interactions due to the presence of additional pairing channels.

Key words: superconductivity; MgB_2; multiple order-parameters; Jahn-Teller effect

Since the discovery of high T_c superconductivity near 40 K in MgB_2,[1] experiments and theories have flourished and exhausted various possible issues on the physical properties of the brand-new MgB_2 superconductor. One of the key issues in MgB_2 is about the origin of high T_c superconductivity, which seems to share little with the previously known Cu-oxide high T_c superconductors. It naturally led to a revival of interest in the highest T_c attainable by the conventional electron-phonon mechanism of superconductivity.

Despite such strong evidences in support of electron-phonon mechanism of superconductivity in MgB_2,[2] however, recent experiments on thermal and spectroscopic properties[3,4] suggested anomalous two-gap superconductivity, which is attributed to the electronic structure of the 2D σ- and 3D π-bands with highly anisotropic electron-phonon couplings[5]. Although the observed superconducting transition temperature of ~40 K by the large electron-phonon coupling is plausible according to several theoretical calculations,[5] however, there still remains some issues on the predicted values of electron-phonon coupling constant λ in comparison with experiments. Further, an important aspect of the electronic structure of MgB_2, that is, the presence and role of the doubly degenerate $p\sigma$ electronic states coupled to the doubly degenerate E_{2g} phonon modes near E_F, has not been addressed properly. In fact, various physical properties of this coupled degenerate states have been known as the $E \otimes e$ Jahn-Teller or vibronic system,[6] but its implications on MgB_2 have not been considered yet.

The MgB_2 system consists of B layers with graphite structure and the intercalated Mg ions between the layers[7]. Due to the hybridization of Mg s and B $p\pi$ states,[5] the electronic structure of MgB_2 exhibits a unique feature of $p\sigma$ states crossing the Fermi level E_F, strongly coupled to the high frequency phonons with $\omega_{E_{2g}} \approx 70$ meV with large anharmonicity. The doubly degenerate $p\sigma$ states belong to the E_g symmetry representation at the Γ-point, where small hole pockets of $p\sigma$-bands form almost two-dimensional Fermi surfaces.

The E_g electron doublet and E_{2g} phonon doublet states for the single hexagonal B unit cell can be represented by the so-called $E \otimes e$ Jahn-Teller model[6]. A typical form of the $E \otimes e$ Hamiltonian can be written by

$$h_0 = \sum_{\alpha=\pm} \omega_0 (a^\dagger_\alpha a_\alpha + \frac{1}{2}) + g\omega_0 \sum_{\alpha=\pm} (a_{-\alpha} + a^\dagger_\alpha) c^\dagger_{-\alpha} c_\alpha \quad (1)$$

where a_α and c_α ($\alpha = \pm$) correspond to the phonon doublet and electron doublet states respectively. It is

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well known that one much take account of the dynamical phase of phonons, i.e., non-adiabaticity, in order to get a proper description of this model. In addition, defining a *pseuo-spin* operator by $J_z = L_z + \frac{1}{2}\tau_z = (n_{a+} - n_{a-}) + \frac{1}{2}(n_{c+} - n_{c-})$ with $n_{a\alpha} = a^\dagger_\alpha a_\alpha$ and $n_{c\alpha} = c^\dagger_\alpha c_\alpha$, one can show that $[h_0, J_z] = 0$, that is, the conservation of pseudo-spin. As results, the ground state with a single electron occupancy retains a two-fold degeneracy and acquires a pseudo-spin quantum number $\tau = \alpha/2 = \pm 1/2$, implying the coupled motion of electron and phonon with right- or left-handed helicity in the phase space. More detailed characteristics of the ground and excited states of this model have been extensively discussed in the literature[6].

When an electron or hole moves from one site to another, the hopping process is affected by the pseudo-spin configuration at each lattice site. For the electron hopping term

$$H_1 = -\sum_{\alpha\langle ij\rangle\sigma} t_0 c^\dagger_{\alpha i\sigma} c_{\alpha j\sigma} \tag{2}$$

where σ represents the *real* spin of electrons, one can perform a unitary transformation projecting the ground state on the pseudo-spin configurations of the Jahn-Teller sites. It is noted that H_1 preserves the pseudo-spin symmetry, i.e., $[H, J_z] = 0$. In the weak coupling limit of Eq. (1) for small g, one can show that the effective pairing-Hamiltonian $H_{\rm eff}$ becomes[8]

$$\begin{aligned} H_{\rm eff} = & \sum_{\alpha\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^\dagger_{\alpha\mathbf{k}\sigma} c_{\alpha\mathbf{k}\sigma} \\ & - \sum_{\alpha\mathbf{k}\mathbf{k}'} V^0_{\mathbf{k}\mathbf{k}'} c^\dagger_{-\alpha\mathbf{k}'\uparrow} c^\dagger_{\alpha-\mathbf{k}'\downarrow} c_{-\alpha-\mathbf{k}\downarrow} c_{\alpha\mathbf{k}\uparrow} \\ & - \sum_{\alpha\mathbf{k}\mathbf{k}'} V^1_{\mathbf{k}\mathbf{k}'} c^\dagger_{\alpha\mathbf{k}'\uparrow} c^\dagger_{-\alpha-\mathbf{k}'\downarrow} c_{-\alpha-\mathbf{k}\downarrow} c_{\alpha\mathbf{k}\uparrow} \\ & - \sum_{\alpha\mathbf{k}\mathbf{k}'} V^2_{\mathbf{k}\mathbf{k}'} c^\dagger_{\alpha\mathbf{k}'\uparrow} c^\dagger_{\alpha-\mathbf{k}'\downarrow} c_{\alpha-\mathbf{k}\downarrow} c_{\alpha\mathbf{k}\uparrow} \end{aligned} \tag{3}$$

Due to the peculiar nature of the residual electron-phonon interactions with the pseudo-spin symmetry, the hopping process generates additional pairing channels, i.e., three distinct channels contributing to the attractive interactions between electrons due to the exchange of phonons. An analogous residual electron-phonon coupling has been suggested for the case of doped C_{60} superconductors in terms of the kinematic constraint imposed by the Berry's phase due to the Jahn-Teller coupling at each site[9].

Since the effective pairing Hamiltonian has an extra pairing symmetry apart from the standard BCS model, one may expect a non-trivial gap structure with multiple order parameters. By solving the gap equations including the symmetry breaking hopping terms,[8] we obtained two-gap solutions, which are responsible for the anomalous behaviors observed in specific heat data[3]. Unlike other theories,[5] both of the gaps are basically isotropic (except for a small anisotropic influence from the $p\pi$ bands located at a different region of the $\mathbf{k}$ space). Two s-wave gaps are allowed here owing to the presence of additional quantum numbers for the pseudo-spin. Without pseudo-spins, there would be only one s-wave gap solution giving the lowest free energy. Our model for the dynamic Jahn-Teller mechanism is distinguished from other exotic cases with multiple order parameters or superconducting gaps, which were studied in relation to the heavy fermion systems.[10] It is emphasized that the dynamic Jahn-Teller state is qualitatively different from the usual electronic states with two-fold degeneracy. The pseudo-spin J_z conservation derived from the Jahn-Teller state acts as a strong constraint in the electron-phonon interactions and pairing interactions as well.

In summary we proposed a mechanism of superconductivity in MgB_2 based on a dynamic Jahn-Teller effect arising from the interplay between the doubly degenerate $p\sigma$ electronic states and the E_{2g} phonon modes. The pseudo-spin constraint imposed on the motion of holes opens up additional pairing channels, which contribute to the non-trivial superconducting properties in MgB_2.

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