Dynamic Jahn-Teller Mechanism of Superconductivity in MgB$_2$

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Following the discovery of high $T_c$ superconductivity near 40 K in MgB$_2$, a lot of efforts have been devoted to revealing the underlying mechanism of this novel superconductor. Now it is widely agreed upon that a relatively strong electron-phonon coupling is responsible for the superconductivity of this material and there exit, at least phenomenologically, two superconducting gaps. It has been proposed that the complex Fermi surfaces having both 2D cylindrical sheets and 3D tubular networks produce two gaps. However, it is still an open question whether one gap is mainly associated with the 2D cylindrical Fermi surfaces and the other is associated with the 3D Fermi surfaces.

In this letter, we propose 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 $e_{2g}$ phonons. The hopping motion of holes of the $p\sigma$ character on the Boron layers is constrained by the ‘pseudo-spin’, which will be defined later, and partial breakdown of the pseudo-spin symmetry is also important in the pairing mechanism. Unlike existing theories, we will explain both high $T_c$ and two distinct gaps in MgB$_2$ without invoking the additional 3D Fermi surface of $p\pi$ character.

According to the band structure calculations, the $p\sigma$ states on the Boron layer form doubly degenerate $E_g$ bands at $\Gamma$ (to be precise, along the $\Gamma A$ line on which the component of $k$ parallel with the Boron plane, $k_{||}$, is zero), where we have small hole pockets presumably responsible for the superconductivity in MgB$_2$. (Splitting of the band degeneracy away from $\Gamma$ will be taken into account later.) These hole states are known to be strongly coupled with $e_{2g}$ phonon modes with $\hbar\omega \approx 70meV$. The $E_g$ hole doublet coupled with $e_{2g}$ phonon doublet states on the Boron layer can be represented by the so-called $E \otimes e$ Jahn-Teller model. A typical adiabatic potential energy surface of the $E \otimes e$ Jahn-Teller model is illustrated in Fig. 1, where $q_\theta$ and $q_e$ correspond to the two phonon coordinates.

It is well known that one must take account of the dynamical phases of the holes and phonons in order to describe the $E \otimes e$ system properly. When the ionic configuration traverses around the potential well in Fig. 1 once, the corresponding orbital wavefunction of the hole (for simplicity of discussion, we leave aside the real spin wavefunction which simply follows the elementary BCS theory) acquires a phase of $-1$, as if the orbital part had spin $1/2$. We call this a pseudo-spin of the hole and denote its projected value by $\alpha = \pm \frac{1}{2}$. This subject was extensively discussed in the literature in the context of the Jahn-Teller effect or Berry’s phase. We also note that the dynamic Jahn-Teller effect in doped C$_60$ superconductors was studied before, although the methods and results there were different from our work.

We introduce a single site Jahn-Teller Hamiltonian per unit cell using mass-weighted coordinate for the sym-

![FIG. 1: Adiabatic potential surface of the $E \otimes e$ Jahn-Teller system and the doubly degenerate pseudo-spin states ($\frac{1}{2}$), ($-\frac{1}{2}$) of the hole.](image-url)
metrized displacement $Q_\gamma (\gamma = \theta, \varepsilon)$, i.e. $q_\gamma = \sqrt{M_s} Q_\gamma$, 

$$h_0 = \frac{1}{2} (p^2 + p^2_z) + \frac{1}{2} \omega_0^2 (q^2_\theta + q^2_\varepsilon) + A (q_\theta \sigma_z + q_\varepsilon \sigma_y), \quad (1)$$

where $A$ is the hole-phonon coupling strength and $\sigma_z$, $\sigma_y$ are Pauli spin matrices for the pseudo-spin representation of $E_g$ hole doublet states. In an analogy to the 2D harmonic oscillator, the vibrational mode in the $(q_\theta, q_\varepsilon)$-space belongs to the eigenmode of the “phonon” angular momentum operator $L_z = (q_\theta p_z - q_z p_\theta)$ with the eigenvalue of $l$, and the principal quantum number $\nu$ becomes $\nu = l + 2k$ ($k$ is a non-negative integer and $-\nu \leq l \leq \nu$). In the present theory of superconductivity, only $\nu = 0, 1, 2$ and $l = 0, \pm 1$ are relevant. Defining the total pseudo-spin of the system by $J_z = L_z + \frac{1}{2} \sigma_z$, it is straightforward to prove $[h_0, J_z] = 0$, that is, the total pseudo-spin of the system is conserved, while individual $L_z$ and $\sigma_z$ are not. (The phonon angular momentum component, $L_z$, can be regarded as a part of the total pseudo-spin in this context.) These pseudo-spin states are derived from the $E \otimes e$ Jahn-Teller coupling between $3d$ holes and $e_{2g}$ phonons, and reflect the non-adiabatic nature of the coupled states. As a consequence, relevant electron and phonon states are expected to be strongly renormalized and contribute to anomalous behaviors (e.g., broad linewidths) observed in recent photoemission spectroscopy and Raman experiments [14, 15].

We generalize the theory to the Bloch state in the $k$-space of a crystal by linear combinations of the local holes of the same pseudo-spin, but mathematical details will be reserved for a longer paper [19]. We first consider the one-phonon ($\nu = 1$) exchange for the Cooper pair formation. Each phonon has $l = \pm 1$ in this case. In the one-phonon absorption or emission, the pseudo-spin of the hole should flip to conserve the total pseudo-spin. The only allowed one-phonon exchange mechanism is the opposite pseudo-spin Cooper pair as illustrated in Fig. 2(a). Pairing of the same pseudo-spin holes violates the conservation law in either one of the two (emission and absorption) processes. Such a selection rule has already been known in the self-energy correction to the Jahn-Teller system [20].

We next consider the two-phonon ($\nu = 2$) case. In MgB$_2$, the two-phonon exchange process has been thought to be important in producing high $T_c$ and included in some previous works [18]. When we properly consider the pseudo-spin symmetry of the Jahn-Teller system such as MgB$_2$, incorporating the two-phonon exchange turns out to be essential in order to obtain two distinct gaps. Unlike the one-phonon exchange process, both opposite- and same- pseudo-spin pairs are allowed here as illustrated in Fig. 2(b) and (c). The total $l$ (sum of two individual $l$’s) of intermediate phonons is restricted to zero (i.e., the hole pseudo-spin change of $\pm 2$ is not possible) to conserve the total pseudo-spin. A new model Hamiltonian with different pseudo-spin channels explicitly labelled is, in the $k$-space representation,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3. \quad (2)$$

$$\mathcal{H}_0 = \sum_{\alpha k \sigma} \varepsilon_{k} c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma}, \quad (3a)$$

$$\mathcal{H}_1 = - \sum_{\alpha k \sigma} V_{kk'} c_{\alpha k \uparrow}^\dagger c_{-\alpha -k \downarrow} c_{-\alpha -k' \downarrow} c_{\alpha k' \uparrow}, \quad (3b)$$

$$\mathcal{H}_2 = - \sum_{\alpha k \sigma} V_{kk'} c_{\alpha k \uparrow}^\dagger c_{-\alpha -k' \downarrow} c_{-\alpha -k \downarrow} c_{\alpha k' \uparrow}, \quad (3c)$$

$$\mathcal{H}_3 = - \sum_{\alpha k \sigma} V_{kk'} c_{\alpha k \uparrow}^\dagger c_{-\alpha -k' \downarrow} c_{-\alpha -k \downarrow} c_{\alpha k' \uparrow}. \quad (3d)$$

$\mathcal{H}_1$, $\mathcal{H}_2$, and $\mathcal{H}_3$ correspond to the diagrams in Fig. 2(a), (b), and (c), respectively. The explicit form of the derived interactions, $V_{kk'}$’s ($i = 0, 1, 2$), can be calculated and will be given elsewhere [19]. To discuss the nature of superconducting states, it suffices here to treat them as given parameters. The additional pairing channels due to the presence of pseudo-spin symmetry can give rise to a non-trivial superconducting ground state. Although the pairing is still based on electron-phonon interactions, the pairing order parameter can now attain more than one symmetry representation leading to the ground state with multi-dimensional order parameters while retaining the conventional $s$-wave type superconductivity.

In the pairing Hamiltonian described above, however, important features of a real crystal are missing. First, the pseudo-spin symmetry is exact only at $k_{||} = 0$ and there occurs small but finite deviation from the exact symmetry for $k_{||} \neq 0$ where Fermi surfaces actually exist. The band splitting at $k_{||} \neq 0$ is a clear manifestation of the breakdown of the rigorous Jahn-Teller theory for Bloch wavefunctions of $k_{||} \neq 0$ in a crystal as opposed to the case of a highly symmetric molecule. Second, higher-order Jahn-Teller coupling terms (not considered so far) do not commute with $J_z$ and break the pseudo-spin conservation [21]. A simple way to incorporate the symmetry breaking effect is to introduce a small symmetry breaking parameter $\phi_k$ ($\phi_{k_{||}} = 0$ and $\phi_{k_{||} \neq 0} \neq 0$) in the hopping Hamiltonian (Eq. (3a)) as follows,

$$\mathcal{H}_0 = \sum_{\alpha k \sigma} \varepsilon_{k} c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma} - \sum_{\alpha k} \phi_{k} \varepsilon_{k} c_{\alpha k \sigma}^\dagger c_{-\alpha k \sigma}. \quad (4)$$
This replacement naturally introduces the symmetry-breaking hopping process which gives the band splitting away from $k_{\parallel} = 0$. (If the pseudo-spin $\frac{1}{2}$ were continuous symmetry ($SU(2)$) for all $k$, there would be a single finite gap plus a zero-gap Goldstone mode, unlike the experimental observation in MgB$_2$.) Now we choose the following two order parameters, one for the opposite pseudo-spin pair and the other for the same pseudo-spin pair,

$$A_k = (c_{\downarrow - k_1} c_{\uparrow + k_1}) = (c_{\downarrow - k_1} c_{- k_1})$$  

$$B_k = (c_{\downarrow - k_1} c_{\uparrow + k_1}) = (c_{\downarrow - k_1} c_{- k_1})$$  

(5a)

(5b)

It is to be noted that the pseudo-spin pairing assumed above is a triplet state (even for exchange of two particles) to preserve the singlet (odd) state of the real spin pair and the s-wave (even) state of the orbital wavefunction. Following the standard mean field approximation, we can derive the effective Hamiltonian $H' (= H - \varepsilon_F N')$,

$$H' = \sum_{\alpha k} \varepsilon_k (c_{\alpha k}^\dagger c_{\alpha k}) + V_{\alpha k}^2 B_k$$

(6)

where $\varepsilon_k = \varepsilon_k - \varepsilon_F$ and the gap-like parameters are expressed as

$$\Delta_{1,k} = \sum_{k'} (V_{kk'}^0 + V_{kk'}^2) A_{k'}$$

$$\Delta_{2,k} = \sum_{k'} V_{kk'}^2 B_{k'}$$

(7)

By fitting to $T_c$ and the specific heat behavior, we are going to obtain below $\lambda_1 = 0.235$, $\lambda_2 = 0.25$ and $\phi = 0.2$ for the assumed value of $\hbar\omega_c = 74.5meV$. The normalized solutions of the above gap equations (with $\sqrt{(\lambda_+ / \lambda_2)} \sim 0.94$ and $\phi = 0.2$) are shown in Fig. 3(a). Our theory gives two distinct gaps of the identical $T_c$ originated from two split-off $p\sigma$ bands alone, in contrast to other theories which invoke the $p\pi$ band to obtain multi-gaps. Furthermore, we predict that there exist two gaps for the same $k$ vector and both gaps are basically isotropic in the Boron plane (except for a small anisotropic influence from the $p\pi$ bands located at different regions of the $k$ space) unlike other theories proposing generically anisotropic gaps. Without pseudo-spins, there would be only one s-wave gap solution giving the lowest free energy. It should be possible, with angle-resolved experimental probes, to test the symmetry or angular dependence of the gap order parameters. Also, it is important in the present theory to include the symmetry-breaking parameter $\phi_k$; otherwise, two gaps should be exactly degenerate and only one gap would manifest itself. With the same degree of approximation as in the BCS formalism, we can derive the expression for $T_c$ (weak coupling limit),

$$k_BT_c \simeq 1.13(\hbar \omega) \exp \left[ - \frac{\lambda_1 + \lambda_2}{2 \lambda_1 \lambda_2} \sqrt{(\lambda_1 - \lambda_2)^2 + 4\phi^2\lambda_1 \lambda_2} \right]$$

(11)
two-phonon couplings lead to effective pairing interactions with additional pseudo-spin channels. As results, the high $T_c$ observed in MgB$_2$ is attributed mainly to the two-phonon exchange mechanism, and further the symmetry breaking hopping term plays a crucial role in producing two gaps which are responsible for the anomalous behaviors observed in experiment including the specific heat measurement.

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FIG. 3: (a) Solution of the self-consistent equations for two gaps $\Delta_+$ and $\Delta_-$, and (b) calculated specific heat for the above gap structure.