Bull. Mater. Sci., Vol. 14, No. 4, August 1991, pp. 1045–1048. © Printed in India.

A mechanism for pairing of RVB excitations

S N BEHERA and D SA
Institute of Physics, Sachivalaya Marg, Bhubaneswar 751 005, India

Abstract. The fluctuations in the RVB order parameter over their meanfield values are considered in the BZA theory which mediate the interaction between the RVB excitations. The condition under which the effective interaction could be attractive and result in superconductivity is investigated. The dependence of the transition temperature on the dopant concentration and the RVB order parameter is calculated.

Keywords. RVB order parameter; RVB excitations; amplitude and phase mode.

1. Introduction

The discovery of high T_c superconductivity (SC) in the perovskite oxides (Bednorz and Muller 1986) has generated a lot of interest to understand the basic properties of these materials and the possible mechanism for it. The evidence in favour of strong electronic correlation together with the low-dimensional nature of these materials led Anderson to propose the resonating valence bond (RVB) state (Anderson 1987) as the ground state for these systems whose elementary excitations (Kivelson *et al* 1987) are (i) the spinons and (ii) the holons. It is proposed that SC might result from (i) the Bose-condensation of the holons for low dopant concentration, (ii) pre-existing real space pairs in the RVB state. Furthermore pairing of the RVB excitations due to the interaction with holes in the oxygen sites has also been proposed (Asai 1988) as a possible mechanism for superconductivity.

In this paper we propose a different mechanism for the pairing of RVB excitations. We assume that the RVB state is described by the BZA meanfield (MF) (Baskaran *et al* 1987) theory. Doping these materials with holes produces (i) RVB excitations which are fermions as well as (ii) the fluctuations in the RVB state whose quanta are bosons. The later excitations can be visualized as the collective modes of the RVB state. These bosons interact with the RVB excitations and can give rise to an effective interaction between the RVB excitations. The condition under which this effective interaction could be attractive and result in SC is investigated. The dependence of the transition temperature on the dopant concentration and the RVB order parameter is calculated.

2. Fluctuations in the RVB state and the mechanism for pairing

It is believed that in the high T_c materials the electrons with strong correlation are described by the Hubbard model.

$$H = -t \sum_{\langle ij \rangle \sigma} C^{\dagger}_{i\sigma} C_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where t and U are the transfer integral and intra-atomic Coulomb repulsion respectively, $\langle ij \rangle$ denotes the summation over the nearest neighbour sites. In the limit

of $U \to \infty$ equation (1) is transferred to the following effective Hamiltonian (Chao *et al* 1977; Cleveland and Medina 1976) which is defined only in the sub-space with the restriction of no double occupancy.

$$H = -t \sum_{\langle ij \rangle \sigma} (1 - n_{i-\sigma}) C^{\dagger}_{i\sigma} C_{j\sigma} (1 - n_{j-\sigma}) + \mu \sum_{i\sigma} n_{i\sigma} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4} n_i n_j) \quad (2)$$

with the antiferromagnetic superexchange interaction of strength $J = 4t^2/U$ between the spins $\mathbf{S}_i$ and $\mathbf{S}_j$. The chemical potential μ is introduced for modelling the doping process later. Now approximating the hopping term $-t(1 - n_{i-\sigma}) C^{\dagger}_{i\sigma} C_{j\sigma} (1 - n_{j-\sigma})$ by $-t\delta C^{\dagger}_{i\sigma} C_{j\sigma}$, δ being the dopant concentration and defining the valence bond singlet pair creation operator by $b^{\dagger}_{ij} = \dfrac{1}{\sqrt{2}} (C^{\dagger}_{i\uparrow} C^{\dagger}_{j\downarrow} - C^{\dagger}_{i\downarrow} C^{\dagger}_{j\uparrow})$, the above Hamiltonian can be reduced to

$$H = -t\delta \sum_{\langle ij \rangle \sigma} (C^{\dagger}_{i\sigma} C_{j\sigma} + \text{h.c.}) + \mu \sum_{i\sigma} n_{i\sigma} - J \sum_{\langle ij \rangle} b^{\dagger}_{ij} b_{ij}. \quad (3)$$

In the MF approximation this Hamiltonian will describe the BZA theory. However the fluctuations in the order parameter are considered. Then following the Nambu operator technique (Kulik *et al* 1981) the Hamiltonian in the momentum representation can be written as

$$\mathscr{H} = \mathscr{H}_{\text{MF}} + \mathscr{H}_{\text{I}}, \quad (4)$$

with

$$\mathscr{H}_{\text{MF}} = \sum_k \psi^{\dagger}_k [(\varepsilon_k - \mu)\sigma_3 - J\Delta\gamma(k)\sigma_1] \psi_k, \quad (5)$$

$$\mathscr{H}_{\text{I}} = \sum_{k,q} \tilde{\gamma}(k - q/2) \psi^{\dagger}_{k+q} [\Delta_{1q}\sigma_1 + \Delta_{2q}\sigma_2] \psi_k, \quad (6)$$

where $\varepsilon_k = -t\delta\gamma(k)$, $\gamma(k) = \sum_{\rho} \exp(i\mathbf{k} \cdot \rho)$, $\tilde{\gamma}(k) = (1/N)\gamma(k)$, ρ being the nearest neighbour vector; the Nambu operator $\psi^{\dagger}_k = (C^{\dagger}_{k\uparrow} C_{-k\downarrow})$, σ_i being the Pauli matrices and Δ_{1q} (Δ_{2q}) are the fluctuations in the amplitude (phase) of the RVB order parameter over their MF values, with

$$\Delta_{iq} = -J/2 \sum_k \langle \psi^{\dagger}_k \sigma_i \psi_{k+q} \rangle. \quad (7)$$

The above MF Hamiltonian can be diagonalized by the usual Bogoliubov transformation and equation (5) reduces to

$$\mathscr{H}_{\text{MF}} = \sum_k E_k (\gamma^{\dagger}_{k0} \gamma_{k0} + \gamma^{\dagger}_{k1} \gamma_{k1}), \quad (8)$$

where the energy of the RVB excitations is $E_k = [(\varepsilon_k - \mu)^2 + \Delta_R^2]^{1/2}$, $\Delta_R(k) = J\Delta\gamma(k)$ is the RVB order parameter, $\gamma^{\dagger}_{k0}(\gamma^{\dagger}_{k1})$ are the creation operator for the fermionic RVB excitations and the coherence factors are $u_k(v_k) = \dfrac{1}{2}\left[1 \pm \dfrac{\varepsilon_k - \mu}{E_k}\right]^{1/2}$. Introducing the bosonic operators for the collective modes of the RVB state equation (6) can be rewritten as

$$\mathscr{H}_{\text{I}} = J \sum_{k,q} \sum_{i=1}^{2} \tilde{\gamma}(k - q/2) \psi^{\dagger}_{k+q} \sigma_i \psi_k (d^{(i)}_q + d^{(i)\dagger}_{-q}) \quad (9)$$

where the fluctuations in the order parameter are identified with the bosonic operators as $\Delta_{iq} = J(d_q^{(i)} + d_{-q}^{(i)\dagger})$. This equation is similar in form to the electron–phonon interaction. Therefore, the effective interaction between the RVB quasi-particles mediated by the exchange of the collective excitations; the amplitude and the phase modes of the RVB state can be calculated by following the standard procedure (Haken 1976) and is given by

$$\mathscr{H}_1^{\text{eff}} = \sum_{k,k'} [F_+(k,k') + F_-(k,k')](\gamma_{k_1}^\dagger \gamma_{-k_1}^\dagger \gamma_{-k'_1} \gamma_{k'_1} + \gamma_{k_0}^\dagger \gamma_{-k_0}^\dagger \gamma_{-k_0} \gamma_{k_0}) \tag{10}$$

where the explicit forms of the strength of interactions arising from the exchange of amplitude (+) and phase (−) modes are

$$F_\pm(k,k') = \pm J^2(k,k')\, U(k,k')(u_k v_{k'} \pm v_k u_{k'})^2, \tag{11}$$

with $J^2(k,k') = J^2\tilde{\gamma}(k,k')$ and $U(k,k') = \dfrac{\omega_{k-k'}}{(E_k - E_{k'})^2 - \omega_{k-k'}^2}$. It is clear from the above expression that the effective interaction arising from the phase mode is negligible and also that the interaction mediated by the amplitude mode is attractive only if the magnitude of difference in the energy of the two interacting quasi-particles is less than the frequency of the amplitude mode. This effective interaction differs from the usual phonon-mediated interaction in having a cut-off equal to the frequency of the RVB amplitude mode instead of the Debye frequency. Therefore the amplitude mode-mediated interaction being attractive can give rise to pairing and hence to sc which is described by the MF BCS-like hamiltonian

$$\mathscr{H}_{\text{MF}} = \sum_{s=0,1} \left[\sum_k E_k \gamma_{k_s}^\dagger \gamma_{k_s} - \sum_k (\Delta_{\text{SC}}(k) \gamma_{k_s}^\dagger \gamma_{-k_s}^\dagger + \Delta_{\text{SC}}^*(k) \gamma_{-k_s} \gamma_{k_s}) \right], \tag{12}$$

where the SC order parameter Δ_{SC} is

$$\Delta_{\text{SC}}(k) = \lambda \sum_{k'} (u_k v_{k'} + v_k u_{k'})^2 \langle \gamma_{-k's} \gamma_{k's} \rangle \tag{13}$$

with $\lambda = J^2(k,k')|U(k,k')|$ is the effective coupling constant. Similarly the equation for chemical potential is

$$\frac{1}{N} \sum_k \frac{\varepsilon_k - \mu}{e_k E_k} \left[2E_k \tanh \frac{\beta e_k}{2} - e_k \right] = \delta, \tag{14}$$

where the SC energy $e_k = [E_k^2 + \Delta_{\text{SC}}(k)^2]^{1/2}$. The gap equation when solved for the transition temperature with the help of the equation for chemical potential yields,

$$k_B T_C = A\hbar\omega_{\text{AM}} \exp\left[-\frac{2}{\lambda N(0)} - \frac{\lambda}{N(0)(2\Delta_R)^2} \left(\frac{\delta}{4\left[1 - \dfrac{1}{2\tanh \dfrac{\Delta_R}{2k_B T_C}}\right]} \right)^2 \right] \tag{15}$$

where $A \cong 0{\cdot}441$, $N(0)$ being the density of states at the Fermi-level and δ the dopant concentration. It is evident from the above expression that the SC transition temperature depends on the RVB order parameter as well as the dopant concentration. In fact it increases as Δ_R becomes larger and decreases with increasing δ. The large

density at the Fermi-level lying just above the RVB gap with higher cut-off frequency of the amplitude mode will give rise to higher SC transition temperature.

3. Conclusion

Pairing of the RVB excitations mediated by the fluctuations in the amplitude of the RVB order parameter is proposed as a mechanism for high T_c superconductivity. An expression is derived for the transition temperature which increases with increasing Δ_R and decreases as the dopant concentration increases.

References

Anderson P W 1987 *Science* **235** 1196
Asai Y 1988 *J. Phys. Soc. Jpn.* **57** 3491
Baskaran B, Zou Z and Anderson P W 1987 *Solid State Commun.* **63** 973
Bednorz J G and Muller K A 1986 *Z. Phys.* **B64** 189
Chao K A, Spalek J and Oles A M 1977 *J. Phys.* **C10** L271
Cleveland C L and Medina R 1976 *Am. J. Phys.* **44** 44
Haken H 1976 in *Quantum field theory of solids* (Amsterdam: North Holland) Ch. VII, Ist Ed., p. 296
Kivelson S A, Rokshar D S and Sethna J P 1987 *Phys. Rev.* **B35** 8865
Kulik I O, Entin-Wohlman O and Orbach R 1981 *J. Low Temp. Phys.* **43** 591