Competition and Coexistence between Néel order and d-wave Singlet RVB

Hiroyuki Yamase,^{*a*, *} Hiroshi Kohno^{*b*}

^a RIKEN (The Institute of Physical and Chemical Research), Wako, Saitama 351-0198, Japan ^b Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

Abstract

The coexistence of antiferromagnetism and *d*-wave superconductivity is known to be realized in the two-dimensional t-J model on the square lattice. It is shown in this paper that this coexistence is not a general feature and is significantly suppressed by t'', the third nearest-neighbor hopping. This effect of t'' is argued on the material dependence of '1/8 anomalies' in high- T_c cuprates.

 $Key \ words: \ \text{antiferromagnetism}, \ \text{superconductivity}, \ \text{coexistence}, \ t\text{-}J \ \text{model}, \ \text{cuprates}$

1. Introduction

The coexistence of antiferromagnetism (AF) and dwave superconductivity (dSC) is known to be realized in the two-dimensional (2D) t–J model[1–3] and extended Hubbard model[4,5]. Since these models are believed to be minimal for high- T_c cuprates, it seems that the coexistence might be a general feature in high- T_c cuprates. However, as we report in this paper, such coexistence is controlled by the long-range hopping integral t''(> 0), and is significantly suppressed with a moderate value of t''.

2. Model and Formalism

We take the 2D t-J model on the square lattice:

$$H = -\sum_{i,j,\sigma} t^{(l)} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \qquad (1)$$

defined in the Fock space with no doubly occupied sites. The $\tilde{c}_{i\sigma}$ (S_i) is an electron (a spin) operator. The hopping integrals, $t^{(l)}$, are assumed between the lth ($l \leq 3$)

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nearest-neighbor (n.n.) sites, and we denote $t^{(1)} = t$, $t^{(2)} = t'$, and $t^{(3)} = t''$. The J (> 0) is superexchange coupling between the n.n. spins. We adopt the slaveboson formalism and introduce the slave particles as $\tilde{c}_{i\sigma}^{\dagger} = f_{i\sigma}^{\dagger} b_i$, where $f_{i\sigma} (b_i)$ is a fermion (boson) operator. The local constraint is described by $\sum_{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} + b_i^{\dagger} b_i = 1$ at every site *i*.

To investigate the interplay between AF and dSC, we analyze this model by introducing the following mean fields: the resonating valence bond (RVB), $\chi^{(l)} \equiv \langle \sum_{\sigma} f_i^{\dagger} \sigma f_j \sigma \rangle$, $\langle b_i^{\dagger} b_j \rangle$ and $\Delta_{\tau} \equiv \langle f_i \uparrow f_{i+\tau \downarrow} - f_i \downarrow f_{i+\tau \uparrow} \rangle$ with $\tau = x$, y, and the AF, $m \equiv \frac{1}{2} \langle \sum_{\sigma} \sigma f_i^{\dagger} \sigma f_i \sigma \rangle e^i \mathbf{Q} \cdot \mathbf{r}_i$ with $\mathbf{Q} = (\pi, \pi)$. These mean fields are taken to be real constants independent of lattice coordinate i. Assuming the boson to be condensed at the bottom of its band and loosing the local constraint to the global one, we determine mean fields self-consistently.

3. Results

Figure 1(a) shows the phase diagram on the plane of temperature versus hole density for the band parameter, t/J = 4, t'/t = -1/6 and t''/t = 0, which will be appropriate to LSCO. The $T_{\rm N}$ and $T_{\rm RVB}^{\rm AF}$ are the onset

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^{*} E-mail: yamase@riken.go.jp

Fig. 1. The mean-field phase diagram in the plane of temperature versus hole density for the band parameters, (a) t/J=4, t'/t=-1/6, t''/t=0, and (b) t/J=4, t'/t=-1/6, t''/t=1/5. The $T_{\rm N}$ and $T_{\rm RVB}^{\rm AF}$ are the onset temperatures of the AF and the coexistence with the *d*-RVB, respectively; $T_{\rm RVB}$ and $T_{\rm RVB}^{\rm noAF}$ are those of the *d*-RVB in the absence of the AF.

temperatures of the AF and the coexistence with the d-wave singlet RVB (d-RVB), respectively; here the d-RVB indicates $\Delta_x = -\Delta_y \neq 0$. The T_{RVB} and $T_{\text{RVB}}^{\text{noAF}}$ are the onset temperatures of the d-RVB in the absence of the AF. The $T_{\text{RVB}}^{\text{AF}}$ is lower than $T_{\text{RVB}}^{\text{noAF}}$, which indicates that the AF ordering suppresses the d-RVB. This 0.6^(a) feature is already seen in the early work[3]. The point t/J = in, this study is that Figo 1(a) is qualitatively changedwith $t/t_{\rm H}$ inclusion of t'' of Realistic magnitude. Fig-0.5 ure 1(b) shows the phase diagram for t/J = 4, t'/t = -1% and t''/t = 1/5 the transfer appropri-ate to KBCO. It is seen that the suppression of $T_{\rm RVB}^{\rm AF}$, namely the d-RVB instability in the AF state, is significant in a sange of moderate hole density. This significant_effect of t'' on the coexistence is also seen in 0.1 ho AF instability in the *d*-RVB state, which is shown by the calculation of the static magnetic susceptibility 0 $0.05(q)^{0.1}$ the d_{RVB}^{1} state of d_{RVB}^{1} 0.3 0.6^(b) t/J = 4, t'/t = -1/6 T_N $T_{\rm RVB}^{\rm AF}$ 4. "Diseussion 0.5 $-T_{\rm RVB}$ temperature[J] $- - T_{RVB}^{noAF}$ 0.4 We have found that possible bulk coexistence of AF 0.3 and d-RVB is controlled by $t'' (\ge 0)$. Such bulk coex-0.2 0.1 0 0.05 0.2 0.1 0.15 0.25 0 0.3 hole density

istence is implied in LSCO with hole density around 1/8[7], known as one of the '1/8 anomalies'. Similar anomaly is reported also in YBCO[8] and Bi2212[9] in the μ SR experiments, which is, however, sharply different from the case of LSCO in that the precession of the muon spin is not observed and the Zn-doping is necessary. Since the μ SR data are taken in the dSC state, this material dependence of '1/8 anomalies' may indicate that the coexistence with AF is less favored in YBCO and Bi2212 than in LSCO. From the previous studies, the existence of moderate value of t'' (> 0) is expected in YBCO and Bi2212, and not in LSCO. Therefore, the material dependence of '1/8 anomalies' will be understood by the present effect of t'', namely an intrinsic effect of the electronic system.

5. Summary

In summary, we have found that possible coexistence of AF and *d*-RVB is controlled by t'' (> 0). The material dependence of '1/8 anomalies' will result from this significant effect of t''.

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References

- G. J. Chen et al., Phys. Rev. B 42 (1990) 2662.
- [2] T. Giamarchi and C. Lhuillier, Phys. Rev. B 43 (1991) 12943.
- [3] M. Inaba et al., Physica C 257 (1996) 299.
- [4] M. Kato and K. Machida, Phys. Rev. B 37 (1988) 1510.
- [5] M. Inui et al., Phys. Rev. B 37 (1988) 2320.
- [6] H. Yamase and H. Kohno, Phys. Rev. B 69 (2004) March.
- [7] H. Kimura et al., Phys. Rev. B 59 (1999) 6517.
- [8] M. Akoshima et al., Phys. Rev. B 62 (2000) 6761.
- [9] I. Watanabe et al., Phys. Rev. B 62 (2000) 14524.