Antiferromagnetic phase transition in high-T_c superconductors

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A random-phase-approximation calculation of the antiferromagnetic phase transition temperature T_N for the Zou-Anderson spinor-holon effective Hamiltonian is given. The calculation includes spin-exchange interaction, which enlarges the bandwidth. The results show that at low temperature $k_B T_N/J$ is a function of $\delta U/2t$, where δ is the doping fraction, t the doping integral, and U the Hubbard U.

Recent high-T_c experiments have shown clearly that the low-temperature phase of high-T_c oxides is antiferromagnetic for small doping.[1,2] Not many calculations have concerned the phase transition between paramagnetism and antiferromagnetism. Hasagawa and Fukuyama have calculated the critical temperature T_N as a function of doping fraction δ using a quasi-two-dimensional tight-binding model.[3] A few different theoretical models for high-T_c oxides, including spin-exchange interaction, have been proposed. Zou and Anderson started from the finite-U Hubbard model and proposed a two-dimensional (2D) effective Hamiltonian for large U.[4] In the following we shall start from the Zou-Anderson effective Hamiltonian and discuss the relation between paramagnetic fluctuation and static susceptibility of high-T_c oxides.

Let us start with the 2D Hubbard model

$$H=-t\sum_{\langle ij\rangle\sigma}C_{i\sigma}^{\dagger}C_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i,\sigma}C_{i\sigma}^{\dagger}C_{i\sigma}\,; \qquad (1)$$

here μ is the chemical potential. By introducing the operator transformation

$$C_{i\sigma}^{\dagger}=e_iS_{i\sigma}^{\dagger}+\sigma d_i^{\dagger}S_{i\bar{\sigma}}\,, \qquad (2)$$

where e and d are holon and double occupation field operators, they are both charged-boson fields and S is a neutral fermion field. Operators S, e, and d are satisfied by the following condition:

$$e_i^{\dagger}e_i+d_i^{\dagger}d_i+\sum_{\sigma}S_{i\sigma}^{\dagger}S_{i\sigma}=1\,. \qquad (3)$$

At the large-U case, Zou and Anderson derived the following effective Hamiltonian:[4]

$$H_{\text{eff}}=H_0-J\sum_{\langle ij\rangle}(S_{i\uparrow}^{\dagger}S_{j\downarrow}^{\dagger}S_{j\downarrow}S_{i\uparrow}+S_{i\uparrow}^{\dagger}S_{j\uparrow}S_{j\downarrow}^{\dagger}S_{i\downarrow})\,,$$
$$H_0=-t\sum_{\langle ij\rangle\sigma}(e_ie_j^{\dagger}-d_id_j^{\dagger})S_{i\sigma}^{\dagger}S_{j\sigma}+U\sum_i d_i^{\dagger}d_i+\mu\sum_i(e_i^{\dagger}e_i-d_i^{\dagger}d_i-1)\,, \qquad (4)$$

where $J=4t^2/U$.

Assuming $e_i\to\langle e_i\rangle=\sqrt{\delta}$ and $d_i\to\langle d_i\rangle=0$, after making Fourier transformation the Zou-Anderson effective Hamiltonian can be written as

$$H_{\text{eff}}=H_t+H_J-\mu N(1-\delta)\,. \qquad (5)$$

In Eq. (5) the corresponding terms can be written as

$$H_t=\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k},\sigma}S_{\mathbf{k}\sigma}^{\dagger}S_{\mathbf{k}\sigma} \qquad (6)$$

and

$$H_J=-\frac{J}{2N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma}\gamma_{\mathbf{q}}[S_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger}S_{\mathbf{k}'-\mathbf{q},\bar{\sigma}}^{\dagger}(S_{\mathbf{k}',\bar{\sigma}}S_{\mathbf{k},\sigma}-S_{\mathbf{k}',\sigma}S_{\mathbf{k},\bar{\sigma}})]\,, \qquad (7)$$

where $\varepsilon_{\mathbf{k},\sigma}=-Zt\delta\gamma_{\mathbf{k}}$, $\gamma_{\mathbf{k}}=(1/Z)\sum_{\delta}e^{i\mathbf{k}\cdot\boldsymbol{\delta}}$, and N is the number of the lattice sites.

In an external magnetic field $\mathbf{B}=\hat{\mathbf{z}}B\cos\mathbf{q}\cdot\mathbf{r}$, where $\mathbf{q}$ and $\mathbf{r}$ are on the XY plane and $\hat{\mathbf{z}}$ is a unit vector. The system has a Zeeman energy

$$H_Z=-\frac{B}{2}[M_Z(\mathbf{q})+M_Z(-\mathbf{q})]\,, \qquad (8)$$

where

$$M_Z(\mathbf{q})=\tfrac{1}{2}g\mu_B\sum_{\mathbf{k}}m_{\mathbf{k},\mathbf{q}} \qquad (9)$$

and

$$m_{\mathbf{k},\mathbf{q}}=S_{\mathbf{k}-\mathbf{q},\uparrow}^{\dagger}S_{\mathbf{k},\uparrow}-S_{\mathbf{k}-\mathbf{q},\downarrow}^{\dagger}S_{\mathbf{k},\downarrow}\,. \qquad (10)$$

Here g is the Landé factor and μ_B is the Bohr magneton.

A random-phase approximation is allowed for $\delta>t/U$ and the resulting susceptibility is

$$\chi(\mathbf{q})=\frac{\chi_0(\mathbf{q})}{1+\tilde{J}(\mathbf{q})\chi_0(\mathbf{q})}\,, \qquad (11)$$

where

$$\chi_0(\mathbf{q})=\frac{g^2\mu_B^2}{4N}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}-f_{\mathbf{k}-\mathbf{q}}}{\tilde{\varepsilon}_{\mathbf{k}-\mathbf{q}}-\tilde{\varepsilon}_{\mathbf{k}}}, \tag{12}$$

$$f_{\mathbf{k}}=\frac{1}{e^{\beta\tilde{\varepsilon}_{\mathbf{k}}}+1}, \tag{13}$$

$$\tilde{J}(\mathbf{q})=\frac{4J\gamma_{\mathbf{q}}}{g^2\mu_B^2}, \tag{14}$$

$$\tilde{\varepsilon}_{\mathbf{k}}=\varepsilon_{\mathbf{k}}-\frac{J}{N}\sum_{\mathbf{k}'}\gamma_{\mathbf{k}-\mathbf{k}'}f_{\mathbf{k}'}. \tag{15}$$

The bare spinor energy has been renormalized and the second term in the right-hand side of Eq. (15) comes from the spin-exchange term

$$\frac{J}{2N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma}\gamma_{\mathbf{q}}S^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}S^{\dagger}_{\mathbf{k}'-\mathbf{q},\bar{\sigma}}S_{\mathbf{k}',\sigma}S_{\mathbf{k},\bar{\sigma}}$$

in Eq. (7). For small doping δ the effective bandwidth $2W=8\delta t$ is also small. By using the logarithmic density-of-states (DOS) approximation, the density of states near the Fermi surface is

$$g(\varepsilon)=\frac{2}{\pi^2 W}\ln\left|\frac{4W}{\varepsilon}\right|. \tag{16}$$

With Eq. (16) as the approximate density of states, at low temperature the spin-exchange contribution could be obtained as

$$-\frac{J}{N}\sum_{\mathbf{k}}\gamma_{\mathbf{k}-\mathbf{k}'}f_{\mathbf{k}'}=-8t(\cos k_x+\cos k_y)\left[\frac{\theta}{\pi^2}(\ln 2+\tfrac{1}{4})\right], \tag{17}$$

where $\theta=2t/U$. When $\delta t>J$, the effect of spin fluctuation is to enlarge the bandwidth. We shall use

$$2\tilde{W}=8t\left[\delta+\frac{4\theta}{\pi^2}(\ln 2+\tfrac{1}{4})\right] \tag{18}$$

as the effective bandwidth in the following calculation.

To calculate the critical temperature T_N for the phase transition between paramagnetism and antiferromagnetism, we take $\mathbf{q}=\hat{\mathbf{Q}}\equiv(\pi/a,\pi/a)$ as usual, here a is the lattice spacing. At low temperature the Van Hove singularity gives

$$\frac{1}{N}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}-f_{\mathbf{k}-\hat{\mathbf{Q}}}}{\tilde{\varepsilon}_{\mathbf{k}-\hat{\mathbf{Q}}}-\tilde{\varepsilon}_{\mathbf{k}}}\cong\frac{2}{\pi^2\tilde{W}}\ln^2\frac{\tilde{W}}{2k_BT}, \tag{19}$$

where k_B is the Boltzman constant. The Néel temperature T_N is

$$\frac{k_BT_N}{J}=\left[\frac{\delta}{\theta}+\frac{4}{\pi^2}(\ln 2+\tfrac{1}{4})\right]\times\exp\left[-\pi\left[\delta+\frac{4\theta}{\pi^2}(\ln 2+\tfrac{1}{4})\right]\Big/2\theta\right]^{1/2}. \tag{20}$$

The above result shows that k_BT_N/J is only the function of δ/θ for large-U Hubbard model at low temperature and $\delta>t/U$. In Fig. 1 we plotted k_BT_N/J as a function of δ/θ, which shows that a small increase of doping will cause a rapid decrease of T_N. This is consistent with Nagaoka's result.[5]

Constraint (3) has not been considered in the above calculations. This is equivalent to our neglecting the chemical potential μ. A more detailed calculation[6] shows that the chemical potential μ will play an important role in changing effective bandwidth for finite δ. But μ can be neglected for small δ ($\delta\le 0.05$).

Figure 2 is the result of the variational Monte Carlo calculation for large-U Hubbard model given by Yokoyama and Shiba.[7] The straight line for $\delta=8t/\pi^2U$ has been

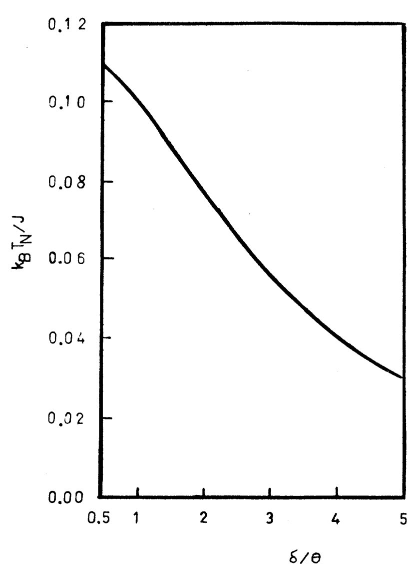

FIG. 1. k_BT_N/J vs δ/θ.

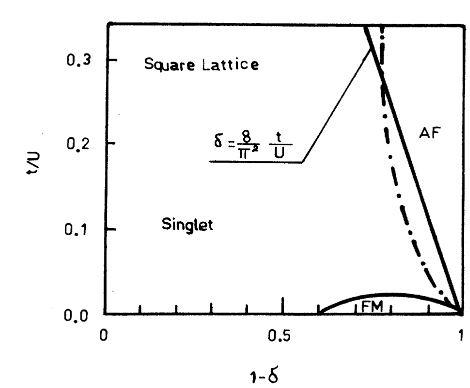

FIG. 2. The phase diagram of 2D square-lattice Hubbard model given in Ref. 7. The straight line was added by us. On the left-hand side of the line RPA calculation is valid.

added by us. We can see that on the left-hand side of the line ($\delta > 8t/\pi^2 U$) there exists a antiferromagnetic region, and a random-phase-approximation (RPA) calculation may apply to the region. On the right-hand side of the line ($\delta < 8t/\pi^2 U$), the RPA scheme is invalid.

Starting from the effective Hamiltonian [Eq. (1)] by solving the Gor'kov equation we can also obtain the spinor-gap equation

$$\Delta(\mathbf{p}) = \frac{ZJ}{N}\sum_{\mathbf{q}} \gamma_{\mathbf{q}} \langle S_{\mathbf{q}-\mathbf{p},\uparrow} S_{\mathbf{p}-\mathbf{q},\downarrow} - S_{\mathbf{q}-\mathbf{p},\downarrow} S_{\mathbf{p}-\mathbf{q},\uparrow}\rangle$$

$$= \frac{ZJ}{N}\sum_{\mathbf{q}} \gamma_{\mathbf{q}} \Delta(\mathbf{p}-\mathbf{q}) \frac{\tanh \frac{1}{2}\beta E_{\mathbf{p}-\mathbf{q}}}{E_{\mathbf{p}-\mathbf{q}}}, \quad (21)$$

where

$$E(\mathbf{p}) = [\xi^2(\mathbf{p}) + \Delta^2(\mathbf{p})]^{1/2},$$

$$\xi_{\mathbf{p}} = \tilde{\varepsilon}_{\mathbf{p}} - \mu - \frac{ZJ}{N}\gamma(0)\sum_{\mathbf{q}} f(\mathbf{q}). \quad (22)$$

This superconducting-gap equation (21) is formally consistent with Ref. 8, provided that we do not stress on the resonating-valence-band assumption. The detailed calculation of the relation between the doping fraction δ and superconducting transition temperature T_{sc} will be discussed in a future paper.[6]

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