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Heat Capacity and Magnetoresistance of a Lightly Doped Two-Dimensional Antiferromagnet in the Noncollinear Phase

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Abstract—The energy spectrum of mobile charge carriers in a two-dimensional Antiferromagnet placed in external magnetic field is analyzed. It is shown that allowing for the magnetic sublattice skew the effective mass of mobile charge carriers in a lightly doped Antiferromagnet. This affects substantially the transport and thermodynamic properties of the system. A insulator–semimetal transition is induced with external magnetic field.

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INTRODUCTION

The kinetic properties of systems with antiferromagnetic ordering are of special interest due to most intermetallides being characterized by antiferromagnetic ordering below 3–6 K [1–3]. Placing such substances in a magnetic field of ~ 20 kOe skews the magnetic sublattice and thus modifies the electronic energy spectrum.

METHOD

The Hamiltonian function for an Antiferromagnet is written as the sum of four summands,

$$\hat{H} = \hat{T} + \hat{H}_{sd} + \hat{H}_{dd} + \hat{H}_h,$$

where $\hat{T} = \sum_{ll'\sigma} t_{ll'} a^+_{l\sigma} a_{l\sigma}$ is kinetic energy operator of collective electrons in Wannier representation; $\hat{H}_{sd} = J\sum_l \vec{S}_l\vec{\sigma}_l$ is the exchange interaction *s-d* operator; $\hat{H}_{dd} = \sum_{ll'} I_{ll'}\vec{S}_l\vec{S}_{l'}$ is the operator of exchange interaction between localized electrons; and $\hat{H}_h = -2\mu_B H\sum_l\left(S^z_l + \sigma^z_l\right)$ is the operator reflecting the energy of Zeeman interaction between localized and collective electrons and an external magnetic field oriented along the *Oz* axis.

In the mean field approximation at $T = 0$, the average value of the projection of sublattice spin moments onto the direction of the magnetic field controlling the sublattice skew takes the form

$$R_\parallel = \frac{\mu_B H}{K_0}, \quad H < \frac{K_0 S}{\mu_B}; \quad R_\parallel = S, \quad H > \frac{K_0 S}{\mu_B}.$$

In this case, the effect of collective electrons on a localized subsystem is not considered.

The Hamiltonian function describing the system of mobile charge carriers is

$$\begin{aligned}\hat{H}_{coll} &= \sum_{ff'\sigma} t_{ff'} a^+_{f\sigma} a_{f'\sigma} + \sum_{\sigma gg'} t_{gg'} b^+_{g\sigma} b_{g'\sigma} \\ &+ \sum_{fg\sigma} t_{fg}\left(a^+_{f\sigma} b_{g\sigma} + b^+_{g\sigma} a_{f\sigma}\right) \\ &+ \sum_{f\sigma} J\left(R_\parallel \sigma a^+_{f\sigma} a_{f\sigma} + \frac{1}{2} R_\perp a^+_{f\sigma} a_{f\bar{\sigma}}\right) \\ &+ \sum_{g\sigma} J\left(R_\parallel \sigma b^+_{g\sigma} b_{g\sigma} - \frac{1}{2} R_\perp b^+_{g\sigma} b_{g\bar{\sigma}}\right) \\ &- 2\mu_B H\left(\sum_{f\sigma} \sigma a^+_{f\sigma} a_{f\sigma} + \sum_{g\sigma} \sigma b^+_{g\sigma} b_{g\sigma}\right).\end{aligned} \tag{1}$$

This is a transition to the two-sublattice form, while the *s–d* exchange interaction between localized and collective subsystems is given in the mean field approximation. After transitioning to a quasi-momentum form, it is easy to obtain the Fermi excitation energy spectrum:

$$E^\pm_{k\sigma} = t_k \pm \sqrt{\left(-\Gamma_k + \sigma\left(JR_\parallel - 2\mu_B H\right)\right)^2 + \frac{1}{4}J^2 R^2_\perp},$$

where $t_k = 2t_2\left(\cos k_x + \cos k_y\right) + 4t_3 \cos k_x \cos k_y$, $\Gamma_k = 4t_1 \cos\left(k_x/2\right)\cos\left(k_y/2\right)$ is the Fourier transform of jump intervals within a sublattice and between different sublattices, $R_\perp = \sqrt{1 - R^2_\parallel}$. In this case, a quasi-momentum ranges over the Brilloin magnetic zone values. Detailed data on the energy spectrum of a noncollinear Antiferromagnet are given in [4].

Here and below, the energy parameters are selected such that the Fermi surface with low doping lies near the points $(0, \pm\pi)$ and $(\pm\pi, 0)$ in the Brilloin magnetic zone,

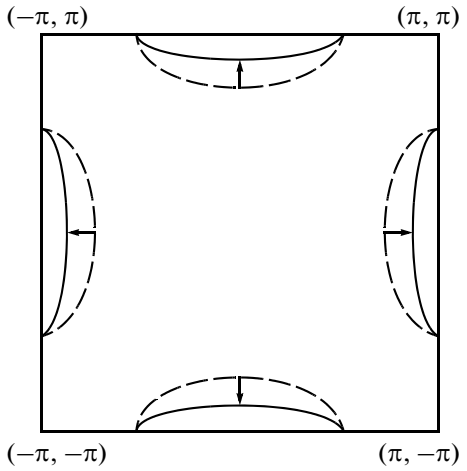

Fig. 1. Fermi surface variations upon applying a magnetic field.

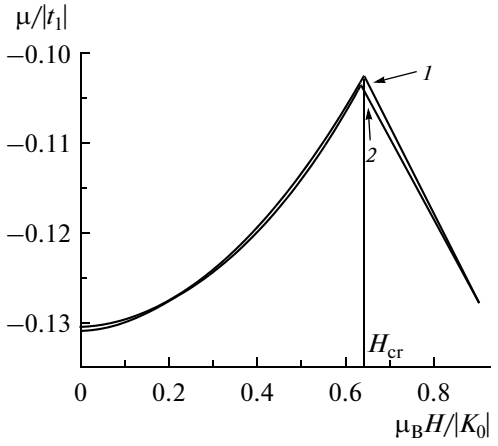

Fig. 2. Dependence of the chemical potential on an external magnetic field in the case of a lightly doped two-dimensional Antiferromagnet. (*1*) Numerically exact solution, (*2*) analytical solution. H_{cr} is the magnetic field value resulting in the intersection of upper and lower subbands.

corresponding to the ARPES data [5] for $YBa_2Cu_3O_{6+x}$ compound. The conditions for selecting parameters then take the form

$$t_2 > 2t_3, \quad 16t_1^2 + \left(\frac{JS}{2}\right)^2 > \left(4t_2 + 8t_3 + \frac{JS}{2}\right)^2.$$

This approach assumes we disregard the Hubbard correlations in order to demonstrate the effect of magnetic sublattice skew. The lower completely filled zone corresponds to the dielectric phase. This means there is no doping, and no current carriers are observed in the system. From the standpoint of energy-band structure, this situation is possible only if the upper and lower antiferromagnetic subbands do not overlap at $H = 0$. The mathematical relation is

$$2t_2 < \frac{JS}{2} + 4t_3.$$

In the relaxation time approximation, the conductivity of a two-dimensional lightly doped Antiferromagnet in a zero magnetic field is determined by the function

$$\sigma = \frac{1}{2}e^2\tau n_h\left(\frac{1}{m_1} + \frac{1}{m_2}\right),$$

where m_1 and m_2 are effective mass values determined by the relation

$$\frac{\hbar^2}{2m_1b^2} = \left(\frac{4t_1^2}{JS} - t_2 - 2t_3\right), \quad \frac{\hbar^2}{2m_2b^2} = (t_2 - 2t_3),$$

where n_h is the concentration of vacant sites in the lower subband and b is the magnetic lattice parameter.

Inclusion of the magnetic field results in considerable variation of the energy spectrum. This effect is especially strong near the upper edge of the lower energy subband. Applying our selected relations between parameters, the lowest effective mass varies considerably (Fig. 1):

$$m_1 = \frac{\hbar^2}{b^2}\frac{JS}{8t_1^2}\sqrt{1 - \left(\frac{\mu_B H}{K_0 S}\right)^2}.$$

Under relatively weak magnetic fields, this results in the appearance of negative magnetoresistance in the system,

$$\sigma(H) = \sigma(0)\left[1 + \frac{1}{2}\left(\frac{\mu_B H}{K_0 S}\right)^2\right], \quad \frac{\mu_B H}{K_0} \ll S.$$

Since the magnetoresistance effect is due to the reconstruction of energy structure of mobile charge carriers, analogous variations ought to be observed in the specific heat of an Antiferromagnet. The electronic specific heat at low temperatures is described by a linear law. Interaction between collective charge carriers and a localized magnetic structure can considerably lower the linear heat capacity upon the application of a magnetic field:

$$C_{mol} = \gamma T, \quad \gamma(H) = \gamma(0)\left[1 - \frac{1}{4}\left(\frac{\mu_B H}{K_0 S}\right)^2\right],$$

$$\gamma(0) = N_A k_B^2 T\frac{\pi^2 g(\varepsilon_F)}{3} = \frac{\pi^3}{6}\left(\frac{k_B T}{t_1}\right)\sqrt{\frac{JS}{t_2 - 2t_3}}N_A k_B.$$

In sufficiently great magnetic fields, less then spin-flip transition value, the intersection of the subbands occur since the minimum of the upper energy subband and the maximum of the lower energy subband are found at different points of quasi-impulse space. An undoped Antiferromagnet (with a completely filled lower subband), being a dielectric material in a zero magnetic field, is transformed into semimetal, while a lightly doped substance is characterized by a rapid increase in the number of carriers in both subbands and a rise in the external magnetic field (Fig. 2). The

relation for the critical magnetic field value of such a transition takes the form

$$JS\sqrt{1-A^2} - 4t_2 + 8t_3 - \frac{2n_h b^2 \pi \sqrt{t_2 - 2t_3}|t_1|}{\sqrt{JS}\sqrt[4]{1-A^2}} = 0,$$
$$A = \frac{\mu_B H_{cr}}{K_0 S}.$$

CONCLUSIONS

A two-dimensional Antiferromagnet placed in an external magnetic field was investigated. Magnetic sublattice skew resulted in variations of the effective mass of the mobile charge carriers in a lightly doped Antiferromagnet. This effect reveals itself in negative magnetoresistance and a drop in the electronic specific heat of the Antiferromagnet. Insulator–semimetall transition occured in relatively strong magnetic field. It should be noted that allowing for the collective subsystem effect on a localized system results in quantitative variation in the stability of qualitative conclusions.

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