Electron paramagnetism in antiferromagnets

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(Submitted 4 April 1989)
Pis'ma Zh. Eksp. Teor. Fiz. **49**, No. 10, 557–559 (25 May 1989)

The nature of the degeneracy of band and localized electron states in an antiferromagnet and their behavior in a magnetic field are analyzed. Structural features have been found in the g-factor: At the edge of the magnetic Brillouin zone, a transverse field does not lift the degeneracy, while localized states at defects are completely nondegenerate.

Measurements of the magnetic susceptibility constitute one of the basic methods for a primary characterization of the electronic properties of materials. Information on the state density at the Fermi level, N_F, is extracted from the Pauli susceptibility χ_P, and the density of localized states, ν, is found from the Curie law:

$$\chi_P = g^2 N_F \qquad \chi_C = g^2 \nu / T. \tag{1}$$

Here T is the temperature, and g is the Zeeman splitting factor ($\pm gH$; the Bohr magneton is 1). For a weak spin-orbit coupling it is natural to assume $g = g_0 \approx 2$.

In this letter we show that spin paramagnetism has several distinctive features when the electrons are studied in an antiferromagnetically ordered crystal. These effects should be manifested in several magnetic semiconductors,[1,2] including high-temperature superconducting compounds of the La_2CuO_4 or $YBa_2Cu_3O_6$ type in an insulating phase, quasi-1D materials with a spin density wave, and other systems with an

intrinsic antiferromagnetic state of band electrons.[3] We formulate several model-independent assertions which can be derived rigorously by a group-theory analysis[4] or which can be found in the weak-coupling model for a spin density wave.

We first consider *band states* for excitations or for small electron (or hole) pockets above the insulator (Hubbard) gap caused by the antiferromagnetic order. It can be shown that the g-factor splits into two components, $g_{\|}$ and $g_{\perp}$, for the different directions of the field $\mathbf{H} = (H_{\|}, H_{\perp})$ with respect to the antiferromagnetic order vector $\mathbf{s}$. The components g_i are always different and generally depend on the position of the wave vector $\mathbf{k}$ in the Brillouin zone. The function $g_{\|}(\mathbf{k})$ generally does not have singularities, and in the weak-coupling model we have $g_{\|}(\mathbf{k}) = g_0$. However, $g_{\perp}(\mathbf{k})$ does exhibit a characteristic property: We have $g_{\perp}(\mathbf{k}) = 0$ on the set of wave vectors $\{\mathbf{k}\}$ which satisfy the condition that the vectors $\mathbf{k}$ and $(\mathbf{k} + \mathbf{Q})$ are equivalent in the symmetry of the nonmagnetic lattice. Here $\mathbf{Q}$ is the magnetic order vector. For an antiferromagnet of the type of a doubling of the period of a square lattice, we would have $\mathbf{Q} = (\pi, \pm\pi)$. Consequently, $g_{\perp}(\mathbf{k})$ vanishes at the boundary of the magnetic Brillouin zone, i.e., for electron and hole states near the edge of the gap opened by the formation of the antiferromagnetism. Upon a deviation by a wave vector δk_x or δk_y from the point of the common position at the boundary of the magnetic Brillouin zone, we have $g_{\perp} \propto \delta k \xi_0$, and at singular points with a Van Hove singularity we have $g_{\perp} \propto \delta k_x \delta k_y \xi_0^2$, where ξ_0 is the coherence length for an antiferromagnetic state.

These results can be derived in an elementary way in the weak-coupling model (Ref. 3, for example) through a diagonalization of the obvious Hamiltonian

$$\begin{pmatrix} \epsilon(\mathbf{k}) + \mathbf{H}\vec{\sigma} & \Delta\, \mathbf{s}\vec{\sigma} \\ \Delta\, \mathbf{s}\vec{\sigma} & \epsilon(\mathbf{k}+\mathbf{Q}) + \mathbf{H}\vec{\sigma} \end{pmatrix}, \tag{2}$$

where $\epsilon(\mathbf{k})$ is the spectrum in the metallic phase, and 2Δ is the gap in the spectrum for the antiferromagnetic phase. We find an equation for the spectrum:

$$(\epsilon - \eta(\mathbf{k}) - \mathbf{H}_{\|}\sigma)^2 - (\xi(\mathbf{k}) - \mathbf{H}_{\perp}\vec{\sigma})^2 - \Delta^2 = 0 \tag{3}$$

$$\eta(\mathbf{k}) = \frac{1}{2}[\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}+\mathbf{Q})], \qquad \xi(\mathbf{k}) = \frac{1}{2}[\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}+\mathbf{Q})] \tag{4}$$

$$\mathbf{H}_{\|} = \mathbf{s}(\mathbf{H}\mathbf{s}), \qquad \mathbf{H}_{\perp} = \mathbf{H} - \mathbf{H}_{\|}.$$

At the boundary of the magnetic Brillouin zone we always have $\xi(\mathbf{k}) \equiv 0$, and with exact nesting, even in 1D systems, the relation $\eta(\mathbf{k}) \equiv 0$ also holds. We see that the assertions formulated above may apply not only for the boundary of the spin zone but also at points of random degeneracy, $\xi(\mathbf{k}) = 0$.

Equations (3) and (4) take a particularly simple form in the case of a 1D system near the edge of the spectrum:

$$\epsilon(\mathbf{q}) = \Delta + \mathbf{H}_{\|}\vec{\sigma} + \frac{1}{2\Delta}(v_F \mathbf{q} + \mathbf{H}_{\perp}\vec{\sigma})^2. \tag{5}$$

We see that $\mathbf{H}_{\perp}$ splits the spectrum not in terms of energy, as an ordinary Zeeman

term would, but in terms of momentum, shifting the minimum of the zone to the points $\pm H_\perp / v_F$. In other words, a transverse magnetic field is equivalent to a disruption of inversion. For non-1D systems with nesting, the value of q in (5) is understood as the deviation from the normal to the boundary of the magnetic Brillouin zone.

A pronounced suppression of the static paramagnetism is seen at large deviations of the direction of **H** from that of **s**. Even at small deviations, however, we should see an anomalous broadening and then a loss of the ESR signal as a result of a dispersion of the resonant frequency in terms of the electron momentum. This effect will occur in both the metallic and thermally activated concentration regimes. Note also the interplay between the static orbital and resonant spin effects due to the change in the g-factor along the constant-energy path of spectrum (5).

Impurity states. We turn now to localized electron states at defects in an antiferromagnetic lattice. With an eye on the CuO_2 plane in a high-temperature superconducting compound, we can consider the cases of (I) site-site and (II) single-site defects corresponding to a replacement of the oxygen and the copper. In the site representation for model (2) the system is described by the Hamiltonian

$$\sum_{\mathbf{n},\mathbf{m}} t(\mathbf{n},\mathbf{m})\, c_{\mathbf{n}}^{+} c_{\mathbf{m}} + \sum_{\mathbf{n}} [\Delta(\mathbf{n})\, e^{i\mathbf{Q}\mathbf{n}}\, c_{\mathbf{n}}^{+}\, \mathbf{s}\vec{\sigma}\, c_{\mathbf{n}} + h.c.] \tag{6}$$

$$t(\mathbf{n},\mathbf{m}) = t(\mathbf{n}-\mathbf{m}) + \tau(\mathbf{n},\mathbf{m}), \quad \mathbf{n} = (n_x, n_y), \quad \Delta(\mathbf{n}) = \Delta + \delta(\mathbf{n}),$$

where $t(\mathbf{I})$ is the Fourier transform of $\epsilon(\mathbf{k})$ in (2), and τ and δ describe the defects of types I and II. It turns out that in case I no bound states form. In case II, bound states appear in the case of nesting or near saddle points. Elementary calculations show that the depth of a bound state, ω, can be found from the condition

$$A\frac{\Delta}{\epsilon_F}\left[\frac{\Delta}{\omega}\right]^{1/2} \propto 1/\lambda, \qquad A \propto \ln\frac{\epsilon_F^2}{\Delta\omega}\,. \tag{7}$$

The expression for A in (7) refers to a system with a saddle point in $\epsilon(\mathbf{k})$. In general, we would have $A \approx \text{const} \propto 1$. The quantity λ determines the strength of a defect: $\delta(\mathbf{n}) = -\lambda\delta_{\mathbf{n},0}$. In the present context, the fact that the degeneracy of the localized states is lifted even without a magnetic field is important. The levels of these states, $\pm(\Delta - \omega)$, are positioned symmetrically in the $(-\Delta, +\Delta)$ gap; each corresponds to only a single projection onto the **s** axis. The absence of a degeneracy is explained on the basis that in the presence of a defect of type II the system loses its symmetry under transformations RT and RI (R is time reversal, T is translation, and I is inversion), which are responsible for an analog of Kramers degeneracy for a pure system and for a defect of type I. Consequently, these states will not contribute to the magnetic susceptibility at all. The observation of a Curie law for χ_C in (1) characterizes the concentrations of only those defects which are unrelated to the antiferromagnetic subsystem.

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Translated by Dave Parsons