Phase separation in magnetically ordered semimetals and half-metals

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Abstract

We derived a free energy functional, which describes the transition from uniformly ordered magnetic state into a phase-separated or phase-modulated state in semimetals and half-metals. Considering the energy of the slightly inhomogeneous electron gas in the Hohenberg-Kohn approximation, we showed that the scale of the phase-separated regions is fixed by the Coulomb screening of the carriers, and is of order of several lattice constants.

Key words: doped magnets; phase separation; EuB_6; manganites

Phase separation (PS) in magnetic systems, with a small concentration, n_0, of electrons per localized spin (LS), e.g. in slightly doped manganites, has attracted considerable attention recently. (For a review, see [1]).

We consider in this paper the properties of phase-separated systems in the vicinity of the transition point (or line). Close to the transition point the electron gas is only slightly inhomogeneous, i.e. the electron density, $n(\mathbf{r})$, has the form $n(\mathbf{r}) = n_0 + \tilde{n}(\mathbf{r})$, with $\tilde{n}(\mathbf{r})/n_0 \ll 1$, and $\tilde{n}_{\mathbf{q}=\mathbf{0}} = 0$, where $\tilde{n}_{\mathbf{q}}$ is the Fourier transform of $\tilde{n}(\mathbf{r})$. Using the Hohenberg-Kohn expression for the free-energy functional (FEF) of a slightly inhomogeneous electron gas [2], we obtain the FEF, $F[\tilde{n}_{\mathbf{q}}]$, of the system as follows

$$F[\tilde{n}_{\mathbf{q}}] = \sum_{\mathbf{q}} r_{\mathbf{q}} \tilde{n}_{\mathbf{q}} \tilde{n}_{-\mathbf{q}} + b \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} \tilde{n}_{\mathbf{q}_1} \tilde{n}_{\mathbf{q}_2} \tilde{n}_{\mathbf{q}_3} \delta(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3) + c \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3 \mathbf{q}_4} \tilde{n}_{\mathbf{q}_1} \tilde{n}_{\mathbf{q}_2} \tilde{n}_{\mathbf{q}_3} \tilde{n}_{\mathbf{q}_4} \delta(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \mathbf{q}_4). \quad (1)$$

Here

$$r(\mathbf{q}) = \frac{\partial^2 f(n,\eta)}{\partial n^2} + \frac{1}{2\mathcal{N}} \left(\frac{\kappa^2}{q^2} + \frac{q^2}{12 k_F^2} \right) = \frac{\partial^2 f(n,\eta)}{\partial n^2} + \frac{1}{2\mathcal{N}} \left[\frac{\kappa}{\sqrt{3} k_F} + \frac{\kappa^2}{q^2} \left(1 - \frac{q^2}{q_0^2} \right)^2 \right], \quad (2)$$

where $f(n,\eta)$ includes the free energy of the magnetic system and the electron kinetic energy, η stands for the temperature, T, magnetic field, H, and other parameters, specifying the free energy, $\mathcal{N}$ is the electron density of states at the Fermi energy, κ^{-1} is the Thomas-Fermi screening length, ϵ_F and k_F are the Fermi energy and the Fermi wave vector, and

$$q_0^2 = 2\sqrt{3} k_F \kappa. \quad (3)$$

b and c in Eq. (1) are constants, which depend on ϵ_F and n_0.

We suppose that the Coulomb interaction is weak, and hence, $\kappa \ll k_F$, $q_0^2 \ll (2k_F)^2$.

The Ginzburg-Landau FEF (1) describes a first order liquid-solid-like transition into a periodic structure, with the magnitude of the reciprocal lattice vectors close to q_0. The transition happens at the the critical line $\eta_c(n_0)$ given approximately by

$$g(n,\eta) \equiv \frac{1}{2\mathcal{N}} \frac{\partial^2 f(n,\eta)}{\partial n^2} = 0. \quad (4)$$

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If the electron spectrum is anisotropic, the inhomogeneous fluctuations at the transition point grow in some special direction. In this case the triad of vectors $\mathbf{q}_0$ cannot be add to zero, and the third-order term in the functional (1) vanishes. As a result, the transition into the PS state becomes a second order phase transition.

Consider now two systems, which can be described by this approach.

Europium hexaboride. This is a ferromagnetic semimetal (FSM), with n_0 of order of $10^{-3} - 10^{-2}$ [3]. The Eu spins (S=7/2) order due to the RKKY indirect coupling. The Fermi energy is much smaller than the s-f exchange energy, JS, which in his turn is smaller than the band width. The polarized carriers act on the LS as a molecular field, proportional to $n(\mathbf{r})$. Hence, the nonuniform fluctuations of $n(\mathbf{r})$ lead to the fluctuation of the free energy of the LS. The function $g(n_0, \eta)$ is [4]

$$g(n_0, \eta) = 1 - \frac{3J^2 n_0}{2\epsilon_F T} B'\Big(\frac{Jn_0 + g\mu_B H}{T}\Big), \qquad (5)$$

where $B(x)$ is the Brillouin function, $B'(x) = dB(x)/dx$.

Fig. 1 shows the phase diagram, which follows in this case from Eqs. (4) and (5).

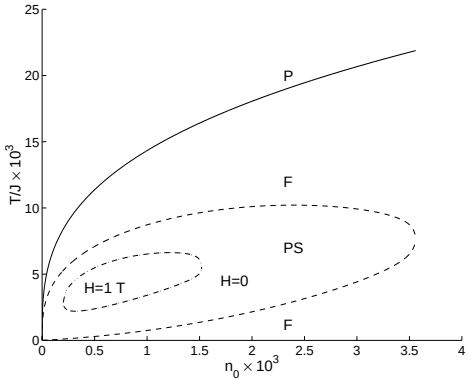

Fig. 1. Phase diagram of a FSM, with $J = 0.1$ eV, $S = 3.5$. The dashed (dashed-dotted) line enclose the phase-separated region, PS, in zero(finite) magnetic field. P and F denote paramagnetic and ferromagnetic phases.

The results account qualitatively for most of the peculiar magnetic properties of EuB_6 [4]. Specifically, they explain naturally the sequence of transition temperatures observed in this ferromagnet [3,5] as well as the strong effect of a magnetic field on the transition temperature into the PS state [3].

Slightly doped manganites. The competition between the antiferromagnetic (AF) exchange, I, and the double exchange in manganites results in canting of the AF ground state [6]. In the G-type AF the canted state is unstable against phase separation at small n. The kinetic energy of the electrons, stabilizes the canted state, if n is larger than $n_c \approx (9/4)^{3/2}(6\pi^2)^{-1} \approx 0.056$ (see Ref. [7] and references therein). The function $g(n_0, \eta)$ depends only on n_0, and is proportional to $n_0^{3/2} - n_c^{3/2}$. Since the electron spectrum in the manganites is anisotropic, we expect that the phase transition into the PS state is of the second order type. In the PS state a stripe-like structure is formed, with the typical scale of the inhomogeneity, $r_0 \sim q_0^{-1}$, determined by the competition between the Coulomb energy, which tends to decrease r_0, and the gradient energy, which tends to increase it. It is understand here that q_0, (3), is properly modified to take into account the anisotropy of the spectrum. The scale r_0 is of order of several lattice constants. In the A-type AF the increase of the kinetic energy with n is weaker than in the G-type AF. The function g does not depend on n_0, and is equal to

$$g(t, t') \propto 9.11\Big(\frac{4IS^2 t'}{t^2}\Big)^{2/3} - 1, \qquad (6)$$

where $t'(t)$ is the hopping integral across (in) the ferromagnetic layer. The canting happens, if t' is larger than some critical value. The above theory holds if t is close to the critical value.

Acknowledgements

I acknowledge discussions with A. Aharony and O. Entin-Wohlman. This work was supported by the German-Israeli Foundation.

References

[1] E. Dagoto, T. Hotta, A. Moreo, Phys. Rep. **344** (2001) 1.

[2] P. Hohenberg, W. Kohn, Phys. Rev. **136** (1964) B864.

[3] S. Süllow *et al.*, Phys. Rev. B **57** (1998) 5860.

[4] I. Ya Korenblit, Phys. Rev. B **64** (2001) 100405(R).

[5] L. Degiorgi *et al.*, Phys. Rev. Lett. **79** (1997) 14541.

[6] P. G. de Gennes, Phys. Rev. **82** (1960) 403.

[7] M. Yu. Kagan, D. I. Khomskii, M. V. Mostovoy, Eur. Phys. J. B **12** (1999) 217.