Magnetic field effect on the phase diagram of electron systems with imperfect nesting

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Fermi surface nesting is a very popular and important concept in condensed matter physics. The existence of two fragments of the Fermi surface, which can be matched upon translation by a certain reciprocal lattice vector (nesting vector), entails an instability of a Fermi liquid state. A superstructure or additional order parameter related to nesting vector is generated due to the instability. The nesting is widely invoked for the analysis of charge density wave (CDW) states, spin density waves (SDW) states, mechanisms of high-T_c superconductivity, fluctuating charge/orbital modulation in magnetic oxides, chromium and its alloys, etc.

It is important to emphasize that in a real material the nesting may be imperfect, i.e. the Fermi surface fragments can only match approximately. One of the earliest studies of imperfect nesting was performed in the context of chromium and its alloys [1]. Quite recently, it was demonstrated that the imperfect-nesting mechanism can be responsible for the nanoscale phase separation in chromium alloys [2], iron-based superconductors [3], and in doped bilayer graphene [4] In this context, the studies of spin and charge inhomogeneities related to the imperfect nesting are currently especially active in the physics of low-dimensional compounds. Other types of inhomogeneous states ("stripes", domain walls) were also discussed in the literature in the framework of similar models. Moreover, it was shown that the possibility of SDW ordering in systems with itinerant charge carriers results in very rich and complicated phase diagrams involving phase-separation [5].

An applied magnetic field *B* alters the quasiparticle states, changing the nesting conditions. In the present paper, we explore the physical consequences of the external magnetic field for electron systems with imperfect nesting. Such study may be relevant, in particular, for recent experiments on doped rare-earth borides [6].

We have found that, when the cyclotron frequency ω_c is comparable to the electron energy gap, Δ_0, the magnetic field effects must be taken into account. The magnetic field enters the model Hamiltonian via two channels: (i) the Zeeman term, and (ii) orbital (or, diamagnetic) contribution. At low field, $\omega_c < \Delta_0$, and not too small *g* factors, one can neglect the latter contribution and take into account only the Zeeman term. We investigated the combined effects of both terms in the limit of ideal electron-hole symmetry and ideal nesting.

Our study demonstrates that in the presence of the Zeeman term, the number of possible homogeneous magnetically-ordered phases significantly increases, compared to the case of B=0. We have found as many as nine possible states with different symmetries. If necessary, this list may be increased by taking into account incommensurate SDW phases and phases with "stripes". Of this abundance, only two ordered homogeneous phases could serve as a ground state of our model [7]. When inhomogeneous states are included into consideration, even the zero-temperature phase diagram becomes quite complex. However, the obtained phase diagram is unlikely to be universal: in the situation where many states with similar energies compete against each other to become the ground state, it is impossible to predict accurately the outcome of this competition. Needless to say, the simplifications of our approach, and the contributions which we have intentionally omitted (lattice effects, realistic shape of the Fermi surface, disorder), can play a quite important role in the final balance. Thus, a broad input from experiments is crucial for the correct identification of different thermodynamic phases.

The orbital contribution to the Hamiltonian leads to the Landau quantization of the single-particle orbits. As a result, we have demonstrated that both order parameters and the Néel temperatures T_N oscillate as the magnetic field changes. This behavior is associated with the oscillatory part of the single-particle density of states, which emerges due to the Landau quantization. The same oscillations of the density of states are also the cause of the de Haas–van Alphen effect. Yet another related phenomenon, the so-called field-induced SDW, is known to occur in quasi-one-dimensional materials [8].

Pronounced oscillations of both order parameters and T_N develop at sufficiently large magnetic fields. This circumstance makes their experimental observation a delicate issue. Indeed, our results were obtained under the assumption of perfect electron-hole symmetry. In a more realistic case, this symmetry is broken, and the magnetic field may cause a transition into a phase with a different order parameter, or destroy the SDW completely before an observable oscillatory trend sets in.

In conclusion, we have demonstrated that in electron systems with imperfect nesting the applied magnetic field leads to a significant increase in the number of possible ordered states. It also affects the inhomogeneous, phase-separated states of the system. At higher fields, the Landau quantization causes oscillations of the SDW order parameters and of the corresponding Néel temperatures.

[1] T.M. Rice, Phys. Rev. B 2, 3619 (1970).
[2] A.L. Rakhmanov, A.V. Rozhkov, A.O. Sboychakov, and F. Nori, Phys. Rev B 87, 075128 (2013).
[3] A.O. Sboychakov, A.V. Rozhkov, K.I. Kugel, A.L. Rakhmanov, and F. Nori, Phys. Rev. B 88, 195142 (2013).
[4] A.O. Sboychakov, A.V. Rozhkov, A.L. Rakhmanov, and F. Nori, Phys. Rev. B 87, 121401(R) (2013).
[5] P.A. Igoshev, M.A. Timirgazin, V.F. Gilmutdinov, A.K. Arzhnikov, and V.Yu. Irkhin, J. Phys.: Condens. Matter 44, 446002 (2015)
[6] N.E. Sluchanko, A.L. Khoroshilov, M.A. Anisimov, A.N. Azarevich, A.V. Bogach, V.V. Glushkov, S.V. Demishev, V.N. Krasnorussky, N.A. Samarin, N.Yu. Shitsevalova, V.B. Filippov, A.V. Levchenko, G. Pristas, S. Gabani, and K. Flachbart, Phys. Rev. B 91, 235104 (2015).
[7]. A.O. Sboychakov, A.L. Rakhmanov, K.I. Kugel, A.V. Rozhkov, and Franco Nori, Phys. Rev. B 95, 014203 (2017).
[8] A.V. Kornilov and V.M. Pudalov, in The Physics of Organic Superconductors and Conductors, A. Lebed ed. (Springer, Berlin, Heidelberg, 2008), pp. 487–527.

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