

Coexistence of Ferromagnetism with Spin Triplet Superconductivity

G. GÓRSKI, K. KUCAB* AND J. MIZIA

Institute of Physics, Rzeszów University
al. Rejtana 16A, 35-959 Rzeszów, Poland

The experimental results for ZrZn₂, URhGe, and in some pressure ranges also for UGe₂, showed that the ferromagnetic superconductors are weak itinerant ferromagnets. Guided by these results we describe the phenomenon of coexistence between equal spin triplet pairing superconductivity and ferromagnetism using the extended Stoner model, which includes in Hamiltonian the on-site Coulomb interaction, U , and occupation dependent hopping integral. We use the Hartree–Fock approximation and the Green functions technique. In the Hartree–Fock approximation the on-site Coulomb interaction plays the role of the on-site exchange (Hund’s) field. All inter-site interactions will have included the inter-site kinetic correlation, $\langle c_{i\sigma}^+ c_{j\sigma} \rangle$, within the Hartree–Fock approximation. We introduce the pressure-dependence to the hopping integral. Numerical results are compared with experimental data for ZrZn₂. The kinetic correlation creates the superconductivity without help of negative values of the Coulomb interactions. The model can explain stimulation of triplet superconductivity by the weak itinerant ferromagnetism. This effect was observed experimentally in ZrZn₂. Numerical analysis also confirms the experimental effect of decrease in critical temperatures (Curie and superconducting) with increasing external pressure.

PACS numbers: 71.10.Fd, 74.20.-z, 75.10.Lp

1. Introduction

The theoretical possibility of ferromagnetism (F) coexisting with the triplet parallel spins superconductivity (SC) was suggested by Fay and Appel for ZrZn₂ [1]. Further theoretical development took place after finding experimental evidence for coexistence of triplet SC with F (see e.g. [2]). It is relatively recently that the so-called ferromagnetic superconductors have been discovered, which at some high pressures exhibit the ferromagnetic and a spin triplet superconducting phases at the same time. At present UGe₂ [3], URhGe [4] and ZrZn₂ [5] belong to the ferromagnetic superconductors. In ZrZn₂ compound the ambient pressure strength affects the Curie temperature. This compound has the quasi-linear dependence of both magnetic moment and Curie temperature on pressure.

2. The model Hamiltonian

Taking into account that the ferromagnetic superconductors are weak itinerant ferromagnets we can describe them by the extended Stoner model (see e.g. [6]), which includes the on-site Coulomb repulsion, U , and occupation dependent hopping integral. We can write the model Hamiltonian as

$$H = - \sum_{\langle ij \rangle \sigma} [t_0 - \Delta t (\hat{n}_{i-\sigma} + \hat{n}_{j-\sigma}) + 2t_{\text{ex}} \hat{n}_{i-\sigma} \hat{n}_{j-\sigma}]$$

$$\times c_{i\sigma}^+ c_{j\sigma} - \mu \sum_i \hat{n}_i + \frac{U}{2} \sum_{i\sigma} \hat{n}_{i\sigma} \hat{n}_{i-\sigma}, \quad (1)$$

where μ is the chemical potential. The Δt and t_{ex} terms correspond to hopping and exchange-hopping interaction respectively, and are given by

$$\Delta t = t_0 - t_1 = t_0(1 - S_1),$$

$$t_{\text{ex}} = \frac{t_0 + t_2}{2} - t_1 = \frac{1}{2} t_0(1 + S_1 S_2 - 2S_1), \quad (2)$$

where $S_1 \equiv t_1/t_0$ and $S_2 \equiv t_2/t_1$. In equations above, t_0 , t_1 , and t_2 are the hopping amplitudes for an electron with spin σ when both sites i and j are empty, when one of the sites i or j is occupied by an electron with opposite spin, and when both sites i and j are occupied by electrons with opposite spin, respectively.

In the calculations below, the constants t_0 , S_1 and S_2 will be assumed pressure-dependent. The kinetic interactions Δt and t_{ex} will also depend on pressure through Eq. (2). The on-site Coulomb repulsion, U , will be assumed pressure-independent. Taking into account the results of [7] giving us the dependence of effective mass, m^* , on the pressure, p , and comparing the dispersion relation in the tight binding approximation (at small k) with the expression $\varepsilon_k = \hbar^2 k^2 / 2m^*$, one obtains the relation

$$t(p) = \frac{t_0}{1 - Ap}, \quad (3)$$

where for ZrZn₂ $A = 0.017 \pm 0.004 \text{ kbar}^{-1}$, and the lattice constant $a = 7.393 \text{ \AA}$ (see [5]). Further on, the depen-

* corresponding author; e-mail: kkucab@univ.rzeszow.pl

dence of hopping integrals on pressure will be suppressed in the notation, i.e. $t(p) \equiv t$, $\Delta t(p) \equiv \Delta t$, $t_{\text{ex}}(p) \equiv t_{\text{ex}}$.

In Hamiltonian (1) there are terms with four and six operators. The terms with four operators will be approximated by the average of two of them multiplied by the remaining two. The averages of the spin-flip type, $\langle c_{i\sigma}^+ c_{j-\sigma} \rangle$, will be ignored. The six-operator term standing at t_{ex} will be approximated by the product of two averages of two operators multiplied by the remaining two operators (see [8]). Using these approximations and dropping in the Hamiltonian spin singlet term and opposite spin triplet term we obtain, after transforming into momentum space, the following form:

$$H = \sum_{k\sigma} (\varepsilon_k^\sigma - \mu + M^\sigma) \hat{n}_{k\sigma} - \sum_{k\sigma} (\Delta_k^\sigma c_{k\sigma}^+ c_{-k\sigma}^+ + \text{h.c.}), \quad (4)$$

where $\varepsilon_k^\sigma = \varepsilon_k b^\sigma$ is the spin-dependent modified dispersion relation, with the band-width factor, b^σ , given by

$$b^\sigma = 1 - \frac{2}{t} [\Delta t n_{-\sigma} - t_{\text{ex}} (n_{-\sigma}^2 - I_{-\sigma}^2 - 2I_\sigma I_{-\sigma})]. \quad (5)$$

The spin-dependent modified molecular field, M^σ , is expressed as

$$M^\sigma = U n_{-\sigma} + 2z I_{-\sigma} (\Delta t - 2t_{\text{ex}} n_\sigma),$$

$$I_\sigma = \langle c_{i\sigma}^+ c_{j\sigma} \rangle, \quad (6)$$

where z is the number of nearest neighbors. The equal spin pairing (ESP) parameter, Δ_k^σ , for the two-dimensional square lattice is given by

$$\Delta_k^\sigma = 4t_{\text{ex}} I_{-\sigma} (\Delta_x^\sigma \sin k_x + \Delta_y^\sigma \sin k_y),$$

$$\Delta_{x(y)}^\sigma = \langle c_{i+x(y)\sigma} c_{i\sigma} \rangle. \quad (7)$$

Solving the Green function equations of motion (see [6]) with Hamiltonian (4) we obtain the following relation for the ESP superconducting critical temperature:

$$1 = 4t_{\text{ex}} I_{-\sigma} \frac{1}{N} \sum_k \left(\frac{\sin^2 k_x}{E_k^\sigma} \tanh \frac{E_k^\sigma}{2k_B T} \right), \quad (8)$$

where $E_k^\sigma = \sqrt{(\varepsilon_k^\sigma - \mu + M^\sigma)^2 + (2\Delta_k^\sigma)^2}$, T is the temperature, and k_B is the Boltzmann constant.

The equations for carrier concentration, n , and magnetization, m :

$$n = n^\sigma + n^{-\sigma}, \quad m = n^\sigma - n^{-\sigma} \quad (9)$$

can be obtained from n^σ :

$$n^\sigma = \frac{1}{2} \times \left[1 - \frac{1}{N} \sum_k \left(\frac{\varepsilon_k^\sigma - \mu + M^\sigma}{E_k^\sigma} \tanh \frac{E_k^\sigma}{2k_B T} \right) \right]. \quad (10)$$

The Fock parameter, $I_\sigma = \langle c_{i\sigma}^+ c_{j\sigma} \rangle$, is given as

$$I_\sigma = \frac{1}{2N} \sum_k \left(\frac{\varepsilon_k^\sigma - \mu + M^\sigma}{zt} \tanh \frac{E_k^\sigma}{2k_B T} \right). \quad (11)$$

3. Numerical results

Solving self-consistently Eqs. (8)–(11) we obtain the phase diagrams showing the dependence of superconducting critical temperature, ferromagnetic critical temperature, and magnetic moment on pressure. In numerical calculations we have used $A = 0.013 \text{ kbar}^{-1}$ in Eq. (3), and the following relations for S_1 and S_2 :

$$S_1 \equiv \frac{t_1}{t_0} = \frac{0.35}{1 - 0.003p}, \quad S_2 \equiv \frac{t_2}{t_1} = \frac{0.25}{1 - 0.003p}. \quad (12)$$

The relation (12) was assumed as the relation similar to the relation describing the pressure dependence of the hopping integral $t(p)$, Eq. (3). The value 0.003 in front of pressure was chosen as to obtain the Curie and superconducting critical temperatures in good agreement with experimental data for ZrZn_2 .

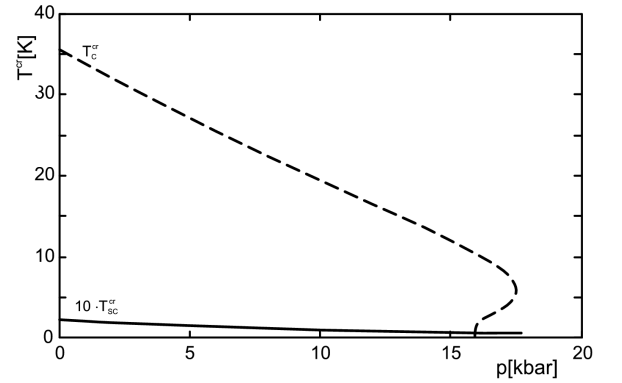


Fig. 1. ESP superconducting (solid line) and ferromagnetic (dashed line) critical temperature vs. pressure. The following values were used: $n = 1.015$, $U = 0.075 \text{ eV}$, and $t_0 = 0.125 \text{ eV}$.

Figure 1 shows the dependence of ESP superconducting, $T_{\text{SC}}^{\text{cr}}$, and ferromagnetic, T_{C}^{cr} , critical temperatures on external pressure. The value of electron occupation $n = 1.015$ was chosen. This value allows obtaining the Curie temperature comparable with experimental data at $p = 0 \text{ kbar}$. The numerical results show that the Curie temperature at zero pressure is decreasing with growing carrier concentration (all remaining parameters being fixed). Let us note that the ESP superconducting critical temperature is magnified 10 times. As we can see, increasing the pressure causes decrease in both superconducting and Curie temperatures. The pressure-dependence of critical temperatures is quasi-linear up to $p \approx 16 \text{ kbar}$. The effect of two values of the Curie temperature at a given pressure above 16 kbar is caused by the specific shape of the density of states (logarithmic) and by the Hartree-Fock (H-F) approximation used in the model. The proper curvature of the Curie temperature dependence on pressure can be obtained by assuming semi-elliptic density of states or by use of the higher-order approximations for four- and six-operator terms in the Hamiltonian (e.g. Hubbard III) (see [6]).

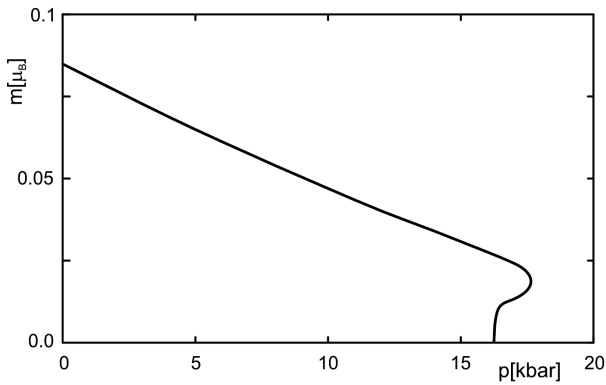


Fig. 2. Magnetic moment (in Bohr's magnetons) vs. pressure. The values used are the same as in Fig. 1, i.e.: $n = 1.015$, $U = 0.075$ eV, and $t_0 = 0.125$ eV.

Figure 2 shows the dependence of magnetic moment on external pressure. As we can see, the dependence $m(p)$ is also quasi-linear up to $p \approx 16$ kbar, in good agreement with experimental data. The strange behavior of this curve above 16 kbar was explained earlier, in the description of Fig. 1.

4. Conclusions

The simple itinerant electron model of Eq. (1) with additional assumption given by Eq. (3) and Eq. (12) can explain the pressure dependence of superconducting critical temperature, ferromagnetic critical temperature, and magnetic moment.

The abrupt decrease in magnetic moment at $p \approx 16.5$ kbar is related to the structural phase transition

(see [9]), which we do not take into account in our model.

It is worthwhile to note in here that taking into account the inter-site correlations (given by the expression $\langle c_{i\sigma}^+ c_{j\sigma} \rangle$) gave us the nonzero values of parameters S_1 and S_2 , and equivalently the nonzero values of parameters Δt and t_{ex} . The last two are responsible for an existence of small superconductivity stimulated by ferromagnetism. Both superconductivity and ferromagnetism have pressure dependence in agreement with the experimental data.

References

- [1] D. Fay, J. Appel, *Phys. Rev. B* **22**, 3173 (1980).
- [2] B.J. Powell, J.F. Annett, B.L. Györfy, *J. Phys. A* **36**, 9289 (2003).
- [3] S.S. Saxena, P. Agarwal, K. Ahilan, F.M. Grosche, R.K.W. Haselwimmer, M.J. Steiner, E. Pugh, I.R. Walker, S.R. Julian, P. Monthoux, G.G. Lonzarich, A. Huxley, I. Sheikin, D. Braithwaite, J. Flouquet, *Nature* **406**, 587 (2000).
- [4] D. Aoki, A. Huxley, E. Ressouche, D. Braithwaite, J. Flouquet, J.-P. Brison, E. Lhotel, C. Paulsen, *Nature* **413**, 613 (2001).
- [5] C. Pfleiderer, M. Uhlarz, S.M. Hayden, R. Vollmer, H.v. Löhneysen, N.R. Bernhoeft, G.G. Lonzarich, *Nature* **412**, 58 (2001).
- [6] J. Mizia, G. Górski, *Models of Itinerant Ordering in Crystals*, 1st ed., Elsevier, London 2007.
- [7] I. Lo, S. Mazumdar, P.G. Mattocks, *Phys. Rev. Lett.* **62**, 2555 (1989).
- [8] L. Arrachea, A.A. Aligia, *Physica C* **289**, 70 (1997).
- [9] M. Uhlarz, C. Pfleiderer, S.M. Hayden, *Phys. Rev. Lett.* **93**, 256404 (2004).