COEXISTENCE OF THE SPIN-TRIPLET SUPERCONDUCTIVITY WITH AN ITINERANT FERROMAGNETISM INDUCED BY THE HUND'S RULE EXCHANGE*

P. Wróbel, J. Spałek

Marian Smoluchowski Institute of Physics, Jagellonian University
Reymonta 4, 30-059 Kraków, Poland

and W. Wójcik

Institute of Physics, Tadeusz Kościuszko Technical University
Podchorążych 1, 30-084 Kraków, Poland

(Received July 10, 2002)

We discuss the local spin-triplet pairing among correlated fermions that is induced by the Hund's rule coupling in orbitally degenerate systems. The appearance of the spin-polarized superconducting phase makes the Stoner threshold a hidden critical point, since the pairing creates a small but detectable uniform magnetization even below this critical point.

PACS numbers: 71.27.+a, 74.20.Mn, 03.65.Pm

The appearance of superconductivity deep inside the weakly ferromagnetic metallic phase in UGe_2 [1], $ZrZn_2$ [2], and in URhGe [3], as well as their simultaneous disappearance as a function of pressure, indicates strongly that the same mechanism is responsible for the onset of both ferromagnetism and superconductivity. Ferromagnetism can be induced by the combined effect of both the local repulsive interaction ($U\sum_{il} n_{il\uparrow}n_{il\downarrow}$) and the local Hund's rule exchange ($-J\sum_{il\neq l'} \boldsymbol{S}_{il}\cdot\boldsymbol{S}_{il'}$) between the electrons located on orbitals labeled by l, l' and the site index i. We have recently proposed [4–6] that the Hund's rule coupling can also be responsible for the triplet pairing in orbitally degenerate narrow band systems, if only the magnitude J on the Fermi surface on the Hund's rule exchange exceeds the magnitude of the antiferromagnetic correlations, *i.e.* for a band filling far away from the half-filled situation.

In the present paper we consider a degenerate-narrow band system characterized by the two coupling constants: the Hubbard intraatomic Coulomb

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

U and the local ferromagnetic exchange magnitude J. Within this two-parameter model we determine the stability regimes of the equal-spin (A) and the totally spin-polarized (A1) phases. We also show that the pairing enhances the magnetic polarization, in effect **hiding** the Stoner critical point for the onset of ferromagnetism in the sense that we observe a gradual growth of the magnetic moment rather than a sharp appearance at the Stoner threshold.

The model is characterized by the Hamiltonian:

$$\mathcal{H} = \sum_{\boldsymbol{k}l\sigma} E_{\boldsymbol{k}l} n_{\boldsymbol{k}l\sigma} + U \sum_{il} n_{il\uparrow} n_{il\downarrow} - J \sum_{ill'(l\neq l')} \left(\boldsymbol{S}_{il} \cdot \boldsymbol{S}_{il'} + \frac{3}{4} n_{il} n_{il'} \right). \tag{1}$$

In this Hamiltonian $E_{\boldsymbol{k}l} = E_{\boldsymbol{k}l} - \mu$ is the single-particle energy in the l-th band, μ is the chemical potential, and the last term contains a full Dirac exchange operator written in the second-quantized form [5]. The hybridization between the orbitals is included in $E_{\boldsymbol{k}l}$. Therefore, U and J represent effective values on the Fermi level rather than bare atomic values. We also omitted the term $(\frac{1}{2}U' \sum_{il\neq l'} n_{il} n_{il'})$, as it reduces to a constant term in the first-order (Hartree–Fock) approximation we make. In what follows, we consider a two-orbital model (the results can be easily generalized to an arbitrary band degeneracy). As before [4], we introduce real-space spin-triplet operators $A^\dagger_{im}$ and A_{im}. In the new notation Hamiltonian (1) takes the form

$$\mathcal{H} = \sum_{\boldsymbol{k}l\sigma} E_{\boldsymbol{k}l} n_{\boldsymbol{k}l\sigma} + U \sum_{il} n_{il\uparrow} n_{il\downarrow} - 2J \sum_{im} A^\dagger_{im} A_{im}\,. \tag{2}$$

Hamiltonian (2) in the Hartree–Fock-BCS approximation reduces to the following form

$$\mathcal{H} = \sum_{\boldsymbol{k}} \boldsymbol{f}^\dagger_{\boldsymbol{k}} \boldsymbol{A} \boldsymbol{f}_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} E_{\boldsymbol{k}2} + N \left(I(\bar{S^z})^2 + \sum_m \frac{|\varDelta_m|^2}{2J)} \right), \tag{3}$$

where $\varDelta_m \equiv 2J\langle A_{im}\rangle$ is the gap parameter of the Cooper pair with the value $S^z = m$, $I \equiv U + 2J$, $\bar{S^z} = \langle S^z_{i1} + S^z_{i2}\rangle/2$ is the magnetic polarization per orbital per site, and $\boldsymbol{A}$ is 4×4 matrix:

$$\boldsymbol{A} = \begin{pmatrix} E_{\boldsymbol{k}1} - I\bar{S^z}, & 0, & \varDelta_1, & \varDelta_0 \\ 0, & E_{\boldsymbol{k}1} + I\bar{S^z}, & \varDelta_0, & \varDelta_{-1} \\ \varDelta_1, & \varDelta_0, & -E_{\boldsymbol{k}2} + I\bar{S^z}, & 0 \\ \varDelta_0, & \varDelta_{-1}, & 0, & -E_{\boldsymbol{k}2} - I\bar{S^z} \end{pmatrix}. \tag{4}$$

The form (4) is derived by introducing a four-dimensional representation [4,5], *i.e.* $\boldsymbol{f}^\dagger_{\boldsymbol{k}} = (f^\dagger_{\boldsymbol{k}1\uparrow}, f^\dagger_{\boldsymbol{k}1\downarrow}, f_{-\boldsymbol{k}2\uparrow}, f_{-\boldsymbol{k}2\downarrow})$. This Hamiltonian can be brought to a diagonal form analytically for an arbitrary band shapes $E_{\boldsymbol{k}1}$ and $E_{\boldsymbol{k}2}$

and for arbitrary $\Delta_\sigma \neq 0$ (only the phases with $\Delta_0 = 0$ are stable for a ferromagnetic superconductor). Namely, the four quasiparticle branches for $\Delta_0 = 0$ are of the form

$$\lambda_{\boldsymbol{k}\sigma 1,2} = \frac{1}{2}\left(E_{\boldsymbol{k}1} - E_{\boldsymbol{k}2}\right) \mp \left[\frac{1}{4}\left(E_{\boldsymbol{k}1} + E_{\boldsymbol{k}2} - \sigma I\bar{S^z}\right)^2 + |\Delta_\sigma|^2\right]^{1/2}, \tag{5}$$

where the sign ($\mp$) corresponds to the label $(1, 2)$ of the eigenvalues $\lambda_{\boldsymbol{k}\sigma 1,2}$. The spectrum separates into two spin subbands with the spin splitting $\delta \equiv \lambda_{\boldsymbol{k}\downarrow i} - \lambda_{\boldsymbol{k}\uparrow i}$, determined mainly by the exchange field. The spectrum is fully gapped if both $\Delta_\uparrow$ and $\Delta_\downarrow$ are nonzero (*i.e.* in the phase called in analogy to the superfluid helium phase A). In the A1 phase (*i.e.* the phase with $\Delta_\uparrow \neq 0$ only) the spin-minority spectrum has the form $\lambda_{\boldsymbol{k}\downarrow 1} = -E_{\boldsymbol{k}2} + I\bar{S^z}$ and $\lambda_{\boldsymbol{k}\downarrow 2} = E_{\boldsymbol{k}1} + I\bar{S^z}$. As we shall see, having $\Delta_\downarrow = 0$ and $\Delta_\uparrow \neq 0$ in the A1 phase does not mean that the system is ferromagnetically saturated, for which $\bar{S^z} = \langle S^z_{i1} + S^z_{i2}\rangle = n/2$, where n is the number of electrons per site.

In Fig. 1 we display the value of the magnetic moment per orbital ($\langle S^z_l\rangle$) and (in the inset) the field dependence of the chemical potential in both A and A1 paired states, as well as the values of the superconducting gaps in A and A1 phases. The magnetic moment follows essentially the same straight-line dependence $\bar{S^z}(B)$ for the both paired states. In view of this last feature of the solution it is not strange that the A1 phase becomes stable even though the system is not yet magnetically saturated.

One very interesting feature of our mean-field approach should be mentioned. Namely, the $\bar{S^z}(B)$ in the paired state dependence *does not* approach exactly the value $\bar{S^z} = 0$ for $B = 0$, even though the system is below the Stoner threshold. The effect is small to become visible in the lower left hand corner of the upper panel, but it is certainly well above the numerical accuracy of the results. To test our conjecture that the pairing itself may introduce a uniform ferromagnetic polarization we have calculated this *remanent* value of the spin magnetic moment in the field $B = 0$ when approaching the Stoner critical point. The result is displayed in Fig. 2.

We observe a beautiful critical dependence of the moment as we approach the Stoner point. So, indeed, the pairing washes out the Stoner critical point, *i.e.* makes it a hidden point. It is interesting to ask to what extent the quantum critical fluctuations could alter this mean-field result. The result also means that the superconducting coherence length becomes infinite at the Stoner point. It remains to be seen whether it is unbound whenever the A1 phase sets in. The results displayed in Fig. 2 contain also one additional feature exhibited in the inset. Namely, the inset shows that if no pairing were present then the mean-field para-ferro-magnetic transition would be discontinuous and directly to the saturated state. The pairing smears out

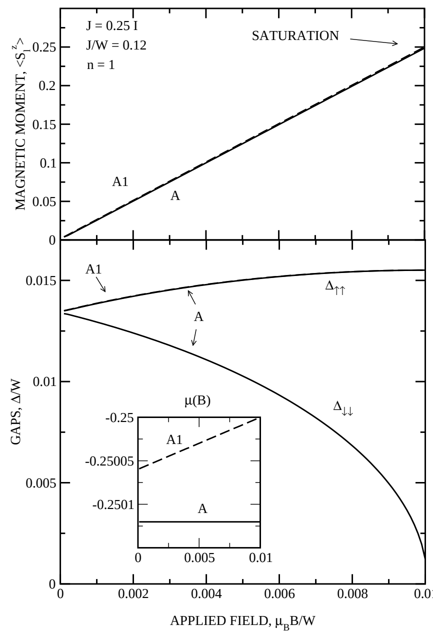

Fig. 1. Upper panel: Magnetic moment $\langle S_l^z \rangle \equiv \bar{S}^z$ in the field; lower panel: Field dependence of the superconducting gaps as marked. Inset: Field dependence of the chemical potential in the A and A1 phases.

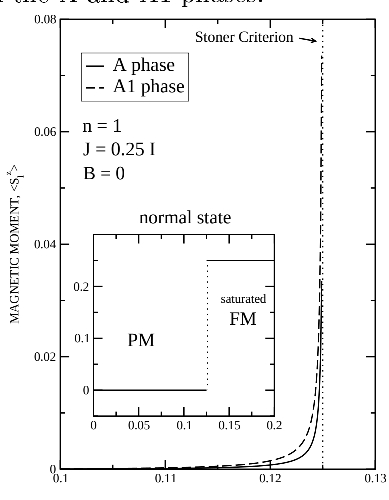

Fig. 2. Magnetic moment $\langle S_l^z \rangle$ induced by the spin-triplet pairing below the Stoner threshold (marked as Stoner criterion, $J/W \approx 0.125$). Inset: magnetic moment *vs.* J/W if the spin-triplet pairing were absent (the para(PM)- to ferro(FM)-magnetic transition is discontinuous at the Stoner point for the constant density of states.

this discontinuity and therefore, we have an extended critical regime for $J/W \to 0.125$. Additionally, because of the absence of the critical point for $\bar{S}^z(J)$ dependence it is difficult to say where the ferromagnetism disappears as a function of *e.g.* pressure. This is exactly what is actually observed for the newly discovered superconducting ferromagnets [1, 2].

In summary, the Hund's rule coupling allows for treating a weak itinerant-electron ferromagnetism and a real-space spin-triplet pairing on an equal footing within a single mechanism. However, the spin fluctuation contribution should be included to see their relative role in scattering the carriers (particularly near $T_{\rm C}$).

The work was supported by the Polish State Committee for Scientific Research (KBN) Grant No. 2 P03B 050 23.

REFERENCES

[1] S.S. Saxena *et al.*, *Nature* **406**, 587 (2000); A. Huxley *et al., Phys. Rev.* **B63**, 144519 (2001); N. Tateiwa *et al., J. Phys. C: Condensed Matter* **13**, L17(2001).

[2] C. Pfleiderer, M. Uhlarz, S.M. Hayden, R. Vollmer, H.v. Löhneysen, N.R. Bernhoeft, G.G. Lonzarich, *Nature* **412**, 58 (2001).

[3] D. Aoki, A. Huxley, E. Ressouche, D. Brithwaite, J. Floquet, J-P. Brison, E. Lhotel, C. Paulsen, *Nature* **413**, 613 (2001).

[4] A. Klejnberg, J. Spałek, *J. Phys. C: Condensed Matter* **11**, 6553 (1999).

[5] J. Spałek, *Phys. Rev.* **B63**, 104513 (2001).

[6] A. Klejnberg, J. Spałek, *Phys. Rev.* **B61**, 15542 (2000).