Renormalization of spin polarised itinerant electron bands in the normal state of a model ferromagnetic superconductor*

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This paper studies the normal state properties of itinerant electrons in a toy model, which is constructed according to the model for coexisting ferromagnetism and superconductivity proposed by Suhl [Suhl H 2001 *Phys. Rev. Lett.* **87** 167007]. In this theory with ferromagnetic ordering based on localized spins, the exchange interaction J between conduction electrons and localized spin is taken as the pairing glue for s-wave superconductivity. It shows that this J term will first renormalize the normal state single conduction electron structures substantially. It finds dramatically enhanced or suppressed magnetization of itinerant electrons for positive or negative J. Singlet Cooper pairing can be ruled out due to strong spin polarisation in the $J > 0$ case while a narrow window for s-wave superconductivity is opened around some ferromagnetic J.

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1. Introduction

The coexistence of ferromagnetism and superconductivity discovered in UGe_2[1] and $ZrZn_2$[2] is of fundamental importance in condensed matter physics. First of all, the magnetic moment of uranium due to f shells in UGe_2 can be considered as localized. In contrast to that, the material $ZrZn_2$ has much less localized d electrons. Therefore attempts to construct superconductivity and ferromagnetism within the same electron system are not very convincing.[3] For example, the single-band mean-field model[4] of coexistent ferromagnetism and s-wave superconductivity is clearly energetically not favoured.[5–7]

Recently, Suhl proposed an alternative model for the coexistence of ferromagnetism and s-wave superconductivity in UGe_2.[8] In this model of localized spins and itinerant electrons, the simultaneous onset of the fascinating coexistence may be explained as a coupling of two conduction electrons via one localized spin. The origin that the small average polarisation of each local spin in a net mean exchange field facilitates binding of electron pairs is assumed to be due to some mechanism not described there. In this scenario for ferromagnetic superconductivity, the exchange interaction $J\sigma_i \cdot S_i$ at lattice site i between conduction electrons spins σ_i and localized spins S_i plays mainly the role of pairing glue for the singlet Cooper pairs of conduction electrons.[3,8] This conclusion is mathematically realized by retaining only the anomalous average of conduction electron operators in the second order product $J^2\sigma_i^+\sigma_i^- S_i^- S_i^+$, where $\sigma_i^\pm$ and $S_i^\pm$ are transverse spin operators. However, it is interesting that this exchange interaction affects the normal state itinerant electrons before superconducting transition occurs.

2. The model and calculation method

In this paper, we study the normal state properties of itinerant electrons to the second order of J. Specifically we adopt the Green's function method to evaluate the normal average of conduction electron operators in the second order product $J^2\sigma_i^+\sigma_i^- S_i^- S_i^+$ in the presence of ferromagnetic ordering based on localized spins.

In order to introduce the magnetic ordering on localized spins explicitly, we constructed a toy model by adding a weak ferromagnetic Heisenberg term $-J_H S_i \cdot S_j$ to the model discussed in Refs. [3] and

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[8]. Note that the fermion representation for the conduction electron spin operators $\sigma_i = (c^{\dagger}_{i\sigma}\sigma^{x}_{i\sigma\sigma'}c_{i\sigma'}, c^{\dagger}_{i\sigma}\sigma^{y}_{i\sigma\sigma'}c_{i\sigma'}, c^{\dagger}_{i\sigma}\sigma^{z}_{i\sigma\sigma'}c_{i\sigma'})$. Then the total Hamiltonian is

$$\begin{aligned} H = & \sum_{ij\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} - J_H \sum_{ij} S_i \cdot S_j \\ & + J \sum_{i} [S^z_i (c^{\dagger}_{i\uparrow} c_{i\uparrow} - c^{\dagger}_{i\downarrow} c_{i\downarrow}) \\ & + S^+_i c^{\dagger}_{i\downarrow} c_{i\uparrow} + S^-_i c^{\dagger}_{i\uparrow} c_{i\downarrow}]. \end{aligned} \tag{1}$$

At zero temperature, this Heisenberg coupling will introduce a magnetization proportional to NS in the localized spin (of spin S) system, where N is the number of lattice sites. We will adopt the linearized Holstein–Primakoff representation[9] ($S^{\dagger}_i = a_i\sqrt{2S}, S^-_i = a^{\dagger}_i\sqrt{2S}, S^z_i = S - a^{\dagger}_i a_i$) for the localized spins. The main quantum effect due to the transverse Heisenberg coupling is the bosonic spin–wave excitations (magnons). Here we just consider the hopping (t) and the exchange interaction (J_H) between nearest-neighbours. Making use of Fourier transformation, we find that the toy model Hamiltonian discussed in this article becomes

$$\begin{aligned} H = & \sum_{\boldsymbol{k}\sigma} \varepsilon_{\boldsymbol{k}\sigma} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} a^{\dagger}_{\boldsymbol{q}} a_{\boldsymbol{q}} \\ & + J\sqrt{2SN^{-1}} \sum_{\mathbf{kq}} \left[a_{-\boldsymbol{q}} c^{\dagger}_{\boldsymbol{k}\downarrow} c_{\boldsymbol{k}+\boldsymbol{q}\uparrow} + \text{h.c} \right]. \end{aligned} \tag{2}$$

Here the three terms account for the spin-polarised conduction electrons, the magnons and coupling between the two subsystems, respectively. In this paper, we will for simplicity work on a square lattice whose number equals the number of both localized spins and itinerant electrons and assume $S = 1$. The conduction electron bands polarised by the z-component of the exchange interaction is

$$\varepsilon_{\boldsymbol{k}\sigma} = -2t (\cos k_x + \cos k_y) - \mu + \sigma JS, \tag{3}$$

where the chemical potential $\mu = 0$ is at half-filling. The magnon energy is

$$\omega_{\boldsymbol{q}} = 8J_H S \left[1 - \frac{1}{2} (\cos q_x + \cos q_y) \right].$$

We define the thermal Green's functions for the spin-polarised conduction electrons as follows:

$$\mathcal{G}_{\sigma} (\boldsymbol{k}, \tau, \tau') = - \left\langle \mathcal{T} \left[c_{\boldsymbol{k}\sigma} (\tau) c^{\dagger}_{\boldsymbol{k}\sigma} (\tau') \right] \right\rangle. \tag{4}$$

So the Matsubara Green's functions for polarized conduction electrons in the absence of the electron–magnon scattering are

$$\mathcal{G}^{\text{o}}_{\sigma} (\boldsymbol{k}, \mathrm{i}\,\omega_n) = \frac{1}{\mathrm{i}\,\omega_n - \varepsilon_{\boldsymbol{k}\sigma}}, \tag{5}$$

with fermionic frequencies $\mathrm{i}\,\omega_n = \mathrm{i}(2n+1)T$, where T is temperature (times Boltzmann constant). Similarly, those for magnons are

$$\mathcal{D} (\boldsymbol{q}, \mathrm{i}\,\nu_m) = \frac{1}{\mathrm{i}\,\nu_m - \omega_{\boldsymbol{q}}} \tag{6}$$

with bosonic frequencies $\nu_m = \mathrm{i}\,2mT$.

We treat the renormalization effects of the third term of Eq. (2) to the spin-polarized conduction electron energy bands by the technique of Feynman diagram. Here, we only discuss the single particle spin-flip processes in the transverse second order product $J^2\sigma^+_i\sigma^-_i S^-_i S^+_i$ and its h.c. term as shown in Fig. 1. Thus, to the second order of the electron–magnon scattering, we obtain the self energies

$$\begin{aligned} \Sigma_{\sigma} (\boldsymbol{k}, \mathrm{i}\,\omega_n) = & -2SJ^2\beta^{-1}N^{-1} \sum_{\mathrm{i}\,\nu_m, \boldsymbol{q}} \mathcal{D} (\boldsymbol{q}, \mathrm{i}\,\nu_m) \\ & \times \mathcal{G}^{\text{o}}_{-\sigma} (\boldsymbol{k} + \sigma\boldsymbol{q}, \mathrm{i}\,\omega_n + \sigma\,\mathrm{i}\,\nu_m) \end{aligned} \tag{7}$$

for the spin-up ($\sigma = +1$) and spin-down ($\sigma = -1$) conduction electrons, respectively.

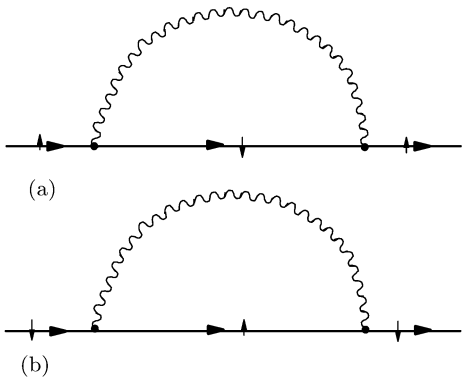


Fig. 1. Feynman diagrams of the second order corrections to the Green's functions of spin-up (a) and spin-down (b) conduction electrons.

The Matsubara imaginary frequency summation is performed by complex integration method[10] using the Fermi and Bose distributions $n(\omega)$ and $f(\varepsilon)$. The self energies are worked out as

$$\begin{aligned} \Sigma_{\uparrow} (\boldsymbol{k}, \mathrm{i}\,\omega_n) = & \; 2SJ^2\beta^{-1}N^{-1} \\ & \times \sum_{\boldsymbol{q}} \frac{n(\omega_{\boldsymbol{q}}) + f(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}\downarrow})}{\mathrm{i}\,\omega_n + \omega_{\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}+\boldsymbol{q}\downarrow}} \mathcal{K} \end{aligned} \tag{8}$$

and

$$\begin{aligned} \Sigma_{\downarrow} (\boldsymbol{k}, \mathrm{i}\,\omega_n) = & \; 2SJ^2\beta^{-1}N^{-1} \\ & \times \sum_{\boldsymbol{q}} \frac{n(\omega_{\boldsymbol{q}}) + f(-\varepsilon_{\boldsymbol{k}-\boldsymbol{q}\uparrow})}{\mathrm{i}\,\omega_n - \omega_{\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}\uparrow}}. \end{aligned} \tag{9}$$

Through the Dyson equation

$$\mathcal{G}_\sigma^{-1}(\boldsymbol{k}, \mathrm{i}\omega_n) = \mathcal{G}_\sigma^{\mathrm{o}-1}(\boldsymbol{k}, \mathrm{i}\omega_n) - \Sigma_\sigma(\boldsymbol{k}, \mathrm{i}\omega_n) \quad (10)$$

and analytic extrapolation $\mathrm{i}\omega_n \to \omega + \mathrm{i}0^+$ in $\mathcal{G}_\sigma(\boldsymbol{k}, \mathrm{i}\omega_n)$, we obtain the spectral functions of the spin-polarized conduction electrons renormalised by the electron–magnon scattering

$$A_\sigma(\boldsymbol{k}, \omega) = -\frac{1}{\pi} \operatorname{Im} \mathcal{G}_\sigma(\boldsymbol{k}, \omega). \quad (11)$$

3. Results and discussions

First, Let us present the conduction electron structures in the absence of the electron-magnon scattering. At half-filling, the Fermi surface of the unpolarised conduction electrons is nested to the MBZ boundary for $J = 0$. The Fermi wave vector along the Brillouin zone diagonal $k_F^{\mathrm{o}} = \pi/2$. The two Fermi surfaces of the spin-polarised conduction electrons given by $\varepsilon_{\boldsymbol{k}\sigma} = 0$ are symmetric around the MBZ boundary. In this case, the two diagonal Fermi wave vectors are defined by $k_F^{\mathrm{o}\sigma} = \cos^{-1}(\sigma JS/4t)$. The two Fermi surfaces are interchanged when the sign of J is reversed. Magnetization of itinerant electrons is directly defined by the area between the two Fermi surfaces with orientation parallel to that of the localized spin system when $J < 0$. We plot the evolution of the Fermi surfaces in Fig. 2. Second, we present our results of self-energy corrections at zero temperature. The Fermi levels defined by $\mathcal{G}_\sigma(\boldsymbol{k}, \mathrm{i}\omega_n)$ are located by positions of maxima of the spectral functions $A_\sigma(\boldsymbol{k}, \omega)$ with $\omega = 0$. The Fermi surfaces of the spin-polarized conduction electrons are modified by the electron-magnon scattering substantially. These features can be seen in Fig. 3. For $J > 0$ shown in Fig 3(a), the two Fermi surfaces are shifted further away from the MBZ boundary in comparison with those in the absence of the electron-magnon scattering. Thus the magnetization of itinerant electrons is dramatically enhanced. This is not surprising since antiferromagnetic J is actually the Kondo s–d exchange. On the contrary, the modified Fermi surfaces for ferromagnetic J displayed in Fig. 3(b) are pushed closer to the MBZ boundary. In other words, the conduction electron magnetization is strongly suppressed by the electron-magnon scattering in the $J < 0$ case.

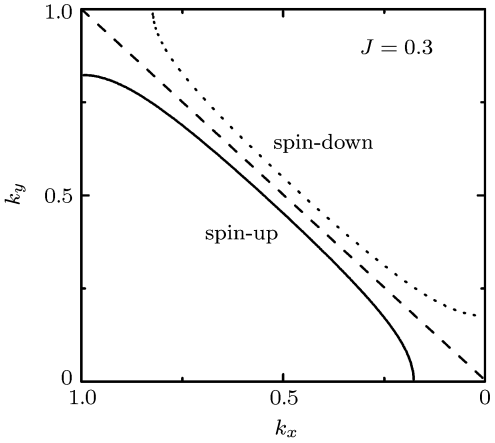


Fig. 2. Fermi surfaces of spin-polarised conduction electrons without the self energy corrections at $J = 0.3t$. The magnetic Brillouin zone (MBZ) boundary is the Fermi surface at $J = 0$. Wave vectors and parameters are in unit of π and t in all figures.

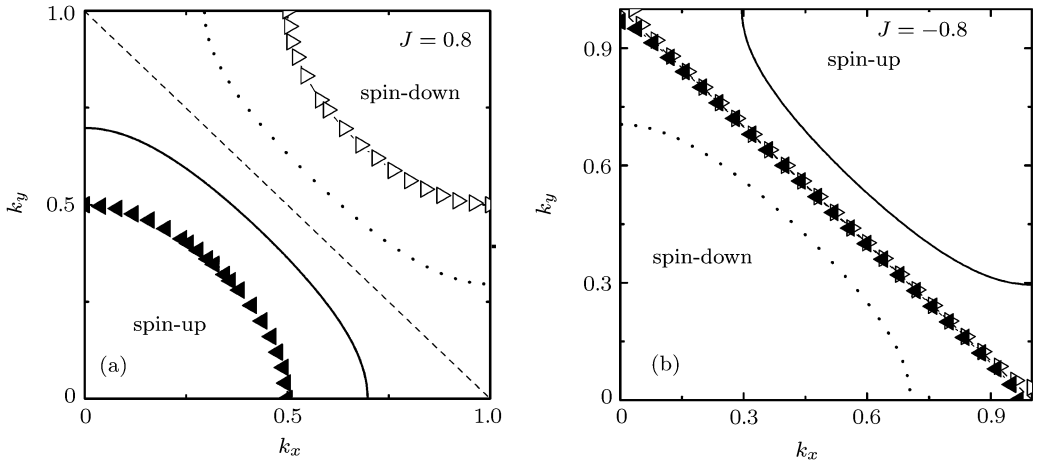


Fig. 3. (a) Fermi surfaces of spin-polarised conduction electrons with (black-solid-up/white-open-down triangles for spin-up/spin-down) and without (lines) modifications due to the electron–magnon scattering. Here, $J_H = 0.001t$ and $J = 0.8t$. (b) The same as (a) except $J = -0.8t$.

A complete view of Fermi surface modifications by the exchange interaction between conduction electron and local spin can be obtained by the J variation of the diagonal Fermi wave vector $k_{\rm F}^{\uparrow}$ of spin-up conduction electron as plotted in Fig. 4.

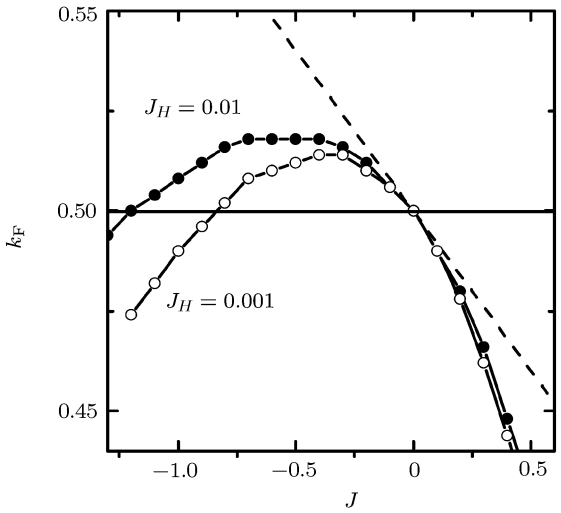


Fig. 4. Spin-up Fermi wave vectors along Brillouin zone diagonal direction versus J with (cirles) and without (dashed line) renormalizations due to the electron-magnon scattering.

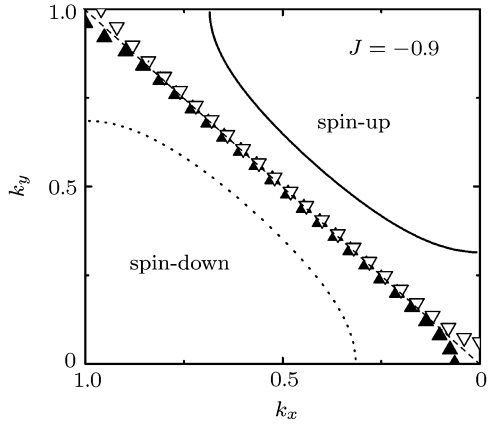


Fig. 5. The same as Fig. 3(a) at $J = -0.9t$. Note, the black-solid-up and white-open-down triangles are shifted across the MBZ boundary in comparison with Fig. 3(b).

In the $J > 0$ region, $k_{\rm F}^{\uparrow}$ ($< k_{\rm F}^{\rm o\uparrow} < k_{\rm F}^{\rm o}$) monotonically decreases as J increases. But for ferromagnetic J, $k_{\rm F}^{\uparrow}$ varies very differently from $k_{\rm F}^{\rm o\uparrow}$. We find that $k_{\rm F}^{\uparrow}$ is renormalized to the paramagnetic $k_{\rm F}^{\rm o}$ again at some critical value $J_{\rm c}(J_H)$ besides the $J = 0$ case. For example, $J_{\rm c}(J_H = 0.01t) \approx -1.2t$ and $J_{\rm c}(J_H = 0.001t) \approx -0.85t$ as found in Fig. 4. We have chosen $J = -0.8t$ close to $J_{\rm c}(J_H)$ in Fig. 3(b). We plot the Fermi surfaces for $J = -0.9t$ by the other side of $J_{\rm c}(J_H)$ in Fig. 5, where the Fermi surfaces of spin-up and spin-down conduction electrons are nearly exchanged across the MBZ boundary in comparison with Fig. 3(b). In other word, the magnetization of itinerant electrons is reversed by the two sides of $J_{\rm c}(J_H)$ due to strong electron-magnon scattering.

Finally, we remark the obvious implications of these effects on Suhl's scenario of ferromagnetic superconductivity. The strong spin polarization in the normal state electronic structures, stems from the self energy corrections, rules out the singlet Cooper pairing for $J > 0$. Binding s-wave electron pairs facilitated by anomalous second order self energy may most likely be realized in the narrow window around some $J_{\rm c}(J_H) < 0$, where the magnetization of itinerant electrons nearly vanishes.

4. Conclusion

In conclusion, we study the normal state properties of itinerant electrons in Suhl's model for coexisting ferromagnetism and superconductivity. We show that the exchange interaction J between conduction electrons and localized spin will firstly renormalize the normal state single conduction electron structures substantially before serving as pairing glue. We find dramatically enhanced or suppressed magnetization of itinerant electrons for positive or negative J. Singlet Cooper pairing can be ruled out due to strong spin polarization in the $J > 0$ case while a narrow window for s-wave superconductivity is opened around some ferromagnetic J.

References

[1] Saxena S S, Agarwal P, Ahilan K, Grosche F M, Haselwimmer R K W, Steiner M J, Pugh E, Walker I R, Julian S R, Monthoux P, Lonzarich G G, Huxley A, Shelkin I, Braithwaite D and Flouquet J 2000 *Nature* (London) **406** 587

[2] Pfleiderer C, Uhlarz M, Hayden S M, Vollmer R, von Lhneysen H, Bernhoeft N R and Lonzarich G G 2001 *Nature* (London) **412** 58

[3] Abrikosov A A 2001 *J. Phys.: Condens. Matter* **13** L943

[4] Karchev N I, Blagoev K B, Bedell K S and Littlewood P B 2001 *Phys. Rev. Lett.* **86** 846

[5] Zhou Y, Li J and Gong C D 2003 *Phys. Rev. Lett.* **91** 069701

[6] Shen R, Zheng Z M and Xing D Y 2003 *Phys. Rev. Lett.* **91** 069702

[7] Joglekar Y N and MacDonald A H 2003 *Phys. Rev. Lett.* **92** 199705

[8] Suhl H 2001 *Phys. Rev. Lett.* **87** 167007

[9] Holstein T and Primakoff H 1940 *Phys. Rev.* **58** 1098

[10] Parks R D 1969 *Superconductivity* (vol.1) (New York: Marcel Decker) p224–226