RKKY interaction in SDW phase of iron-based superconductors

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Using the multiband model we analyze the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the magnetic impurities in layered ferropnictide superconductors. In the normal state the interaction is spin isotropic and is dominated by the nesting features of the electron and hole bands separated by the antiferromagnetic momentum, $Q_{AF}$. In the AF state the RKKY interaction maps into an effective anisotropic XXZ-type Heisenberg exchange model. The anisotropy originates from the breaking of the spin-rotational symmetry induced by the AF order and its strength depends on the size of the AF gap and the structure of the folded Fermi surface. We discuss our results in connection to the recent experiments.

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I. INTRODUCTION

The oscillatory Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction\cite{1,2} of the localized magnetic moments in a metal has always played an important role in revealing the nature of the magnetic interaction in metals with partially unfilled $d$- and $f$-electron shells. This indirect interaction is the result of the spin polarization of conduction electrons produced by the exchange interaction of the localized moments with conduction electrons where the distance between two localized moments controls the strength of their effective exchange. Originally formulated for the three-dimensional spherical Fermi surface, RKKY interaction has been also analyzed for the two-dimensional (2D)\cite{3,4} as well as one-dimensional (1D)\cite{5} electron gas. A particular interesting situation arises in a highly anisotropic Fermi surface with nesting. In particular, it was shown that the RKKY interaction in such a case consists of several terms originating from flat regions in the fermionic spectrum (van Hove regions) and those which describe the interference between contributions from their vicinities\cite{6}. Note that the latter terms have an overall prefactor $\cos(Q \cdot r)$ with $Q = (\pi, \pi)$. In the nearly nested situation this last term is present down to the interatomic distances and favors the commensurate antiferromagnetic ordering of the localized moments.

It is important to bear in mind that in order to evaluate the RKKY interaction at the distances $r$ the details of the fermionic dispersion on a scale of $1/r$ in the $k$-space is required. As a result the fine details of the Fermi surface are only important at largest distances while even the approximate knowledge of the electronic spectrum over the whole Brillouin zone is often enough for a good description of the RKKY interaction at the interatomic distances in $r$ space. In this regard it is quite instructive to analyze the RKKY interaction in recently discovered Fe-based superconductors\cite{7}. Band structure calculations\cite{8} and experimental probes such as angle-resolved photoemission (ARPES)\cite{9} and quantum oscillation\cite{10,11} experiments show that to a good approximation the Fermi surface topology of iron-based superconductors consists of the small sized circular hole pockets centered around the $\Gamma$–point $(0, 0)$, and elliptic electron pockets centered around the $(\pm \pi, 0)$, and $(0, \pm \pi)$-points of the unfolded Brillouin zone (BZ). The pockets are nearly of the same size which results in the nesting properties of the electron and hole bands at wave vectors, $Q_1$ ($Q_1 = (\pi, 0)$, and $Q_2 = (0, \pi)$, i.e. $\varepsilon_{k_+} \simeq -\varepsilon_{k_-}$). Given the electronic structure of ferropnictides, it is natural to assume that magnetic order emerges, at least partly, due to near-nesting between the dispersions of holes and electrons\cite{10,11}.

Here we analyze the novel aspects of the RKKY interaction in iron-based superconductors which arise due to the peculiar Fermi surface topology in these systems. The origin of the local moments in ferropnictides can be either $4f$-electrons in ReFeAsO series (Re- is a rare-earth element\cite{12,13}) or possibly partially localized $d$-electrons which arise due to proximity to a Mott insulator\cite{14}.
coexist with itinerant ones. Our primary interest is to investigate the evolution of the oscillatory behavior of the RKKY interaction in the presence of nesting in the normal and in the antiferromagnetic states of iron-based superconductors. Analyzing the RKKY interaction in the antiferromagnetic state we find spin space anisotropy of the interaction, a feature that has not been reported so far. We will also study in detail the influence of the model parameters like ellipticity of the electron pockets, and SDW gap size on the spatial variation of the RKKY interaction.

The paper is organized as follows: In Sec. II we evaluate the RKKY interaction for a three band model and present its analytical form for SDW and normal state regimes. Using these results we evaluate the RKKY interaction numerically in Sec. III and discuss its relevance for the experiments. We finally present a summary and conclusion in Sec. IV.

II. MULTI BAND RKKY INTERACTION IN THE NORMAL AND SPIN DENSITY WAVE STATES

In this investigation we employ a minimal model of interacting 3d electrons and local moments in ferropnictides with a circular 3d hole Fermi surface (FS) centered around Γ-point (a-band) and two elliptical electron FS pockets centered around (±π, 0) and (0, ±π) points in the unfolded BZ (b-bands) (See Fig.1).

The Hamiltonian of the system of localized magnetic moment impurities in the multi band conduction electron sea is defined by

\[ H = H_c + H_{imp} + H_{int}, \]

where \( H_c = H_c^0 + H_c' \) is the conduction electron Hamiltonian which is given by:

\[
H_c^0 = \sum_{k, \sigma} \varepsilon_k \hat{c}_k^{\dagger} \hat{c}_k \]

\[
= \sum_{k, \sigma} \left[ \varepsilon_k \hat{a}_k^{\dagger} \hat{a}_k + \varepsilon_k^e \hat{b}_k^{\dagger} \hat{b}_k + \varepsilon_k^h \hat{b}_k^{\dagger} \hat{b}_k \right].
\]

Here, \( \hat{c}_k^{\dagger} \) refers to the creation operators of the conducting electrons. In particular, \( \hat{a}_k^{\dagger} (\hat{b}_k^{\dagger}) \) creates an electron with spin \( \sigma \) in the hole (electron) band. The tight-binding energy dispersion of the electron and hole bands can be parametrized as follows

\[ \varepsilon_k^e = \varepsilon_0 + \mu_e \]

\[ \varepsilon_k^h = \varepsilon_0 + \mu_h \]

\[ \varepsilon_k = \varepsilon_0 + \mu_e \left(1 - \epsilon \right) \cos(k_x + \pi) + \left(1 - \epsilon \right) \cos(k_y) \]

\[ \varepsilon_k = \varepsilon_0 + \mu_e \left(1 + \epsilon \right) \cos(k_x + \pi) + \left(1 + \epsilon \right) \cos(k_y) \]

where \( \epsilon \) accounts for the ellipticity of the electron pockets and \( \varepsilon_0 = 0.05 \text{eV} \) is the chemical potential for zero doping. Following our previous analysis, we use the following hopping matrix elements \( t_h = 0.85 \text{eV}, t_e = -0.68 \text{eV}, \mu_h = 1.44 \text{eV}, \) and \( \mu_e = -1.23 \text{eV} \) which accounts for the Fermi velocities and sizes of the Fermi pockets, see Ref.9.

The interaction part of the conduction electron Hamiltonian contains density-density interactions between hole and electron bands which give rise to a SDW order between the hole pocket and one of the electron pockets located around \((\pi, 0)\) point of the BZ. Assuming the experimentally observed \( Q_{AF} = Q = (\pi, 0) \) SDW ordering wave vector a standard mean-field decoupling yields the self-consistency condition for the SDW order parameter

\[ W \propto \sum_{k, \sigma} \langle \hat{a}_k^{\dagger} \hat{b}_{1k+Q, \sigma} \rangle. \]

The resulting mean-field Hamiltonian has the form

\[ H_c^{MF} = H_c^0 + \sum_{k, \sigma} W \sigma \left[ a_k^{\dagger} b_{1k+Q, \sigma} + H.c. \right], \]

where the spin index \( \sigma = \pm 1 \) refers to the spin up and down, respectively. Now applying the unitary transformations

\[ a_k = v_k c_{k\sigma} - u_k d_{k\sigma} \]

\[ b_{k+Q, \sigma} = \sigma \left[ u_k c_{k\sigma} + v_k d_{k\sigma} \right] \]

the mean-field Hamiltonian for the conducting electrons can be diagonalized and the coefficients of the transfor-
FIG. 3. (color online) The intra-band (upper panel, (a) $J_{n}^{11}$, (b) $J_{n}^{22}$, (c) $J_{n}^{33}$) and inter-band (lower panel (d) $J_{n}^{12}$, (e) $J_{n}^{13}$, and (f) $J_{n}^{23}$) contributions to the RKKY interaction in the normal state for $\epsilon = 0.5$ and 5% of the electron doping.

FIG. 4. (color online) The intra-band (upper panel (a) $J_{x}^{11}$, (b) $J_{x}^{22}$, (c) $J_{x}^{33}$) and interband (lower panel (d) $J_{x}^{12}$, (e) $J_{x}^{13}$, and (f) $J_{x}^{23}$) contributions to the RKKY interaction, $J^x$ in SDW state $x$-direction for $W = 40\text{meV}$, $\epsilon = 0.5$, and 5% of the electron doping.

The diagonalized Hamiltonian has the form

$$\mathcal{H}_{c}^{MF} = \sum_{k, \sigma} \left[ E_{k}^{1} c_{k \sigma}^\dagger c_{k \sigma} + E_{k}^{2} d_{k \sigma}^\dagger d_{k \sigma} + E_{k}^{3} b_{2k \sigma}^\dagger b_{2k \sigma} \right],$$

with

$$u_{k}^{2} = \frac{1}{2} \left[ 1 + \frac{(\epsilon_{k}^{h} - \epsilon_{k}^{e1})}{\sqrt{(\epsilon_{k}^{h} - \epsilon_{k}^{e1})^2 + 4W^2}} \right]$$

$$v_{k}^{2} = \frac{1}{2} \left[ 1 - \frac{(\epsilon_{k}^{h} - \epsilon_{k}^{e1})}{\sqrt{(\epsilon_{k}^{h} - \epsilon_{k}^{e1})^2 + 4W^2}} \right].$$
The magnetic anisotropy of the form $J_x = J_y \neq J_z$ in this expression appears through the SDW order which is polarized along $z$-spin quantization axis. Specifying $\mathbf{R}_i = \mathbf{0}$ and $\mathbf{R}_j = \mathbf{r} = (x, y)$ these effective exchange couplings are given by

$$J_{ij} = J_{ij}^y = \sum_{\gamma \gamma'} \gamma \gamma' \left[ \frac{f(\mathbf{k}, \gamma) - f(\mathbf{k}', \gamma')}{E_k - E_{k'}} \right],$$

$$J_{ij}^z = \sum_{\gamma \gamma'} \gamma \gamma' \left[ \frac{f(\mathbf{k}, \gamma) - f(\mathbf{k}', \gamma')}{E_k - E_{k'}} \right].$$

Here $f(\mathbf{k}, \gamma)$ is the Fermi function, and the SDW coherence factors, $\eta_{kk', \sigma', \sigma}$, are defined as

$$\eta_{kk, \sigma, \sigma}^{(11)} = u_k v_{k'} + \sigma' e^{\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} + \sigma e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'},$$

$$\eta_{kk, \sigma, \sigma}^{(12)} = -u_k v_{k'} - \sigma' e^{\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} - \sigma e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'},$$

$$\eta_{kk, \sigma, \sigma}^{(21)} = -u_k v_{k'} - \sigma' e^{\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} - \sigma e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'},$$

$$\eta_{kk, \sigma, \sigma}^{(22)} = u_k v_{k'} - \sigma' e^{\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} - \sigma e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'},$$

$$\eta_{kk, \sigma, \sigma}^{(13)} = u_k e^{\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i},$$

$$\eta_{kk, \sigma, \sigma}^{(31)} = u_k e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i},$$

$$\eta_{kk, \sigma, \sigma}^{(23)} = -u_k e^{\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i},$$

$$\eta_{kk, \sigma, \sigma}^{(32)} = -u_k e^{-\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i} v_k u_{k'} e^{\mathbf{i} \mathbf{Q} \cdot \mathbf{R}_i},$$

$$\eta_{kk, \sigma, \sigma}^{(12)} = 1$$

Setting $W = 0$ it is easy to verify that in the paramagnetic or normal state regime the RKKY interaction simplifies to the usual expression in two-dimensional metals with nesting properties.

$$\mathcal{H}_{RKKY}^{ij} = J_{ij}^y S_i \cdot S_j$$
where the interaction is now isotropic in the spin space ($J_x = J_y = J_z \equiv J_n$). The effective exchange couplings are then given by

$$J_n^{ij} = \sum_{\gamma\gamma'} J_n^{\gamma\gamma'}(\mathbf{r}) = J_{xx}^2 \text{Re} \left( \sum_{\gamma\gamma'} e^{iQ_{\gamma'} - Q_{\gamma}} \mathbf{r} \chi^{\gamma\gamma'}(\mathbf{r}) \right),$$

(15)

here $Q_{\gamma} = Q_1$, $Q_{\gamma'} = Q_2$, $Q_0 = 0$, and $\chi^{\gamma\gamma'}(\mathbf{r})$ is magnetic spin susceptibility of conduction electrons (Lindhard response function) which is given by

$$\chi^{\gamma\gamma'}(\mathbf{r}) = \sum_{\mathbf{k}k'} e^{i(k-k') \cdot \mathbf{r}} \left[ \frac{f(\mathbf{k}, \gamma) - f(\mathbf{k}', \gamma')}{\varepsilon_k - \varepsilon_{k'}} \right].$$

(16)

### III. NUMERICAL RESULTS AND DISCUSSION

Based on the equations above we present in the following the results of the numerical evaluation of the RKKY interaction in the SDW and the normal state phases. We first present an overall behavior of the RKKY interaction. In particular, Fig. 2 shows the contour mesh of the RKKY interaction for 5% electron doping and ellipticity parameter $\epsilon = 0.5$ as a function of interatomic distances for both SDW and normal state regimes. In addition to the breaking of the spin rotational symmetry, there is another important difference in the behavior of the RKKY interaction between the normal and the SDW state of iron-based superconductors. This concerns the absence of tetragonal symmetry in the SDW state. As clearly seen by comparing Fig. 2(a) and Fig. 2(b)-(c) the $C_4$ symmetry present in the normal state is broken down to $C_2$ symmetry. Apart from these differences the RKKY interaction show also some similarities. In particular, close to the impurity position the effective interaction is ferromagnetic(FM) in both cases and becomes antiferromagnetic(AF) at a distance comparable to the lattice constant. In the asymptotic regime ($x/a, y/a \gg 1$) the oscillatory behavior from FM to AF and vice versa sets in. As expected the amplitude of oscillations decreases with increasing distance between the local moment impurities.

For clarification of the role played by the interband and intraband scattering we display in Fig. 3 the contribution of each term separately in the normal state. These figures show that the inter band contribution to the RKKY interaction is much larger at shorter distances than the intraband one. This arises again due to pronounced nesting features of the electron and hole bands. In addition, observe that a finite ellipticity introduces some asymmetry along $x$ and $y$ direction for each component of the RKKY interaction where electron pockets are involved. This asymmetry, however, averages out in the full RKKY interaction which possesses again the tetragonal symmetry.

This is not any longer the case in the SDW state as shown in Fig. 4 for $J_z$ component. Here, the intraband-interband contributions to the RKKY are strongly anisotropic. This originates from the fact that the SDW has $Q_1 = (\pi, 0)$ ordering wave vector and as a result of its ordering the tetragonal symmetry is broken. It is interesting to notice that such effect was found recently in EuFe$_2$As$_2$ where the magnetic anisotropy of the Eu magnetic moments was changing across the SDW transition temperature. This change in the magnetic anisotropy is in direct agreement with our results. Note also that the sum of all contributions is anisotropic along $a$ and $b$ crystallographic directions in both $J_x$ and $J_z$ components of the interactions. In particular, as clearly shown in Fig. 4(b)-(c) the ferromagnetic interaction is extended in both $J_x$ and $J_z$ along the $y$ direction which is perpendicular to the AF ordering of the Fe-plane.

To see the changes on the quantitative level we show...
The nature of this difference is both SDW order and the
structure of the remaining small pockets that occur due
in the SDW state are unequal along \( \mathbf{x} \) and \( \mathbf{y} \) directions. We ob-
served that the amplitude of the oscillations increases in
the SDW state but overall the dependence remains the
same. Namely, it is ferromagnetic for short distances
and then oscillates between positive (AF) and negative
(FM) values. In addition, \( J_z \) and \( J_x \) RKKY interac-
tions have slightly different period which results in the
fact that they may have opposite signs for a given inter-
impurity distance. This difference is associated with the
structure of the SDW matrix elements which appear in
the \( J_z^2 \) and \( J_x^2 \) components of the RKKY interaction dif-
dently (see Eqs.(11)-(12)). An additional effect of the
SDW is shown in Fig.6 where we plot the behavior of
\( J_z \) and \( J_x \) along \( \mathbf{a} \) and \( \mathbf{b} \) crystallographic directions. As
clearly seen from this figure, the period of the oscillation
is not only different for \( J_z \) and \( J_x \) components but also
for each of them in the \( \mathbf{x} \) and \( \mathbf{y} \) crystallographic direc-
tions. In particular, the antiferromagnetic XXZ regime
with negative anisotropy at \( z \approx 2a \) is observed along
(0, 1) direction. On the other hand for (1,0)-direction
the XXZ ferromagnetic Heisenberg model is dominant
and the effective interaction changes to AF behavior only
around \( y \approx 2.5a \). Thus through SDW spin-space and
real space anisotropies are correlated. Furthermore along
(1,0)-direction the magnetic anisotropy changes sign for
the first time at a distance of about \( y \approx 0.75a \) and it pre-
vails for a longer period as compared to (0,1) direction.
The nature of this difference is both SDW order and the
structure of the remaining small pockets that occur due
to folding of hole and one electron pocket located at \((\pi,0)\)
point of the BZ. Due to larger hopping of this electron
band along \( \mathbf{x} \)-direction the \( k_F \) values of the folded bands
in the SDW state are unequal along \( \mathbf{x} \) and \( \mathbf{y} \)-direction
which is then reflected in the periodicity of the RKKY
interaction.

Furthermore we show the effect of the ellipticity in
Fig.7 where one could clearly observe the increasing pe-
riod of the oscillations for larger values of \( \epsilon \). The same
effect is observed for increasing electron doping. This is
natural as both ellipticity and doping for a given value
of \( W \) make the remnant pockets and the corresponding
values of \( k_F \) along \( \mathbf{x} \) and \( \mathbf{y} \) direction larger. This effect
is almost absent in the normal state (not shown) which
points out that in the SDW state the interaction between
magnetic impurities will be strongly modified.

The natural question arises whether the effects of the
SDW state on the RKKY interaction become more
pronounced for increasing size of the SDW gap and cor-
responding increase of the magnetic moment. In Fig.8
we show the evolution of the oscillatory behavior of
the RKKY \( J_z \) interaction for different value of \( W \). Note that
the amplitude of the oscillations weakens upon increase
of the SDW gap. This is due to the shrinkage of the remnant
electron and hole FS pockets which arise due to folding
of the BZ in the SDW. The larger becomes the SDW gap
the smaller will be the remnant pocket size. As a matter
of fact for some critical value of \( W \) the pockets involved
in the SDW completely disappear from the Fermi surface.
Therefore the only contribution to the RKKY will arise
in this case due to electron pocket located at \((0,\pi)\), not
involved in the SDW formation. This explains why \( J_z \)
shows weaker oscillations along \( \mathbf{x} \)-direction, while along
\( \mathbf{y} \)-direction the oscillations are almost the same. This is
because the oscillatory behavior of \( J_z \) along \((0,1)\) direction
is determined by the electron pocket which remains
intact in the SDW state while along \((1,0)\) direction the
SDW order gaps completely the FS and only slight oscil-
lations are still visible.

IV. SUMMARY AND CONCLUSION

In conclusion we analyze the changes of the RKKY
interaction in the SDW state of iron-based superconduc-
tors. The generalized RKKY interaction in these com-

FIG. 8. (color online) Influence of the SDW gap magnitude on the RKKY interaction parameter, \( J_z \), for (100)-direction (a); and for (010)-direction (b).
pounds is of an effective XXZ Heisenberg-type where the $O(3)$ symmetry is broken but $U(1)$ symmetry of the interaction for rotation around an axis parallel to the SDW polarization vector $\hat{W}$ is still preserved. We show that for small distances between the local moments, $r < a$, the interaction between local spins is ferromagnetic but for larger $r$ it oscillates between AF and FM regimes with different periods and amplitudes which depend strongly on ellipticity or doping of electron pockets. In addition, the period of the oscillation strongly depends on the magnitude of the SDW gap and the structure of the Fermi surface in the folded BZ.

Our main observation is that the RKKY interaction between magnetic impurities in SDW state become anisotropic below $T_{SDW}$. As a result, the magnetization of the rare-earth magnetic moments, already anisotropic by itself due to crystalline electric field effects, will experience additional temperature dependent anisotropy induced by the conduction electrons below $T_{SDW}$. Quite generally the effect of SDW ordering of Fe spins on the rare-earth subsystem was found in several studies.\cite{Yamada1997,Novosel2007}

However, the effect of induced anisotropy below $T_{SDW}$ on the rare-earth magnetization was observed only recently in EuFe$_2$(As$_{1-x}$P$_x$)$_2$ system by measuring magnetic anisotropy of the Eu$^{2+}$ ions above and below $T_{SDW}$. In particular, it was found that upon decreasing temperature the ratio the magnetization anisotropy of Eu spins, $M_{ab}/M_c$, becomes temperature dependent below $T_{SDW}$ reflecting the influence of the SDW order.\cite{Novosel2007}

This is in direct agreement with our results. Our further observation that the magnetic anisotropy is then also reflected in the spatial anisotropy was not yet observed as it requires the use of unwinned crystals or the use of the local probes such as nuclear magnetic resonance (NMR). It would be interesting to check this effect experimentally.

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