Mass modification of itinerant carriers in RKKY oscillations induced by finite range exchange interactions

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We investigate the Ruderman-Kittel-Kasuya-Yosida oscillations of the itinerant carrier spin density in a system where those oscillations appear only due to a finite distribution of a localized spin. The system represents a half-infinite one-dimensional quantum wire with a magnetic impurity located at its edge. In contrast to the conventional model of a point-like exchange interaction the itinerant carrier spin density oscillations in this system exist. We analytically demonstrate that when the radius of the exchange interaction is less than the wave length of the itinerant carriers living on the Fermi surface, the long range behavior of the oscillations is identical to the one taking place in the zero radius limit of the same exchange interaction but for an infinite one-dimensional quantum wire where, in comparison with the original half-infinite system, the mass of the itinerant carriers is strongly modified by the exchange interaction radius. On the basis of our analysis we make a suggestion on directionality of surface Ruderman-Kittel-Kasuya-Yosida interaction shown in recent experiments: we believe that in general the anisotropy of the Ruderman-Kittel-Kasuya-Yosida interaction could result not only from the anisotropy of the Fermi surface of itinerant carriers but also from the anisotropy of the spin carrying atomic orbitals of magnetic impurities.

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I. INTRODUCTION

Systems with interacting localized magnetic moments play an important role in modern spintronics. Among those systems the ones where the interaction between localized spins is due to the itinerant carriers are very attractive for semiconductor spintronics because the magnetic properties of the systems can be manipulated by the itinerant carrier density. The latter in semiconductors can be easily varied using external gate voltage.

This, so-called itinerant magnetism, is provided by the exchange interaction introduced by Ruderman and Kittel in the context of the hyperfine interaction between a localized nuclear spin and conduction electrons and later by Kasuya and Yosida in the context of the \( s-d \) interaction between conduction electrons and magnetic ions of transition metals.

The essence of the Ruderman-Kittel-Kasuya-Yosida (RKKY) itinerant magnetism is that the exchange interaction between localized spins and paramagnetic itinerant carrier system induces oscillations of the itinerant carrier spin density. These oscillations propagating in an originally non-magnetic system couple localized spins and create a magnetic structure. This type of interaction becomes relevant when the direct spin-spin coupling is weak, \( i.e., \) in diluted systems. For example ferromagnetism in bulk diluted magnetic semiconductors is of the RKKY type. It was investigated in Ga\(_{1-x}\)Mn\(_x\)As using high-resolution scanning tunneling microscopy.

The RKKY effect has also been widely studied in mesoscopic systems both without spin-orbit interactions and with spin-orbit interactions. In the latter case spin-orbit interactions make the RKKY spin density oscillations anisotropic. Impact of electron-electron interactions on the RKKY range function in one-dimensional quantum wires (1D QW) was considered in Refs. It was shown that the range function is different from the one in non-interacting 1D QWs. It turns out that due to electron-electron interactions the range function decays slower than in the non-interacting case.

However, in spite of considerable amount of scientific research on the RKKY interaction a little attention has been paid to the fact that the exchange interaction responsible for the RKKY interaction is actually non-local in space but has a finite range \( r_0 \) given by the spatial spin distribution around the localization center. In theoretical models of the RKKY interaction it is almost always assumed that \( r_0 = 0 \) and the exchange interaction has a point-like character which is modeled by the Dirac delta-function. Of course, in many cases it is a very good
approximation when the wave function of a magnetic impurity is well localized which means that \( r_0 \) is less than all other relevant lengths present in the system. However, in semiconductors there is one important length, namely the wave length of the itinerant carriers living on the Fermi surface, \( l_F \), which can be varied in a wide range. This can be done, e.g., by changing the carrier density with the help of a gate voltage. Therefore, one can reach a situation where \( l_F < r_0 \).

What is more interesting is that even in the case when \( l_F > r_0 \) it can happen that in a given system the RKKY spin density oscillations appear only due to a finite value of \( r_0 \) and cannot appear if \( r_0 = 0 \). Such a situation takes place, for example, when magnetic impurities are deposited on a surface of a paramagnetic bulk sample. The wave function of the itinerant carriers in the sample is equal to zero on its surface and therefore for a point-like model of the exchange interaction, \( r_0 = 0 \), the RKKY spin density oscillations do not appear and cannot couple the spins of the magnetic impurities on the surface. Therefore, no magnetic ordering will take place.

However, in reality \( r_0 \neq 0 \) and the exchange interaction will definitely produce the spin density oscillations with the subsequent magnetic structure of the impurity spins on the surface of the sample. Thus, in this system a finite value of \( r_0 \) creates itinerant surface magnetism.

Some efforts to consider a finite range of the exchange interactions were made in the research devoted to ferromagnetism in Heusler alloys\(^{17–21} \). An essential drawback of the models of the exchange interactions in those attempts was that in the limit \( r_0 \to 0 \) the models did not reproduce point-like exchange interactions. However, it is desirable to reproduce the Dirac delta-function in the limit \( r_0 \to 0 \) because it is often used in many theoretical models and therefore one would like to make a comparison with traditional theories in the limit \( r_0 \to 0 \).

A finite range exchange interaction which in the limit \( r_0 \to 0 \) gives the traditional Dirac delta-function model has been used in Ref.\(^{22} \) to calculate the RKKY exchange integrals and in Ref.\(^{23} \) to study the RKKY spin density oscillations in a mesoscopic ring. In particular, in Ref.\(^{22} \) it has been demonstrated that a finite value of \( r_0 \) removes an unphysical divergency of the RKKY integral at zero distance while in Ref.\(^{23} \) it has been shown that any finite value of \( r_0 \) always becomes important if the number of the electrons in the ring is large enough. However, the research in Ref.\(^{22} \) represented mainly a numerical experiment and, as a result, did not clarify the physical role played by the localization radius of the impurity spin. In addition, the RKKY spin density oscillations in that study were also present in the limiting case \( r_0 \to 0 \) and therefore a finite value of \( r_0 \) did not play any key role in the formation of the RKKY spin density oscillations.

In the present work we use the model of Ref.\(^{23} \) for a finite range exchange interaction in a system where the RKKY spin density oscillations appear only if \( r_0 \neq 0 \). The system represents a half-infinite 1D QW with a magnetic impurity on its edge. Since the wave function of the itinerant carriers (electrons to be definite) is zero on the edge of the wire, the RKKY spin density density oscillations exist only if \( r_0 \) is finite. To understand the physical role played by the impurity spin localization radius in the RKKY spin density oscillations we solve the problem analytically in the case when \( l_F > r_0 \) and calculate the coordinate dependence of the RKKY oscillations in this system. We demonstrate that at large distances this dependence is identical to the one of the RKKY oscillations which one would obtain in the limiting case \( r_0 = 0 \) of our model but for an infinite 1D QW with electrons whose mass is strongly modified by the localization radius of the impurity spin.

The paper is organized as follows. In Section II we mathematically formulate the problem and solve it in Section III using the Feynman diagram approach. In connection with recent experiments we make a suggestion in Section IV about directionality of surface RKKY interaction. Conclusions are given in Section V.

## II. FORMULATION OF THE PROBLEM

As mentioned in the introduction the system represents (see Fig. I) a half-infinite 1D QW with, e.g., a magnetic ion on its edge. It could be also another object, natural or artificial (e.g., a quantum dot with odd electron number) with non-vanishing total spin \( S \). The electrons in a half-infinite 1D QW have eigenenergies

\[
\epsilon_{q_F} = \frac{q_F^2}{2m},
\]

where \( m \) is the effective mass of the conduction electrons and \( q_F \) is not the electron momentum because the translational invariance is broken. The quantum number \( q_x \) takes all real values except zero, \( q_x \neq 0 \). The eigenstates \( |q_x \sigma \rangle \), where \( \sigma \) is the spin quantum number, in the coordinate representation are

\[
\langle x\sigma'|q_x \sigma \rangle = \begin{cases} 
\delta_{\sigma'\sigma} \frac{1}{L} \sin \left( \frac{\pi q_x x}{L} \right) & x \geq 0 \\
0 & x < 0
\end{cases},
\]

where \( L \) is the size of the system. To consider a half-infinite system we take the limit \( L \to \infty \) in the subsequent calculations. Since the momentum operator is \( \hat{p}_x = -i\hbar \partial / \partial x \), one can see that \( \langle x\sigma'|q_x \sigma \rangle \) is not the eigenfunction of \( \hat{p}_x \) and thus, as mentioned above, the quantum number \( q_x \) is not the electron momentum.

The electronic density vanishes on the edge of the wire. Far from the edge it has the value which it would have in an infinite 1D QW with the Fermi momentum \( q_F \) (in the infinite case it would be real momentum),

\[
n_0 = \frac{2q_F}{\pi\hbar}.
\]

In the region close to the edge the electronic density shows oscillations known as the Friedel oscillations.
The half-infinite quantum wire can be modeled by the following potential:

\[ u(x) = \begin{cases} 0, & x > 0, \\ \infty, & x \leq 0. \end{cases} \]  

(3)

The second quantized Hamiltonian of the half-infinite 1D QW without the magnetic impurity thus reads in the coordinate basis as

\[
\hat{H}_0 = \sum_{\sigma} \int dx \left( \hat{\psi}^\dagger \sigma(x) \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \hat{\psi}_\sigma(x) + \right. \\
+ \left. \sum_{\sigma} \int dx u(x) \hat{\psi}^\dagger \sigma(x) \hat{\psi}_\sigma(x), \right)
\]  

(4)

where \( \hat{\psi}^\dagger \sigma(x) \) and \( \hat{\psi}_\sigma(x) \) are the electronic creation and annihilation field operators of the half-infinite 1D QW.

When the magnetic impurity is deposited on the edge of the half-infinite 1D QW, the electronic spin density interacts through the exchange interaction with the impurity spin. The corresponding second quantized Hamiltonian is

\[
\hat{H}_{ex} = \sum_{\sigma,\sigma'} S^i(\sigma|\sigma'|) \int dx \, J(x) \hat{\psi}^\dagger \sigma(x) \hat{\psi}_{\sigma'}(x),
\]  

(5)

where \( \hat{\sigma} \) is the vector of the Pauli matrices and for \( J(x) \) we use the model of Ref. 23.

\[
J(x) = \frac{J}{r_0 \sqrt{\pi}} \exp \left[ -\left( \frac{x}{r_0} \right)^2 \right].
\]  

(6)

The total Hamiltonian describing the RKKY electronic spin density oscillations is given by the sum

\[
\hat{H} = \hat{H}_0 + \hat{H}_{ex}.
\]  

(7)

To get the RKKY oscillations and understand the physical role of the finite impurity spin distribution \( r_0 \) on those oscillations one may consider \( \hat{H}_{ex} \) as a perturbation. In the next section we will implement this perturbation theory on the language of the Feynman diagram expansion.

III. DIAGRAMMATIC SOLUTION

To obtain the electronic spin density we first have to find the imaginary-time (or Matsubara) one-particle Green’s function,

\[
\mathcal{G}_{\sigma\sigma'}(\imath \tau | \imath \tau') = \langle T \hat{\psi}_{\sigma}(x, \tau) \hat{\psi}^\dagger_{\sigma'}(x', \tau') \rangle,
\]  

(8)

where the angular brackets stand for the thermal average and the electronic field operators are in the imaginary-time Heisenberg representation,

\[
\hat{\psi}_\sigma(x, \tau) = e^{\imath \tau (\hat{H} - \mu N)} \hat{\psi}_\sigma(x) e^{-\imath \tau (\hat{H} - \mu N)},
\]

\[
\hat{\psi}^\dagger_\sigma(x, \tau) = e^{\imath \tau (\hat{H} - \mu N)} \hat{\psi}^\dagger_\sigma(x) e^{-\imath \tau (\hat{H} - \mu N)},
\]  

(9)

where \( \mu \) is the chemical potential.

The exact electronic spin density is obtained from the imaginary-time Green’s function as

\[
\sigma_{\text{exact}}^i(x) = -\text{Tr}[\hat{\sigma}^i \mathcal{G}(\imath \tau | \imath \tau + 0)],
\]  

(10)

where the trace is taken in the spin space.

The RKKY oscillations of the electronic spin density are contained in the contribution to \( \mathcal{G}_{\sigma\sigma'}(\imath \tau | \imath \tau') \) of the first order in the perturbation Hamiltonian \( \hat{H}_{ex} \). The corresponding Feynman diagram is shown in Fig. 2. The wavy lines in this diagram are the electronic propagators \( \mathcal{G}^{(0)}_{\sigma\sigma'}(\imath \tau | \imath \tau') \) of the half-infinite 1D QW without the magnetic impurity. They include the Friedel oscillations of the electronic density and can be found using a trick suggested in Ref. 24. The trick is based on the image charge technique. The result is

\[
\mathcal{G}_{\sigma\sigma'}^{(0)}(\imath \tau | \imath \tau') = \mathcal{G}^{(0)}_{\sigma\sigma'}(\imath \tau | \imath \tau') - \mathcal{G}_{\sigma\sigma'}^{(0)}(\imath \tau - \imath \tau')
\]  

(11)

for \( \imath \tau \geq 0 \) and \( \imath \tau' \geq 0 \),

\[
\mathcal{G}_{\sigma\sigma'}^{(0)}(\imath \tau | \imath \tau') = 0
\]  

(12)

for \( \imath \tau < 0 \) or \( \imath \tau' < 0 \). In Eq. (11) \( \mathcal{G}_{\sigma\sigma'}^{(0)}(\imath \tau | \imath \tau') \) is the imaginary-time Green’s function of the corresponding infinite 1D QW without the magnetic impurity.

Using the rules for the analytic reading of Feynman diagrams we obtain from the diagram shown in Fig. 2 the first order contribution to \( \mathcal{G}_{\sigma\sigma'}(\imath \tau | \imath \tau') \), i.e., \( \mathcal{G}_{\sigma\sigma'}^{(1)}(\imath \tau | \imath \tau') \) and calculate the electronic spin density

\[
\sigma^i(x) = -\text{Tr}[\hat{\sigma}^i \mathcal{G}^{(1)}(\imath \tau | \imath \tau + 0)].
\]  

(13)

It is easily verified that the result is given by the following expression:

\[
\sigma^i(x) = \frac{16mJS^i}{\pi^2 \hbar^2} \times \\
\int_0^\infty dq_x \int_0^\infty dq'_x \sin \left( \frac{1}{\hbar} q_x x \right) \sin \left( \frac{1}{\hbar} q'_x x \right) \times \\
\times Q_4 q_x q'_x n_{q_x} - n_{q'_x} q_x^2 - q_x'^2,
\]  

(14)
where \( x \geq 0 \), \( n_{q_x} \) is the Fermion occupation number,

\[
n_{q_x} = \frac{1}{e^\beta (\epsilon_{q_x} - \mu) + 1}
\]  

(15)

with \( \beta = 1/k_B T \) being the inverse temperature and the matrix \( Q_{q_x q'_x} \) is

\[
Q_{q_x q'_x} = \frac{1}{4} \left[ e^{\frac{-q_x^2}{4\hbar^2} (q_x - q'_x)^2} - e^{\frac{-q_x^2}{4\hbar^2} (q_x + q'_x)^2} \right].
\]

(16)

Therefore the dependence of the electronic spin density on the impurity spin distribution comes through the matrix \( Q_{q_x q'_x} \).

One can see from Eq. (16) that when \( r_0 = 0 \), the matrix \( Q_{q_x q'_x} \) vanishes and no RKKY spin density oscillations appear in the system. This is in agreement with our earlier qualitative discussions.

Below we only consider the most interesting case of zero temperature \( T = 0 \). Using Eq. (16) we obtain from Eq. (14) in the zero temperature limit the following expression for the electronic spin density:

\[
\sigma^i(x) = \frac{8mJS^i}{\pi^2 \hbar^2} \times \\
\times \int_0^1 dq_x \int_0^\infty dq'_x \sin \left( \frac{q_F x}{\hbar} q_x \right) \sin \left( \frac{q_F x}{\hbar} q'_x \right) \times \\
\times e^{\frac{-q_x^2}{4\hbar^2} (q_x - q'_x)^2} - e^{\frac{-q_x^2}{4\hbar^2} (q_x + q'_x)^2} \times \\
= 0. Using Eq. (16) we obtain from Eq. (14) in the zero temperature limit the following expression for the electronic spin density:
\]

(17)

\[
I(x) = \\
= \int_0^1 dq_x \int_0^\infty dq'_x \sin \left( \frac{x}{l_F} q_x \right) \sin \left( \frac{x}{l_F} q'_x \right) \times \\
\times e^{\frac{-q_x^2}{4\hbar^2} (q_x - q'_x)^2} - e^{\frac{-q_x^2}{4\hbar^2} (q_x + q'_x)^2} \times \\
q_x^2 - q'_x^2,
\]

(18)

where \( l_F = \hbar/2q_F \), can be calculated analytically in the case \( r_0/l_F \ll 1 \). To do this we perform the expansion

\[
e^{-\left( \frac{q_x^2}{4\hbar^2} \right)} (q_x - q'_x)^2} - e^{-\left( \frac{q_x^2}{4\hbar^2} \right)} (q_x + q'_x)^2} \approx \left( \frac{r_0}{l_F} \right)^2 q_x q'_x.
\]

(19)

Let us denote through \( J(x) \) the integral \( I(x) \) approximated using this expansion,

\[
J(x) = \left( \frac{r_0}{l_F} \right)^2 \times \\
\times \int_0^1 dq_x \int_0^\infty dq'_x \sin \left( \frac{x}{l_F} q_x \right) \sin \left( \frac{x}{l_F} q'_x \right) \times \\
\times \frac{q_x q'_x}{q_x^2 - q'_x^2}.
\]

(20)

The analytical expression for the integral \( J(x) \) is

\[
J(x) = \frac{\pi}{16} \left( \frac{r_0}{l_F} \right)^2 \left[ \frac{2\cos(2x/l_F)}{x/l_F} - \frac{\sin(2x/l_F)}{(x/l_F)^2} \right].
\]

(21)

To demonstrate that the integral \( J(x) \) is really a good approximation to the exact integral \( I(x) \) we calculate the integral \( I(x) \) numerically and show two situations in Figs. 3 and 4 for the two cases \( r_0/l_F < 1 \) and \( r_0/l_F > 1 \), respectively. Even when \( r_0/l_F = 0.4 \), i.e., is not too much smaller than 1, the integral \( J(x) \) gives a good precision and for smaller \( r_0/l_F \) the difference between \( J(x) \) and \( I(x) \) decreases rapidly. On the other side, as one can see from Fig. 4 in the case \( r_0/l_F = 5 \) the integral \( J(x) \) gives values much larger than the exact integral \( I(x) \) and at small distances it even predicts a wrong qualitative coordinate dependence.

In the case when \( r_0/l_F < 1 \) we therefore obtain the
RKKY oscillations of the electronic spin density,
\[ \sigma^i(x) = J S^i \left( \frac{r_0}{l_F} \right)^2 \frac{2m \cos(2x/l_F)}{\pi \hbar^2} \left( \frac{\sin(2x/l_F)}{2x/l_F} - \frac{\sin(2x/l_F)}{(2x/l_F)^2} \right). \]  
(22)

In diluted magnetic systems one is interested in the long range behavior of the RKKY oscillations. From Eq. (22), it follows that the long range behavior of the RKKY oscillations is
\[ \sigma^i(x) = J S^i \left( \frac{r_0}{l_F} \right)^2 \frac{2m \cos(2x/l_F)}{\pi \hbar^2} \frac{\sin(2x/l_F)}{2x/l_F}. \]  
(23)

Comparison of the long range behavior of the RKKY spin density oscillations, Eq. (23), with the one in a point-like Dirac’s delta-function model of the exchange interaction in an infinite 1D QW allows us to make the following conclusion. The RKKY oscillations induced by finite range exchange interactions, \( r_0 \neq 0 \), in a half-infinite 1D QW are identical to the ones which would take place in the limit \( r_0 = 0 \) of our model but in an infinite 1D QW with conduction electrons having a modified mass
\[ m^* = \left( \frac{r_0}{l_F} \right)^2 m. \]  
(24)

This modification is quite strong because in semiconductors the quantity \( r_0/l_F \) may be tuned in a wide range and it can be made much less than 1.

Eq. (24) clarifies the physical role of the finite magnetic impurity spin distribution in the formation of the RKKY spin density oscillations. One can still use a point-like Dirac’s delta-function model of the exchange interaction between the magnetic impurity spin and conduction electrons. However, the electron mass \( m \) must be replaced by the modified mass \( m^* \).

IV. A SUGGESTION ON DIRECTIONALITY OF SURFACE RKKY INTERACTION

In recent experiments\textsuperscript{28} surface RKKY interaction was studied using cobalt adatoms on platinum (111). A strong directional dependence of the RKKY spin density oscillations was observed. The anisotropic behavior was attributed only to the anisotropy of the Fermi surface of platinum.

In connection with our analysis we would like to note that since the wave function of the itinerant carriers in platinum is equal to zero on its surface, the RKKY spin density oscillations in the experiments of Ref. \textsuperscript{28} are definitely only due to a finite spin distribution of cobalt adatoms. As we have shown above for a simple one-dimensional model, the RKKY spin density oscillations existing only due to a finite value of \( r_0 \) are created by electrons whose mass is strongly modified by the radius of the exchange interaction \( r_0 \). Therefore, in addition to the Fermi surface anisotropy the anisotropic behavior of the RKKY spin density oscillations could also be produced by the fact that the itinerant carrier mass for different directions suffers different modification.

It is not difficult to generalize our model, Eq. (20), to take into account the anisotropy of the spin carrying atomic orbitals of a magnetic impurity. The simplest possibility for the case of magnetic adatoms on a two-dimensional surface is
\[ J(x, y) = \frac{J}{r_0^x r_0^y \pi} \exp \left[ - \left( \frac{x}{r_0^x} \right)^2 - \left( \frac{y}{r_0^y} \right)^2 \right], \]  
(25)

where \( r_0^x \neq r_0^y \). Other more adequate models taking into account the real angular distribution of the magnetic impurity spin are also possible.

Since in general the symmetries of the Fermi surface of itinerant carriers and the spin carrying atomic orbitals of a magnetic impurity are different, it is experimentally challenging to distinguish these two different kinds of symmetries in the RKKY spin density oscillations. The experimental observation of traces of the symmetry of the spin carrying atomic orbitals of a magnetic impurity could prove that a finite spin distribution of the impurity spin plays a significant role in the formation of the RKKY interaction.

V. SUMMARY

We have studied the Ruderman-Kittel-Kasuya-Yosida (RKKY) spin density oscillations in a system where these oscillations appear only due to a finite spin distribution of a magnetic impurity. It has been shown that the physical role played by the finite spin distribution is to modify the mass of the itinerant carriers in the system.

Making use of this result we have made a suggestion on the anisotropic behavior of surface RKKY interaction observed in recent experiments which were explained only from the point of view of the anisotropy of the Fermi surface of itinerant carriers. We assume that the anisotropy of the spin carrying atomic orbitals of a magnetic impurity could result in an anisotropic itinerant carrier mass modification and thus it could also contribute to an anisotropic behavior of surface RKKY interaction but with the impurity atomic orbital symmetry which is in general different from the symmetry of the Fermi surface of the itinerant carriers.

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