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Flow equations and the Ruderman-Kittel-Kasuya-Yosida interaction

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Abstract. The method of continuous unitary transformations is applied to obtain the indirect exchange coupling between local magnetic moments in an electron gas. The derivation of the exact analytical expression for the resulting Ruderman-Kittel-Kasuya-Yosida interaction is presented for general dimensionality. In odd dimensions, the result can be shown explicitly to exhibit universal $2k_F$ oscillatory behaviour on all length scales.

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1 Introduction

Over four decades ago, Ruderman and Kittel [1], followed by Kasuya [2] and by Yosida [3], investigated the indirect exchange coupling between localized magnetic moments immersed in a metallic host. They derived the resulting oscillatory long-range magnetic interaction mediated by the polarization of the conduction electrons, which then became known as the Ruderman-Kittel-Kasuya-Yosida or RKKY interaction. In their original work, these authors restricted themselves to consider explicitly the spatial dependence of the interaction in three dimensions, while the two-dimensional case was solved much later by Korenblit and Shender [4] and also by Béal-Monod [5]. The solution in one dimension was obtained by Kittel [6], with several subtleties of his derivation later clarified by Yafet [7]. All these results in special dimensions are based on second order perturbation theory for the magnetic response function. In the derivation of the effective magnetic interaction between the localized spins, they employ a perturbative expression for the nonuniform static susceptibility of the electron gas [6], *i.e.* the Lindhard function. In this framework, an analytical result for the RKKY interaction in generalized dimensionality has been obtained only very recently by Aristov [8], utilizing a Landau-type representation of the electronic Green's function.

In this Rapid Note we present the derivation of the RKKY interaction in general dimension d based on the method of continuous unitary transformations [9,10]. We intend to show that this alternative approach allows to obtain the general analytical expression for the spatial dependence of the coupling between magnetic moments in a very elegant and transparent way. This implies to start *ab initio* from the Hamiltonian of the electron gas coupled to magnetic impurities via a Kondo term. Unlike the usual approach, no prior results for this system need to be invoked, including the electronic propagator and the two-particle correlation function. The derivation is performed completely on the Hamiltonian level. Additionally, we show for odd dimensions that the spatially dependent result for the RKKY susceptibility can be expressed in an analytical form which makes the typical $2k_F$ oscillations explicit for all distances.

2 The flow equations

To describe the coupling of free electrons to local magnetic moments, we consider the Kondo-like Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\sigma}\, c_{\mathbf{k}\sigma} + \frac{J}{2} \sum_{a\mathbf{r}\sigma\sigma'} S^a_{\mathbf{r}}\, c^\dagger_{\mathbf{r}\sigma}\, \sigma^a_{\sigma\sigma'}\, c_{\mathbf{r}\sigma'}. \qquad (1)$$

The $c^\dagger, c$ are fermionic operators and the S^a denote Cartesian components of the localized spins. Accordingly, we choose the dispersion

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m^*} - \epsilon_F. \qquad (2)$$

It is also assumed that the magnetic coupling acts on an energy scale very close to the Fermi edge, $J \ll \epsilon_F$.

To proceed with the original Hamiltonian (1), we apply a properly chosen continuous unitary transformation, $U(\ell)$, which introduces a flow parameter $\ell \geq 0$. Due to this transformation, which aims at the elimination of those scattering terms which do not conserve the electronic energy, the Hamiltonian itself becomes ℓ-dependent, $\mathcal{H}(\ell) = U(\ell)\, H\, U^\dagger(\ell)$. Additionally to the original contributions in (1), $\mathcal{H}(\ell)$ also contains newly generated terms which describe the indirect exchange between the magnetic moments or more complicated interactions. One thus has

$$\mathcal{H}(\ell) = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \; :c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}: + \frac{1}{2} \sum_{a\mathbf{k}\mathbf{k}'} \chi_{\mathbf{k}\mathbf{k}'}(\ell)\; S^a_{\mathbf{k}-\mathbf{k}'} S^a_{\mathbf{k}'-\mathbf{k}} + \frac{1}{2} \sum_{a\mathbf{k}\mathbf{k}'\sigma\sigma'} J_{\mathbf{k}\mathbf{k}'}(\ell)\; S^a_{\mathbf{k}-\mathbf{k}'} : c^\dagger_{\mathbf{k}\sigma} \sigma^a_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} :, \quad (3)$$

where $: \ldots :$ denotes normal ordering with respect to the Fermi sea, corresponding to zero temperature. All terms generated by the transformation are written in normal ordered form. Interaction terms others than those given in (3) are disregarded after normal ordering, since they do not contribute to the magnetic susceptibility in the order we work, $\mathcal{O}(J^2)$. The coupling functions in (3) obey the initial conditions $J_{\mathbf{k}\mathbf{k}'}(0) = J$ and $\chi_{\mathbf{k}\mathbf{k}'}(0) = 0$. Both $J_{\mathbf{k}\mathbf{k}'}$ and $\chi_{\mathbf{k}\mathbf{k}'}$ depend on two momenta, as is enforced by the transformation properties. The flow of the Hamiltonian under the continuous transformation is described by the differential equation [9]

$$\frac{\mathrm{d}}{\mathrm{d}\ell}\mathcal{H}(\ell) = [\eta(\ell), \mathcal{H}(\ell)], \quad (4)$$

where $\eta(\ell)$ is the antihermitean generator which has to be chosen appropriately. In order to eliminate those terms from the Hamiltonian which couple the magnetic impurities to the electron gas, we adopt the choice

$$\eta(\ell) = \frac{1}{2} \sum_{a\mathbf{k}\mathbf{k}'\sigma\sigma'} J_{\mathbf{k}\mathbf{k}'}(\ell)(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) S^a_{\mathbf{k}-\mathbf{k}'} : c^\dagger_{\mathbf{k}\sigma} \sigma^a_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} : . \quad (5)$$

This form of the generator ensures that the nondiagonal ($|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}| > 0$) contributions in (3) are eventually removed. The basic flow equation (4) then results in the following differential equation for the nondiagonal coupling function

$$\frac{\mathrm{d}}{\mathrm{d}\ell} J_{\mathbf{k}\mathbf{k}'}(\ell) = -J_{\mathbf{k}\mathbf{k}'}(\ell)\; (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})^2 + \sum_{\mathbf{q}} n_{\mathbf{q}}\; J_{\mathbf{k}\mathbf{q}}(\ell) J_{\mathbf{q}\mathbf{k}'}(\ell) \big(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}'} - 2\epsilon_{\mathbf{q}}\big). \quad (6)$$

Here $n_{\mathbf{k}} = \theta(k_F - k)$ and $k = |\mathbf{k}|$. The flow of the magnetic susceptibility is given by

$$\frac{\mathrm{d}}{\mathrm{d}\ell} \chi_{\mathbf{k}\mathbf{k}'}(\ell) = J^2_{\mathbf{k}\mathbf{k}'}(\ell)(n_{\mathbf{k}} - n_{\mathbf{k}'})(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}). \quad (7)$$

Note that the occupations $n_{\mathbf{k}}$ enter the flow equations as a consequence of the normal ordering procedure. The electronic energies $\epsilon_{\mathbf{k}}$ do not depend on the transformation flow, since the homogeneous magnetization of the local spins is assumed to vanish.

To obtain the solutions of these differential equations, we restrict ourselves to the contributions to the susceptibility which are of second order in the initial magnetic coupling, *i.e.* of order $\mathcal{O}(J^2)$. To the order $\mathcal{O}(J)$ relevant for the $J_{\mathbf{k}\mathbf{k}'}$, from (6) one then finds an exponential decay of the Kondo coupling,

$$J_{\mathbf{k}\mathbf{k}'}(\ell) = J \exp\big(-\ell\; (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})^2\big) + \mathcal{O}(J^2), \quad (8)$$

which highlights the continuous elimination of all non-degenerate ($k \neq k'$) terms as $\ell \gg 1$. As is apparent from (7), only these non-degenerate scattering processes enter into the effective magnetic interaction, in accordance with the Pauli principle. Although Eq. (6) contains contributions which are of higher order in J, these are not sufficient to obtain the accurate higher order corrections of $J_{\mathbf{k}\mathbf{k}'}(\ell)$. The reason for this is that with the generator (5) new (normal ordered) terms are generated in the transformed Hamiltonian, which do not contribute to the $\mathcal{O}(J^2)$ result for the susceptibility and are therefore neglected, but become important in higher orders. With this solution for $J_{\mathbf{k}\mathbf{k}'}(\ell)$, the magnetic susceptibility is given by

$$\chi_{\mathbf{k}\mathbf{k}'}(\ell) = \frac{J^2}{2} \frac{n_{\mathbf{k}} - n_{\mathbf{k}'}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}} \left(1 - \exp\big(-2\ell\; (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})^2\big)\right). \quad (9)$$

The physical result for $\chi_{\mathbf{k}\mathbf{k}'}$ is now obtained from this expression by taking the limit $\ell \to \infty$.

To compare the results of the continuous transformation via flow equations with the corresponding single-step transformation of the Hamiltonian, note that commuting the generator (5) with itself at different ℓ reproduces its own operator structure after normal ordering,

$$[\eta(\ell), \eta(\ell')] = \frac{1}{2} \sum_{a\mathbf{k}\mathbf{k}'\sigma\sigma'} g_{\mathbf{k}\mathbf{k}'}(\ell, \ell')\, S^a_{\mathbf{k}-\mathbf{k}'} : c^\dagger_{\mathbf{k}\sigma} \sigma^a_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} : . \quad (10)$$

Here, as in (3), more complicated interaction terms are neglected. For $g_{\mathbf{k}\mathbf{k}'}(\ell, \ell')$ one has the result

$$g_{\mathbf{k}\mathbf{k}'}(\ell, \ell') = \sum_{\mathbf{q}} n_{\mathbf{q}} (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}})(\epsilon_{\mathbf{q}} - \epsilon_{\mathbf{k}'}) \times \big(J_{\mathbf{k}\mathbf{q}}(\ell) J_{\mathbf{q}\mathbf{k}'}(\ell') - J_{\mathbf{k}\mathbf{q}}(\ell') J_{\mathbf{q}\mathbf{k}'}(\ell)\big). \quad (11)$$

Since $[\eta(\ell), \eta(\ell')] = \mathcal{O}(J^2)$, one finds that up to terms of this order the unitary transformation $U(\ell) = \exp S(\ell)$ is given by $S(\ell) = \int_0^\ell \mathrm{d}\ell'\, \eta(\ell')$, where

$$S(\ell) = \frac{1}{2} \sum_{a\mathbf{k}\mathbf{k}'\sigma\sigma'} \frac{J - J_{\mathbf{k}\mathbf{k}'}(\ell)}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}} S^a_{\mathbf{k}-\mathbf{k}'} : c^\dagger_{\mathbf{k}\sigma} \sigma^a_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} : . \quad (12)$$

This finding indicates that with respect to the transformed Hamiltonian in $\mathcal{O}(J^2)$ the continuous transformation in the $\ell \to \infty$ limit and the transformation $U(\infty)$ performed in a single step are equivalent.

3 The general solution

From the result (9) for the magnetic interaction in momentum space, the spatial dependence is obtained by

$$\chi_{\mathbf{r}}(\ell) = \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}}\, \chi_{\mathbf{k}\mathbf{k}'}(\ell). \quad (13)$$

Performing first the two polar integrations, one arrives at the useful representation

$$\chi_{\mathbf{r}}(\ell) = \frac{a^{2d}}{(2\pi)^d\, r^{d-2}} \int_0^\infty \mathrm{d}k\, k^{\frac{d}{2}} \int_0^\infty \mathrm{d}k' k'^{\frac{d}{2}} \times \chi_{\mathbf{k}\mathbf{k}'}(\ell)\, \mathcal{J}_{\frac{d}{2}-1}(kr)\, \mathcal{J}_{\frac{d}{2}-1}(k'r), \quad (14)$$

which encapsulates the general dimensional dependence. Here a^d is the volume of the d-dimensional unit cell. We adopt the notation that $\mathcal{J}$ and $\mathcal{N}$ denote Bessel and Neumann functions, respectively. This expression for the spatially varying susceptibility involves integrations over products of Bessel functions which can be evaluated analytically [11]. One obtains the result

$$\chi_{\mathbf{r}}(\infty)=\frac{\pi J^2}{4\epsilon_F}\left(\frac{k_F a^2}{2\pi r}\right)^d\frac{(k_F r)^2}{d-1}\,\Phi_d(k_F r), \tag{15}$$

which is in agreement with [8]. The interesting spatial dependence is contained in the function

$$\Phi_d(x)=\mathcal{J}_{\frac{d}{2}-1}(x)\,\mathcal{N}_{\frac{d}{2}-1}(x)+\mathcal{J}_{\frac{d}{2}}(x)\,\mathcal{N}_{\frac{d}{2}}(x). \tag{16}$$

This result is a continuous function both of the distance r and the dimensionality d. It is valid for general $d>0$. In the asymptotic regime, $k_F r\gg 1$, the expression (15) reduces to

$$\chi_{\mathbf{r}}(\infty)\simeq\frac{J^2}{4\epsilon_F}\left(\frac{k_F a^2}{2\pi r}\right)^d\sin(2k_F r-\pi d/2), \tag{17}$$

where the characteristic $2k_F$-governed oscillations are apparent on long distances. Therefore, one has $\chi_{\mathbf{r}}\sim r^{-d}$ for $r\to\infty$, while $\chi_{\mathbf{r}}\sim r^{2-d}$ for $r\to 0$ and $d>2$. From the result in general dimension (15), one immediately recovers the previously known special solutions for $d=1,2,3$. Utilizing a result for the free electron gas,

$$\left(\frac{k_F a}{2\pi}\right)^d=\frac{\Gamma(\frac{d}{2}+1)}{2\pi^{d/2}}, \tag{18}$$

in $d=3$ one finds the well-known expression

$$\chi_{\mathbf{r}}(\infty)=\frac{9\pi J^2}{4\epsilon_F}\frac{2k_F r\,\cos(2k_F r)-\sin(2k_F r)}{(2k_F r)^4}. \tag{19}$$

For $d=2$, one rederives

$$\chi_{\mathbf{r}}(\infty)=\frac{\pi J^2}{4\epsilon_F}\times\big(\mathcal{J}_0(k_F r)\,\mathcal{N}_0(k_F r)+\mathcal{J}_1(k_F r)\,\mathcal{N}_1(k_F r)\big). \tag{20}$$

In one dimension, due to the vanishing denominator in (15), the calculation involves derivatives of the Bessel and Neumann functions with respect to their index [12]. The correctly reproduced result then reads

$$\chi_{\mathbf{r}}(\infty)=\frac{\pi J^2}{16\epsilon_F}\,\mathrm{si}(2k_F r), \tag{21}$$

with the sine integral $\mathrm{si}(x)=-\int_x^\infty \mathrm{d}t\,t^{-1}\sin t$.

For odd integer spatial dimensionality, a general statement about the oscillatory behaviour of the susceptibility (15) is possible. Defining the nth-degree polynomials $\mathcal{Q}_n(x)$ in terms of generalized hypergeometric functions,

$$\mathcal{Q}_n(x):=\ {}_2F_0[n+1,-n;1/x], \tag{22}$$

which are monotonically increasing on the negative real axis, the function $\Phi_d(x)$ in odd dimensions d can be expressed by

$$\Phi_{2n+1}(x)=\frac{(-1)^{n+1}}{\pi x}\times\Im\left[\exp(2ix)\left(\mathcal{Q}_n^2(2ix)-\mathcal{Q}_{-n}^2(2ix)\right)\right]. \tag{23}$$

Here $n+1$ is a natural number and $\Im$ denotes the imaginary part. This result for $d=2n+1$ shows explicitly that the oscillatory part of the magnetic interaction exhibits the typical $2k_F$ dependence.

More generally, consider the momentum dependent susceptibility

$$\chi_{\mathbf{q}}(\ell)=a^{-d}\sum_{\mathbf{r}}e^{-i\mathbf{q}\mathbf{r}}\,\chi_{\mathbf{r}}(\ell), \tag{24}$$

which can be represented as a Mellin transform,

$$\chi_{\mathbf{q}}(\infty)=\frac{\pi J^2}{4\epsilon_F}\frac{\Gamma(\frac{d}{2}+1)}{d-1}\left(\frac{2k_F}{q}\right)^{\frac{d}{2}-1}\times\int_0^\infty \mathrm{d}x\,x^{2-\frac{d}{2}}\,J_{\frac{d}{2}-1}(\frac{qx}{k_F})\,\Phi_d(x). \tag{25}$$

Readily evaluated, the integration yields the result

$$\chi_{\mathbf{q}}(\infty)=-\frac{dJ^2}{4\epsilon_F}\,\varphi_d(\frac{q}{2k_F}), \tag{26}$$

with the function $\varphi_d(x)$ given by

$$\varphi_d(x)=\theta(1-x)\,{}_2F_1[1,1-\frac{d}{2};\frac{3}{2};x^2]+\theta(x-1)\,\frac{1}{dx^2}\,{}_2F_1[1,\frac{1}{2};1+\frac{d}{2};1/x^2]. \tag{27}$$

Note that in even integer dimensions $\varphi_{2n}(x)$ in the range $x<1$ is a $(n-1)$th-degree polynomial in x^2. More specifically, for $x<1$ it can be expressed as

$$\varphi_{2n}(x)=\frac{(-2)^{n-1}(n-1)!}{(2n-1)!!}\,P_{n-1}^{(\frac{1}{2}-n,\frac{1}{2})}(2x^2-1), \tag{28}$$

where the $P_m^{(\alpha,\beta)}$ are Jacobi polynomials.

4 Final remarks

In this Rapid Note we have presented a derivation of the RKKY interaction for general spatial dimension, utilizing the method of flow equations based on continuous unitary transformations. To emphasize the conceptual elegance of this method, the calculations have been performed explicitly in order $\mathcal{O}(J^2)$ and for the free electron gas. However, the general expressions derived in section 2 remain valid in a straightforward manner also for a more complicated electron dispersion, but then the resulting momentum integrations are much more difficult to solve analytically. To extend the derivation beyond the second order of the coupling J, a number of additional new interaction terms must be included in the transformed Hamiltonian and the generator. This leads to higher-order corrections of the flow equations for the couplings $J_{\mathbf{kk}'}$ and $\chi_{\mathbf{kk}'}$, as well as to new flow equations for the additional couplings. Although this extended set of flow equations again can be solved exactly order by order of J, the final multiple momentum integrals become quite intractable. However, also at this level the calculations remain much more transparent than standard many-body perturbation theory.

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