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Advanced Condensed Matter Theory — SS10

Exercise 6

1.0. The Rudermann-Kittel-Kasuya-Yosida (RKKY) Interaction

This exercise is concerned with the derivation of the form of the RKKY interaction. The RKKY is a particular kind of magnetic interaction between magnetic ions which are separated by a finite distance. In this case there can be of course no direct interaction between the ions. They can, however, *indirectly* interact through mediation by the quasi-free, mobile electrons of the conduction band, in which the two magnetic ions are assumed to be embedded. The Hamiltonian for such an interaction has the form

$$H = H_s + H_{sf} = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - J \sum_{i=1}^{2} \mathbf{s}_i \cdot \mathbf{S}_i \tag{1}$$

where here H_s is the Hamiltonian for the conduction electrons, while $\mathbf{s}_i$ and $\mathbf{S}_i$ are the spin operators for the electrons and magnetic ions respectively.

a) Show the general relation

$$H_{sf} = -J \sum_{i=1}^{2} \mathbf{s}_i \cdot \mathbf{S}_i = -J \sum_{i=1}^{2} \left\{ s_i^z S_i^z + \frac{1}{2}(s_i^+ S_i^- + s_i^- S_i^+) \right\} \tag{2}$$

b) Expressing the electron spin operators in terms of the creation and annihilation operators in the usual way, i.e., $s_i^z = \frac{\hbar}{2}(c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow})$, $s_i^+ = \hbar c^\dagger_{i\uparrow} c_{i\downarrow}$, and $s_i^- = \hbar c^\dagger_{i\downarrow} c_{i\uparrow}$ and performing a Fourier transformation of the creation and annihilation operators into wavevector space, show that (2) can be written in the form

$$H_{sf} = -\frac{J\hbar}{2N} \sum_i \sum_{\mathbf{k},\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{R}_i} \left\{ S_i^z \left(c^\dagger_{\mathbf{q}+\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{q}+\mathbf{k}\downarrow} c_{\mathbf{k}\downarrow} \right) + S_i^+ c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} + S_i^- c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} c_{\mathbf{k}\downarrow} \right\} \tag{3}$$

We want to perform a perturbation calculation upon the interaction Hamiltonian H_{sf} between the localized f-electrons and the conduction band electrons. In other words, we want to calculate the energy correction due to H_{sf} up to 2nd order. These quantities are defined in the usual manner: For the 1st order correction we have

$$E_0^{(1)} = \langle\, 0; f \mid H_{sf} \mid 0; f \,\rangle \tag{4}$$

and the 2nd order expression is

$$E_0^{(2)} = \sum_{(A,f') \neq (0,f)} \frac{\mid \langle\, 0; f \mid H_{sf} \mid A; f' \,\rangle \mid^2}{E_0^{(0)} - E_A^{(0)}} \tag{5}$$

For this purpose we need to carefully define the unperturbed *unpolarized* ground state $\mid 0; f\,\rangle$ and excited state $\mid A; f'\,\rangle$ of the *total* system. We first see that the space and spin parts can be separated: $\mid 0; f\,\rangle \equiv \mid 0\,\rangle \mid f\,\rangle$ and analogously for the excited state. The ground state of the unperturbed *electronic* system (corresponding to the filled Fermi sphere) is defined in the usual way as $\mid 0\,\rangle = \frac{1}{N!}\sum_{\mathcal{P}}(-1)^p\mathcal{P}\mid \mathbf{k}_1^{(1)}m_{s1}^{(1)}, \mathbf{k}_2^{(2)}m_{s2}^{(2)}, \ldots \mathbf{k}_N^{(N)}m_{sN}^{(N)}\,\rangle$ and analogously for the excited state, where the kets $\mid \mathbf{k}_i^{(i)}m_{si}^{(i)}\,\rangle \equiv \mid \mathbf{k}_i^{(i)}\,\rangle \mid m_{si}^{(i)}\,\rangle$ are single electron states where i is a electron label.

c) Based on the information given above, argue that (4) vanishes.

d) We note that the expression for the 2nd order energy correction involves matrix elements which connect ground and excited states $\langle\, 0; f \mid H_{sf} \mid A; f'\,\rangle$. Due to the orthonormality of the single particle states the matrix element splits into expressions of the form $\langle\, 0 \mid \mathcal{O} \mid A\,\rangle \Rightarrow \langle\, \mathbf{k}'m_s' \mid \mathcal{O} \mid \mathbf{k}''m_s''\,\rangle$. Argue, in the same way as in question (c), that the following matrix elements take the forms

$$\langle\, \mathbf{k}'m_s' \mid c^\dagger_{\mathbf{q}+\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{q}+\mathbf{k}\downarrow}c_{\mathbf{k}\downarrow} \mid \mathbf{k}''m_s''\,\rangle \to \Theta(k_F - |\mathbf{k}+\mathbf{q}|)\Theta(|\mathbf{k}| - k_F)\delta_{\mathbf{k},\mathbf{k}''}\delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'}\frac{2}{\hbar}\langle\, m_s' \mid s_z \mid m_s''\,\rangle$$

$$\langle\, \mathbf{k}'m_s' \mid c^\dagger_{\mathbf{q}+\mathbf{k}\uparrow}c_{\mathbf{k}\downarrow} \mid \mathbf{k}''m_s''\,\rangle \to \Theta(k_F - |\mathbf{k}+\mathbf{q}|)\Theta(|\mathbf{k}| - k_F)\delta_{\mathbf{k},\mathbf{k}''}\delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'}\frac{2}{\hbar}\langle\, m_s' \mid s_+ \mid m_s''\,\rangle$$

$$\langle\, \mathbf{k}'m_s' \mid c^\dagger_{\mathbf{q}+\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} \mid \mathbf{k}''m_s''\,\rangle \to \Theta(k_F - |\mathbf{k}+\mathbf{q}|)\Theta(|\mathbf{k}| - k_F)\delta_{\mathbf{k},\mathbf{k}''}\delta_{\mathbf{k}+\mathbf{q},\mathbf{k}'}\frac{2}{\hbar}\langle\, m_s' \mid s_- \mid m_s''\,\rangle$$

e) Putting together the different pieces into (5) and using the completeness relations $\sum_{f'} \mid f'\,\rangle\,\langle\, f' \mid = 1$ and $\sum_{m_s''} \mid m_s''\,\rangle\,\langle\, m_s'' \mid = 1$ show that we have the intermediate result

$$E_0^{(2)} = \frac{J^2}{4N^2}\sum_{\mathbf{k},\mathbf{q}}\sum_{i,j}\sum_{m_s'}\frac{\Theta_{\mathbf{k},\mathbf{k}+\mathbf{q}}e^{-i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}}{\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})}\,[\,\langle\, f \mid \langle\, m_s' \mid \{\, S_i^z(4S_j^z(s_z)^2 + 2S_j^+(s_zs_-) + 2S_j^-(s_zs_+)) +$$
$$+ S_i^+(2S_j^z(s_-s_z) + S_j^+(s_-)^2 + S_j^-(s_-s_+)) + S_i^-(2S_j^z(s_+s_z) + S_j^+(s_+s_-) + S_j^-(s_+)^2)\,\}\mid m_s'\,\rangle \mid f\,\rangle\,]$$

f) Using the fact that $s_i = \frac{\hbar}{2}\sigma_i, i = x, y, z$ and the relations $s_+ = \frac{\hbar}{2}(\sigma_x + i\sigma_y), s_- = \frac{\hbar}{2}(\sigma_x - i\sigma_y)$ show that

$$E_0^{(2)} = \frac{J^2\hbar^2}{2N^2}\sum_{\mathbf{k},\mathbf{q}}\sum_{i,j}\Theta_{\mathbf{k},\mathbf{k}+\mathbf{q}}e^{-i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\frac{\langle\, f \mid \mathbf{S}_i\cdot\mathbf{S}_j \mid f\,\rangle}{\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})} \tag{6}$$

from which one can read off the coupling constant J_{ij}^{RKKY} in the effective Hamiltonian

$$H_f^{RKKY} = -\sum_{i,j} J_{ij}^{RKKY}\mathbf{S}_i\cdot\mathbf{S}_j \tag{7}$$

g) Evaluate J_{ij}^{RKKY}. Do this in the *effective mass approximation* $\varepsilon(\mathbf{k}) = \frac{\hbar^2k^2}{2m^*}$ and by first converting the two summations into integrations, i.e., $\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{q}} \to \frac{V^2}{N^2(2\pi)^6}\int d^3k\int d^3q$ to obtain the intermediate result

$$J_{ij}^{RKKY} = \frac{m^*J^2V^2}{N^24\pi^4R_{ij}^2}\int_0^{k_F}\int_{k_F}^{\infty}dk\,k\frac{\sin(k'R_{ij})\sin(kR_{ij})}{k^2-k'^2} \tag{8}$$

h) Set the lower integral limit in the second integral to zero in (8). Use (or first prove!)

$$\int_0^{\infty}dk\,k\frac{\sin(kR_{ij})}{k^2-k'^2} = \frac{\pi}{2}\cos(k'R_{ij}) \tag{9}$$

to find the final expression for J_{ij}^{RKKY}.