University of Regensburg Summer Term 2018

Quantum Theory of Condensed Matter I

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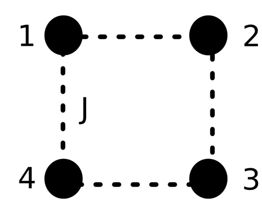
Sheet 6

1. Heisenberg Model: Small System .... [9P]

Solve the Heisenberg model for a system consisting of four electrons ($S = 1/2$) coupled with $J > 0$ as depicted in the figure. It is described by the Hamiltonian

$$H = J \sum_{n=1}^{4} \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \qquad \text{with } \mathbf{S}_1 \equiv \mathbf{S}_5.$$



(a)(3P) Calculate the eigenenergies of H. *Hint:* Rewrite H using $\mathbf{S}_{13} = \mathbf{S}_1 + \mathbf{S}_3$ and $\mathbf{S}_{24} = \mathbf{S}_2 + \mathbf{S}_4$.

(b)(3P) Determine the corresponding eigenstates. *Hint:* Look up Clebsch-Gordan coefficients.

(c)(3P) Compare the ground state energy with the energy of the state where two pairs of electrons, e.g., $(1, 2)$ and $(2, 4)$, are in a singlet state, respectively. Why can we call the ground state *valence-bond state*?

2. Rudermann-Kittel-Kasuya-Yosida Interaction .... [13P]

Assume a system of distributed localized magnetic ions ($\mathbf{S}_i$) where the inter-ion separation is too large for a direct exchange mechanism (their corresponding *unperturbed* Hamiltonian is thus $H_S \equiv 0$). In the following we are going to calculate an indirect exchange interaction between two ion spins which is mediated by quasi-free electrons of the conduction band. The unperturbed part of the model consists of

$$H_s = \sum_{\mathbf{k},\sigma} \epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{1}$$

for the conduction electrons, with $c^\dagger_{\mathbf{k}\sigma}(c_{\mathbf{k}\sigma})$ the creation (annihilation) operator of an electron with wave vector $\mathbf{k}$ and spin σ. This Hamiltonian is perturbed by the exchange interaction between the electrons and two localized ions. The corresponding perturbation operator is taken to be of Heisenberg type and thus given by

$$H_{sS} = -J \sum_{i=i}^{2} \mathbf{s}_i \cdot \mathbf{S}_i. \tag{2}$$

(a)(2P) Show that H_{sS} can be written as

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

with N the number of positions $\mathbf{R}_i$ in the volume V.
Hint: Write down the spin operators in second quantization: $s^z_i = (\hbar/2)(c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow})$, $s^+_i = \hbar c^\dagger_{i\downarrow} c_{i\downarrow}$ etc. Perform a Fourier transformation into wavevector space.

(b)(6P) The unperturbed ground state $|0,\gamma\rangle$ of the *total* system can be separated into the Slater determinant of the single electron (s-type) states $|\mathbf{k}_i^{(i)}, m_{s_i}^{(i)}\rangle$, written down as

$$|0\rangle := \frac{1}{N!}\sum_{\mathcal{P}}(-1)^p \mathcal{P}\,|\mathbf{k}_1^{(1)} m_{s1}^{(1)}, \mathbf{k}_2^{(2)} m_{s2}^{(2)}, \ldots, \mathbf{k}_N^{(N)} m_{sN}^{(N)}\rangle\,, \tag{4}$$

and the spin part $|\gamma\rangle$: $|0,\gamma\rangle = |0\rangle\,|\gamma\rangle$, which is an eigenstate of $H_S + H_s$. Here, $m_{s_i} = \pm 1/2$ is the magnetic quantum number and the superscript referring to the particle number. Since the electron spins of the unperturbed ground state do not interact, the spin part $|\gamma\rangle$ contains all possible relative spin orientations.

Show that the perturbation correction in first order vanishes and the second is given by

$$E_0^{(2)} = \frac{J^2\hbar^2}{2N^2}\sum_{\mathbf{kq}}\sum_{i,j}\theta(k_F - |\mathbf{k}+\mathbf{q}|)\theta(|\mathbf{k}| - k_F)\frac{\langle\gamma|\,\mathbf{S}_i\cdot\mathbf{S}_j\,|\gamma\rangle}{\epsilon(\mathbf{k}+\mathbf{q}) - \epsilon(\mathbf{k})}e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \tag{5}$$

with the Heaviside function θ and the Fermi wave vector k_F.
Hint: To get the 2nd order correction one has to evaluate $\langle 0,\gamma\,|H_{sS}|\,A,\gamma'\rangle$ with $|A,\gamma'\rangle$ being the excited state. The evaluation of the matrix elements simplifies due to to the orthonormality of the single particle states: $\langle 0\,|.|\,A\rangle \to \langle\mathbf{k}' m_s'\,|.|\,\mathbf{k}'' m_s''\rangle$

(c)(5P) The result from (b) allows for the definition of an effective Hamiltonian

$$H^{\mathrm{RKKY}} = -\sum_{ij} J_{ij}^{\mathrm{RKKY}}\mathbf{S}_i\cdot\mathbf{S}_j \tag{6}$$

with the eigenvalue $E_0^{(2)}$. Using the effective mass approximation, $\epsilon(\mathbf{k}) = \hbar^2 k^2/(2m^*)$, show that the *RKKY-coupling constant* is given by

$$J_{ij}^{\mathrm{RKKY}} = \frac{J^2 k_F^6}{\epsilon_F}\frac{\hbar^2 V^2}{N^2(2\pi)^3}F(2k_F R_{ij}) \tag{7}$$

where $\epsilon_F = \epsilon(k_F)$, $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$ and

$$F(x) = \frac{\sin(x) - x\cos(x)}{x^4}. \tag{8}$$

Hint: Use $(1/N^2)\sum_{\mathbf{kq}} \to V^2/(N^2(2\pi)^6)\int \mathrm{d}^3k \int \mathrm{d}^3q$ and $\mathbf{R}_{ij}$ as the polar axis in polar coordinates. An intermediate result is

$$J_{ij}^{\mathrm{RKKY}} = m^*\left(\frac{JV}{2\pi^2 N R_{ij}}\right)^2\int_0^{k_F}\mathrm{d}k'\,k'\int_{k_F}^{\infty}\mathrm{d}k\,k\frac{\sin(k'R_{ij})\sin(kR_{ij})}{k^2 - k'^2}. \tag{9}$$

Why can we set the lower integral limit in the second integral to zero? Further, prove and use

$$\int_0^{\infty}\mathrm{d}k\,k\frac{\sin(kR_{ij})}{k^2 - k'^2} = \frac{\pi}{2}\cos(k'R_{ij}). \tag{10}$$