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Theorie zu Magnetismus, Supraleitung und Elektronische Korrelation in Festkörpern

Sommersemester 2019

Blatt 8

(Abgabe: 11.06.2019)

Aufgabe 1 (**Intra-atomic exchange and the Hund's rule coupling**) (10=5+5 Punkte)

Consider the general two-particle operator of the the Coulomb interaction

$$H = V = \frac{1}{2}\sum_{i\neq j} V_c(\vec{r}_i, \vec{r}_j), \tag{1}$$

where the indices i, j label the interacting electrons.

i) For the case of three interacting t_{2g} orbitals, due to symmetry there are only three independent Coulomb integrals for appropriatly chosen real wave functions of the t_{2g} orbitals

$$U = \langle mm|V_c|mm\rangle = \int d^3r d^3r' \; \phi_m(\vec{r})\phi_m(\vec{r'})V_c(\vec{r},\vec{r'})\phi_m(\vec{r'})\phi_m(\vec{r}), \tag{2}$$

$$U' = \langle mm'|V_c|mm'\rangle = \int d^3r d^3r' \; \phi_m(\vec{r})\phi_{m'}(\vec{r'})V_c(\vec{r},\vec{r'})\phi_{m'}(\vec{r'})\phi_m(\vec{r}), \tag{3}$$

$$J = \langle mm'|V_c|m'm\rangle = \int d^3r d^3r' \; \phi_m(\vec{r})\phi_{m'}(\vec{r'})V_c(\vec{r},\vec{r'})\phi_m(\vec{r'})\phi_{m'}(\vec{r}) \tag{4}$$

Rewrite the Coulomb interaction in terms of second quantization with creation/annihilation operators $d^\dagger_{m\sigma}, d_{m\sigma}$ for the t_{2g} orbitals m and identify the terms of the Kanamori Hamiltonian

$$\begin{aligned} H_K = {} & U\sum_m n_{m\uparrow}n_{m\downarrow} + U'\sum_{m\neq m'} n_{m\uparrow}n_{m'\downarrow} + (U'-J)\sum_{m<m',\sigma} n_{m\sigma}n_{m'\sigma} \\ & - J\sum_{m\neq m'} d^\dagger_{m\uparrow}d_{m\downarrow}d^\dagger_{m'\downarrow}d_{m'\uparrow} + J\sum_{m\neq m'} d^\dagger_{m\uparrow}d^\dagger_{m\downarrow}d_{m'\downarrow}d_{m'\uparrow}. \end{aligned} \tag{5}$$

What is the physical interpretation of each term?

ii) Using the definition of the total charge, spin and orbital isospin generators

$$N = \sum_{m\sigma} n_{m\sigma} \tag{6}$$

$$\vec{S} = \frac{1}{2}\sum_m\sum_{\sigma\sigma'} d^\dagger_{m\sigma}\vec{\tau}_{\sigma\sigma'}d_{m\sigma'} \tag{7}$$

$$L_m = i\sum_{m'm''}\sum_\sigma \epsilon_{mm'm''}d^\dagger_{m'\sigma}d_{m''\sigma}, \tag{8}$$

where $\vec{\tau}$ are the Pauli matrices, one can show that the Kanamori Hamiltonian H_K can be written as

$$\begin{aligned} H_K = {} & \frac{1}{4}(3U'-U)N(N-1) + (U'-U)\vec{S}^2 + \frac{1}{2}(U'-U+J)\vec{L}^2 \\ & + \left(\frac{7}{4}U - \frac{7}{4}U' - J\right)N + (U'-U+2J)\sum_{m\neq m'} d^\dagger_{m\uparrow}d^\dagger_{m\downarrow}d_{m'\downarrow}d_{m'\uparrow}. \end{aligned} \tag{9}$$

(You can get 5 bonus points for the derivation of Eq. (9))

Show that the requirement of Eq. (9) to be spin-rotationally invariant leads to $U' = U - 2J$. One possibility is to consider the state of two electrons in the Eigenstates of σ_x, i.e. $|\sigma_x^+ \sigma_x^-\rangle = c^\dagger_{\sigma_x^+} c^\dagger_{\sigma_x^-} |0\rangle = \frac{1}{2}\left(c^\dagger_\uparrow + c^\dagger_\downarrow\right)\left(c^\dagger_\uparrow - c^\dagger_\downarrow\right)|0\rangle$ and show that it is not an eigenstate of the last term in Eq. (9).

Show that in this case the Kanamori Hamiltonian reduces to

$$H_K = (U - 3J)\frac{N(N-1)}{2} - 2J\vec{S}^2 - \frac{J}{2}\vec{L}^2 + \frac{5}{2}JN. \tag{10}$$

Check if this Hamiltonian obeys the Hund's rules of maximal S, then maximal L.