Energy Spectrum of the Ferromagnet with Threefold Orbital Degeneracy

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For the detailed theoretical investigation of magnetic and electrical phenomena, in particular, the metal-insulator transition, in family of doped fullerides, the model [1] which took into account peculiarities of narrow-band materials, namely an orbital degeneracy of electronic energy levels, an intra-atomic Coulomb repulsion and a correlated hopping of electrons has been proposed. Ferromagnetic ordering in the noted materials attracts much attention [?] therefore the model [1] is to be developed further by taking into account interatomic exchange interaction J besides the Hund's rule coupling J_H. In the regime of week to moderate Coulomb interaction the use of modified mean field approach [2] within the Green function method has allowed us to obtain the single electron energy spectrum:

$$E^{\lambda\sigma}\left(\vec{k}\right) = -\tilde{\mu}_{\lambda\sigma} + \alpha^{\lambda\sigma} t\left(\vec{k}\right),$$

where the normalized chemical potential

$$\tilde{\mu}_{\lambda\sigma} = \mu - \beta'_{\lambda} - \beta''_{\lambda\sigma} - Un_{\lambda\bar{\sigma}} - 2U'n_{\bar{\lambda}\bar{\sigma}} - 2\left(U' - J_H\right)n_{\bar{\lambda}\sigma} + zJ\sum_{\lambda} n_{\lambda\sigma},$$

and the correlation band narrowing factor

$$\alpha^{\lambda\sigma} = 1 - \tau_1 n - 4\tau' n_{\bar{\lambda}} - 2\tau'' n_{\lambda\bar{\sigma}} - \frac{zJ}{w}\sum_{j\sigma}\left\langle a^{+}_{j\alpha\sigma} a_{p\alpha\sigma}\right\rangle.$$

are introduced. In line with the terminology of the paper [2] we treat $\beta''_{\lambda\sigma}$ as a spin-dependent shift of a band center. The correlated hopping, being the essential peculiarity of the model, is characterized by the dimensionless parameters $\tau' = t'_{pj}/\left|t_{pj}\right|$, $\tau'' = t''_{pj}/\left|t_{pj}\right|$. The half band width of the energy band is given by the relation $w = z\left|t_{pj}\right|$, where z stands for the nearest neighbor s number, n is electron concentration. Filling factors for single-electron states, electron concentration and the system magnetization m are related by the equations $n_{\alpha\uparrow} + n_{\alpha\downarrow} + n_{\beta\uparrow} + n_{\beta\downarrow} + n_{\gamma\uparrow} + n_{\gamma\downarrow} = n$, $n_{\alpha\uparrow} + n_{\beta\uparrow} + n_{\gamma\uparrow} - n_{\alpha\downarrow} - n_{\beta\downarrow} - n_{\gamma\downarrow} = m$. From these equations in the case of absence of the orbital order the concentrations of electrons in particular spin and orbital states are obtained $n_{\alpha\uparrow} = (n+m)/3$, $n_{\alpha\downarrow} = (n-m)/3$.

The obtained energy spectrum is used to derive an analytical expression for the ground state energy E_0:

$$E_0 = \frac{1}{2N}\sum_{\vec{k}\lambda\sigma}\left(t_{\vec{k}}(n) + E^{\lambda\sigma}_{\vec{k}}\right)\left[1 + \exp\left(\left(E^{\lambda\sigma}\left(\vec{k}\right) - \mu\right)/kT\right)\right]^{-1}$$

Dependencies of the ground state energy of the model under investigation on the energy parameters U, J_H, zJ, correlated hopping parameters, electron concentration and magnetization has been studied in detail and the equilibrium ground state magnetization m_{GS} has been found.

References

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2. L. Didukh, V. Hankevych, O. Kramar, Yu. Skorenkyy, Jour. of Phys.: Cond. Matter **14**, 827 (2002).