New mean field approximation in the theory of strongly correlated systems

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Approach which develops ideas of papers [1–3] is proposed. In framework of the proposed approximation the single electron Green function for the Hubbard model is obtained, in particular. This function for the case of half filled band (mean number of electrons per site $n = n_\uparrow = n_\downarrow = 1$) and absence of the magnetic ordering has the following form

$$G_{\mathbf{k}} = \frac{1}{4\pi}\left(\frac{A_{\mathbf{k}}}{E - E_1(\mathbf{k})} + \frac{B_{\mathbf{k}}}{E - E_2(\mathbf{k})}\right),$$

where $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ depend on the energy parameters $t(\mathbf{k})$ (hopping integral) and U (intraatomic Coulomb repulsion) as well as on the polar states concentration d (concentrations of doublons and holes are equal),

$$E_{1,2}(\mathbf{k}) = \frac{(\epsilon_1 + \epsilon_2)}{2} + (1-2d)t(\mathbf{k}) \mp \frac{1}{2}\sqrt{(U + \epsilon_2 - \epsilon_1)^2 + (4dt(\mathbf{k}))^2},$$

$$\epsilon_1 = \frac{n_\downarrow}{N}\sum_{\mathbf{k}} \frac{t^2(\mathbf{k})}{E - \frac{U}{2} - t(\mathbf{k})}, \quad \epsilon_2 = \frac{n_\uparrow}{N}\sum_{\mathbf{k}} \frac{t^2(\mathbf{k})}{E + \frac{U}{2} - t(\mathbf{k})}.$$

Two latter expressions are written with taking into account possible magnetic ordering ($n_\uparrow \neq n_\downarrow$) in presense of magnetic field. In the two-pole approximation they are the shifts of the "atomic" levels. In consequence of this the activation energy of hole-doublon pair is renormalized ($U \to U + \epsilon_2 - \epsilon_1$). The obtained two-pole spectrum is exact in atomic and band limits, temperature dependent, reproduces the Hartree-Foch spectrum in the regime of weak interactions and the spectrum calculated with use of perturbation theory in the case of strong interactions ($t - J$ model for $n = 1$), describes the metal-insulator transition.

Taking into account the Hubbard center $\leftrightarrow$ Hubbard band transitions beyond the two-pole approximation leads not only to the "atomic" levels shifts, but also to the levels broadening and quasiparticle damping.

1. Didukh L. Journ. of Phys. Studies, vol.1 241 (1997).
2. Didukh L. phys. stat. solidi (b), vol.206 R5 (1998).
3. Didukh L. Acta Physica Polonica (B), vol.31 3097 (2000).