Self-consistent description of simplified pseudospin-electron model

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A method of the self-consistent calculation of the thermodynamical and correlation functions is presented. This approach is based on the GRPA (generalized random phase approximation) scheme with the inclusion of the mean field corrections. The numerical research shows that interaction between the electron and pseudospin subsystems leads to the possibility of the dipole (pseudospin) and charge-density instabilities as well as phase separation into the uniform and/or chess-board phases.

The aim of this article is to calculate the correlation functions, pseudospin and particle number mean values as well as the grand canonical potential for the simplified \((U = 0)\) pseudospin-electron model (PEM) within the one self-consistent approach.

PEM includes the local interaction of the conducting electrons with some two level subsystem described by pseudospins \(S^z = \pm 1/2\) (e.g. anharmonic vibrations of the apex oxygen ions in YBaCuO-type crystals) \([2]\). On the other hand, PEM can be transform into the binary alloy type model as well as into the Falikov-Kimball model (FKM) and they can be also studied analytically within the framework of the developed scheme.

The model Hamiltonian is the following:

\[
H = \sum_i H_{i0} + \sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma},
\]

\[
H_{i0} = -\mu \sum_{\sigma} n_{i\sigma} + g \sum_{\sigma} n_{i\sigma} S_i^z - h S_i^z,
\]

where an interaction with pseudospins \((g\text{-term})\) placed in some longitudinal field \(h\) (chemical potential for ions in FKM) are included in the single-site part; \(\mu\) is the chemical potential. The second term in the Hamiltonian describes an electron hopping from site to site.

The calculations are performed in the strong coupling case \((g \gg t)\) using single-site states as the basic one. A formalism of the electron annihilation (creation) operators \(a_{i\sigma} = c_{i\sigma} P^+_i\), \(\hat{a}_{i\sigma} = c_{i\sigma} P^-_i\) \((P^\pm_i = 1/2 \pm S_i^z)\) acting at a site with the certain pseudospin orientation is introduced.

Expansion of the calculated quantities in terms of the electron transfer leads to an infinite series of terms containing the averages of the \(T\)-products of the \(a_{i\sigma}, \hat{a}_{i\sigma}\) operators. The evaluation of such averages is made using the corresponding Wick’s theorem. The results are expressed in terms of the products of the nonperturbed Green’s functions and averages of the projection operators \(P_i^\pm\) which are calculated by means of the semi-invariant expansion \([3]\).

The calculation of the correlation functions is performed within a self-consistent scheme in the framework of the generalized random phase approximation \([4]\) with the inclusion of the mean field type contributions coming from the effective pseudospin interaction via conducting electrons, i.e. all zero-order correlators (second order semi-invariants) as well as pseudospin mean value are calculated by the mean-field Hamiltonian:

\[
H_{MF} = \sum_i H_{i0} + \alpha_1 P^+_i + \alpha_2 P^-_i,
\]

\[
\alpha_1 P^+_i + \alpha_2 P^-_i = \frac{2}{N\beta} \sum_{n,k} \frac{t_{ik}^2}{g_n^{-1} - t_{ik}} \left[ \frac{P^+_i}{\omega_n - \varepsilon_1} + \frac{P^-_i}{\omega_n - \varepsilon_2} \right],
\]

\[
g_n = \frac{\langle P^+ \rangle}{\omega_n - \varepsilon_1} + \frac{\langle P^- \rangle}{\omega_n - \varepsilon_2}, \quad \varepsilon_{1,2} = -\mu \pm \frac{g}{2}.
\]

Diagram equation on pseudospin correlator \(\langle S^z S^z \rangle_q\) is following:

![Diagram equation on pseudospin correlator](image)

This equation differs from the one for the Ising model in MFA by the replacement of the exchange
interaction by the electron loop (which describes an interaction between pseudospins via conducting electrons). In the analytical form its solution is equal

$$\chi_{S^zS^z}(\omega_m, q) = \frac{\delta(\omega_m)(P^+)(P^-)}{T - \Theta(T, q)},$$

$$\Theta(T, q) = -\frac{2}{\beta} \sum_n \frac{1}{N} \sum_k \Lambda_n^2 \tilde{t}_n(k) \tilde{t}_n(k + q),$$

$$\Lambda_n = g \sqrt{\langle P^+ \rangle \langle P^- \rangle} \frac{\tilde{t}_n(k)}{(1 - g_n \tilde{t}_n(k))}.$$

Equation for pseudospin mean value in the uniform case ($\langle S_i^z \rangle = \langle S^z \rangle$) is following:

$$\langle S^z \rangle = \frac{1}{2} \tan \left\{ \frac{\beta}{2} (h + \alpha_2 - \alpha_1) + \ln \frac{1 + e^{-\beta \epsilon_1}}{1 + e^{-\beta \epsilon_2}} \right\}$$

We also calculate particle number mean value and grand canonical potential [3]. All quantities can be derived from the grand canonical potential by

$$\frac{d\Omega}{d(-h)} = \langle S^z \rangle,$$

$$\frac{d\langle S^z \rangle}{d(\beta h)} = \langle S^z S^z \rangle_{q=0},$$

which show the thermodynamical consistence of the proposed approximations.

The analysis of the pseudospin correlator temperature behaviour shows that high temperature phase become unstable with respect to fluctuations with wave-vector $q = (\pi, \pi)$ (for some model parameters values) that indicates the possibility of the phase transition into a modulated (chess-board) phase. On the other hand, the phase transition between the uniform phases with different pseudospin mean values (bistability) is possible [3].

From the comparison of the grand canonical potential $\Omega$ values for uniform and chess-board phases ($\mu=$const regime), the ($\mu, \hbar$) phase diagram is obtained (Fig. 1a).

Chess-board phase exists as intermediate one between the uniform phases with different $\langle S^z \rangle$ and $\langle n \rangle$ values. The transition between different uniform phases (bistability) is of the first order (Fig. 1a, dashed line), while the transition between the uniform and modulated ones is of the first (dotted line) or second (solid line) order.

On the other hand, the minimum of the free energy $F = \Omega + \mu N$ is the equilibrium condition in

![Figure 1. Phase diagrams: (a) $\mu - h$, (b) $n - h$. I – uniform phase, II – chess-board phase, PS – phase separation area. ($T/g = 0.005$, $t/g = 0.2$)](image)

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