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Bose–Fermi–Hubbard model: Pseudospin operator approach

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ARTICLE INFO

Article history:
Received 4 January 2011
Received in revised form
14 February 2011
Accepted 15 February 2011

Keywords:
Bose–Fermi–Hubbard model
Phase transitions
Supersolid phase

ABSTRACT

The thermodynamics of the Bose–Fermi–Hubbard model with direct interaction between neighbour bosonic particles is considered in this work at finite temperature. The hard-core boson case is considered and the pseudospin formalism is used. Charge susceptibility of the system is calculated and the possibilities of the transitions to the charge density wave order, superfluid and supersolid phases are analysed. We derive an analytic formula for the grand canonical potential and analyse the thermodynamically stable states.

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1. Introduction

Bose–Fermi–Hubbard(BFH)-type models have been widely used in condensed matter physics. An example of the real system where this model can be applied is a crystal intercalated by ions (for example, TiO_2 crystals, intercalated by lithium, such systems can be used as rechargeable high-energy-batteries [1]). The pseudospin-electron model (which is similar to the BFH model with hard-core bosons) of intercalation was formulated in our previous works [2,3]. In such systems ions interact with electrons and effective interaction between ions is formed. In this work we also consider the direct interaction between ion (boson) particles and investigate phase transitions at finite temperature.

BFH-type models can also be used to describe mixtures of bosonic and fermionic atomic species in optical lattices [4–9]. By varying the strength of the periodic potential created by the laser beams it is possible to change the interatomic interactions. During the last decade, such systems have been intensively studied both theoretically and experimentally. Extended Bose–Hubbard-type models include an additional interaction between particles at different sites (long-range interaction), this interaction exists in dipolar cold atoms or polar molecules. Such systems have a long-range boson–boson interaction mediated by their dipole moment, which can be approximated by a nearest neighbour interaction. The possibility of using excited states of optical lattices to generate nearest neighbour interaction between particles was discussed in Ref. [10]. In the Bose–Fermi–Hubbard model the interaction between bosons is mediated by fermionic atoms in a mixture of bosonic and fermionic atoms [9,11]. The additional interaction between bosonic particles leads to the appearance of a supersolid phase, when a superfluid order parameter and crystal order coexist. Interest in the supersolid phase has increased since the observation of the supersolid-like behaviour in the low-temperature He-experiments [12]. It should be noted that there are rather few studies of the BFH model at finite temperature and away from the half-filling case.

2. Model and results

The Hamiltonian of the model is

$$H = -\sum_{ij} \Omega_{ij} S_i^+ S_j^- + \sum_{ij} J_{ij} S_i^z S_j^z + \sum_i g S_i^z n_i - \sum_{ij} t_{ij} c_i^+ c_j - \sum_i \mu n_i - \sum_i h S_i^z. \quad (1)$$

In this work we consider infinite on-site boson–boson interaction and use the pseudospin formalism ($S_i^z = 1/2$ when there is a boson in a site i and $S_i^z = -1/2$ in the opposite case), c_i^+ and c_i are fermion creation and annihilation operators, respectively. The first and second terms in Eq. (1) are responsible for nearest neighbour boson hopping and boson–boson interaction, respectively; g-term accounts for the boson–fermion interaction energy, we also take into account the kinetic energy of the fermions with t denoting the nearest neighbour ~~tunnelling~~. The last two terms involve the chemical potentials of the fermions and bosons, respectively, these terms are used to change the filling of the corresponding particles.

The Hamiltonian is decomposed into two parts [11]:

$$H = H_0 + H_{int}, \quad (2)$$

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doi:10.1016/j.physb.2011.02.042

where the unperturbed Hamiltonian H_0 is obtained in the mean field approximation (MFA)

$$gn_iS_i^z \to g\langle n_i\rangle S_i^z + gn_i\langle S_i^z\rangle - g\langle n_i\rangle\langle S_i^z\rangle$$

$$\Omega_{ij}S_i^+S_j^- \to \Omega_{ij}\langle S_i^+\rangle S_j^- + \Omega_{ij}S_i^+\langle S_j^-\rangle - \Omega_{ij}\langle S_i^+\rangle\langle S_j^-\rangle$$

$$J_{ij}S_i^zS_j^z \to J_{ij}\langle S_i^z\rangle S_j^z + J_{ij}S_i^z\langle S_j^z\rangle - J_{ij}\langle S_i^z\rangle\langle S_j^z\rangle. \quad (3)$$

The Hamiltonian H_0 is diagonalised in the $\boldsymbol{k}$-representation using the unitary transformation in the pseudospin subspace

$$S_i^z = \sigma_i^z\cos\theta + \sigma_i^x\sin\theta,$$

$$S_i^x = \sigma_i^x\cos\theta - \sigma_i^z\sin\theta,$$

$$\sin\theta = -\frac{2\Omega\langle S^x\rangle}{\lambda}, \quad \cos\theta = \frac{h-gn-2J\langle S^z\rangle}{\lambda},$$

$$\lambda = \sqrt{(h-gn-2J\langle S^z\rangle)^2 + (2\Omega\langle S^x\rangle)^2},$$

$$\Omega \equiv \Omega_{\boldsymbol{q}=0}, \quad J \equiv J_{\boldsymbol{q}=0},$$

$$H_0 = -\sum_{\boldsymbol{k}}(t_{\boldsymbol{k}} + \mu - g\langle S^z\rangle)c_{\boldsymbol{k}}^+c_{\boldsymbol{k}} - \sum_i \lambda\sigma_i - Ng\langle S^z\rangle\langle n\rangle + N\Omega\langle S^x\rangle^2 - NJ\langle S^z\rangle^2, \quad (4)$$

$$H_{int} = \sum_i g(S_i^z - \langle S^z\rangle)(n_i - \langle n\rangle) - \sum_{ij}\Omega_{ij}[(S_i^x - \langle S^x\rangle)(S_j^x - \langle S^x\rangle) + S_i^yS_j^y] + \sum_{ij}J_{ij}(S_i^z - \langle S^z\rangle)(S_j^z - \langle S^z\rangle), \quad (5)$$

with N denoting the number of lattice sites.

To calculate the density–density correlator $\mathfrak{G}_{ij}(\tau) = \langle T_\tau S_i^z(\tau) S_j^z(0)\rangle$, we perform an expansion in powers of H_{int}

$$\langle T_\tau S_i^z(\tau)S_j^z(0)\rangle = \frac{\langle T_\tau S_i^z(\tau)S_j^z(0)\sigma(\beta)\rangle_0}{\langle\sigma(\beta)\rangle_0},$$

$$\exp(-\beta H) = \exp(-\beta H_0)\sigma(\beta),$$

$$\sigma(\beta) = T_\tau \exp\left[-\int_0^\beta H_{int}(\tau)\,d\tau\right], \quad (6)$$

the averaging $\langle\ldots\rangle_0$ is performed over the distribution with H_0, where T_τ is the imaginary time ordering operator and $\beta = 1/T$ is the inverse temperature. To calculate the average values of the T_τ-products, we utilize the diagram technique and Wick's theorem for both the spin and fermi operators [13]. To calculate the mean value of the products of the σ^z operators we perform a semi-invariant expansion, for example, $\langle T_\tau\sigma_l^z(\tau)\sigma_m^z(0)\rangle_0 = \langle\sigma^z\rangle^2 + M_{lm}$, where $M(\omega_n) = \beta\delta_{\omega_n,0}(\frac{1}{4} - \langle\sigma^z\rangle^2)$ is the semi-invariant in the frequency representation (ω_n is a bosonic Matsubara frequency), and $\langle\sigma^z\rangle = \frac{1}{2}\tanh(\beta\lambda/2)$ is the average value of the pseudospin.

At the summation of diagrams we restrict ourselves in the spirit of the random phase approximation (RPA) to the diagrams having a structure of multi-loop chains (fore more details, see Ref. [11]). The junctions between boson (pseudospin) Green's functions $\langle T_\tau\sigma_l^+(\tau)\sigma_m^-(0)\rangle_0 = -2\langle\sigma^z\rangle K_{lm}(\tau)$ (where $K(\omega_n) = 1/(i\omega_n - \lambda)$) and semi-invariants are realised by the boson ~~tunnelling~~ $\Omega_{\boldsymbol{q}}$, direct boson interaction $J_{\boldsymbol{q}}$ and the fermionic loop $\Pi_{\boldsymbol{q}}(\omega_n) = (1/N)\sum_{\boldsymbol{k}}(n(t_{\boldsymbol{k}}) - n(t_{\boldsymbol{k}+\boldsymbol{q}}))/(i\omega_n + t_{\boldsymbol{k}} - t_{\boldsymbol{k}+\boldsymbol{q}})$.

The Dyson equation for Green's function $G_{lm}^{\alpha\beta} = -\frac{1}{2}\langle T_\tau\sigma_l^\alpha(\tau)\sigma_m^\beta(0)\rangle$ can be written in the following form:

$$G_{\boldsymbol{q}}^{\alpha\beta}(\omega_n) = G_{(0)\boldsymbol{q}}^{\alpha\beta}(\omega_n)\Delta^{\alpha\beta} + G_{(0)\boldsymbol{q}}^{\alpha\delta}(\omega_n)\Sigma_{\boldsymbol{q}}^{\delta\gamma}(\omega_n)G_{\boldsymbol{q}}^{\gamma\beta}(\omega_n), \quad (7)$$

where $\Sigma_{\boldsymbol{q}}^{\alpha\beta}(\omega_n) = \Pi_{\boldsymbol{q}}^{\alpha\beta}(\omega_n) + \Omega_{\boldsymbol{q}}^{\alpha\beta}$ is a self-energy part and $\Delta^{\alpha\beta} = 0$ or 1 depending on the values of α,β ($\alpha,\beta = +,-,z$). The matrix elements $\Pi_{\boldsymbol{q}}^{\alpha\beta}(\omega_n)$ and $\Omega_{\boldsymbol{q}}^{\alpha\beta}$ are similar to the ones obtained in Ref. [11] with the substitution $g^2\Pi_{\boldsymbol{q}} \to g^2\Pi_{\boldsymbol{q}} + 2J_{\boldsymbol{q}}$. For example,

$$\Pi_{\boldsymbol{q}}^{-+}(\omega_n) = \Pi_{\boldsymbol{q}}^{+-}(\omega_n) = \Pi_{\boldsymbol{q}}^{++}(\omega_n) = \Pi_{\boldsymbol{q}}^{--}(\omega_n) = (g^2\Pi_{\boldsymbol{q}}(\omega_n) + 2J_{\boldsymbol{q}})\frac{\sin^2\theta}{2}$$

$$\Omega_{\boldsymbol{q}}^{++} = \Omega_{\boldsymbol{q}}^{--} = -\Omega_{\boldsymbol{q}}(\cos^2\theta - 1). \quad (8)$$

In a similar fashion, we can derive expressions for other matrix elements. The matrix equations (7) form three independent sets of equations of the third order which can be separately solved. After some tedious algebra we can derive the expression for the density–density correlator $\mathfrak{G}_{\boldsymbol{q}}(\omega_n)$ which is similar to that obtained in Ref. [11] when we perform the above-mentioned substitution.

As reported in Ref. [11], the diagrammatic method allows us to derive the terms proportional to $\delta_{\omega_n,0}$ which are important and should be considered in the static limit $\omega \to 0$. The equation of motion method for two-time Zubarev Green's functions and decoupling procedure does not allow us to reveal these terms. This is due to the nonergodicity of the considered model.

In the following we consider a three-dimensional case (with a lattice constant $a = 1$), and in our calculations we choose a half width of the fermionic band W to be our energy scale ($-W < t_{\boldsymbol{k}} < W$). At finite temperature we can consider the transition from the uniform nonsuperfluid normal phase (NR) (at low temperature this is a Mott insulating phase) to the charge density wave (CDW) phase for small values of the bosonic hopping parameter $\Omega < 2T$, this inequality is also valid in the considered here case $J_{\boldsymbol{q}} \neq 0$ [11].

Lines of the instability with respect to the transition into the charge-ordered phase with different values of the modulation wave vectors $\boldsymbol{q} = (q,q,q)$ can be obtained using the condition of divergence of the static density–density correlator $\mathfrak{G}_{\boldsymbol{q}}(\omega = 0)$. At half fermionic filling $n_f = 1/2$ the chess-board phase with the wave vector $q = (\pi,\pi,\pi)$ has the highest temperature of the instability. In Fig. 1, we show lines of the instability at the fixed non-half fermionic filling $n_f \neq 1/2$ for two cases: (a) the case of a non-superfluid phase (Fig. 1(a)) and (b) the case of a superfluid (SF) phase (Fig. 1(b)). As it was shown in Ref. [11] in the regime of the fixed fermionic chemical potential, the highest temperature of the instability with respect to the transition into the incommensurate modulated phase with $q \neq (\pi,\pi,\pi)$ is obtained at non-half bosonic filling. Here, we consider the case of the fixed fermionic concentration and the highest temperature of the instability is reached at half bosonic filling $n_B = S^z + 1/2 = 1/2$, see Fig. 1(a). We did not reveal the existence of the supersolid (SS) phase with incommensurate wave vector of modulation $\boldsymbol{q} \neq (\pi,\pi,\pi)$ and the supersolid phase with modulation wave vector $\boldsymbol{q} = (\pi,\pi,\pi)$ has the highest temperature of the instability, see Fig. 1(b). The appearance of the incommensurate modulated phase is connected with the competition between the effective boson interaction via fermions and the direct boson–boson interaction (it is known that the repulsive direct interaction between bosons leads to the modulated phase with the wave vector of modulation $\boldsymbol{q} = (\pi,\pi,\pi)$ only). The presence of the supersolid phase is due to the effective interaction between bosons mediated by fermions and the direct interaction between nearest neighbour hard-core bosons does not lead to the appearance of the supersolid phase.

Now our focus is on the chess-board phase. We consider two sublattices: $\langle n_{i\alpha}\rangle = n_\alpha$, $\langle S_{i\alpha}^z\rangle = \langle S_\alpha^z\rangle$, $\langle S_{i\alpha}^x\rangle = \langle S_\alpha^x\rangle$, here $\alpha = 1,2$ is a sublattice index and i is an elementary cell index. Using the Hamiltonian H_0, we can obtain the equations for averages $\langle n\rangle$, $\langle S^z\rangle$, $\langle S^x\rangle$

$$n_\alpha = \frac{1}{N}\sum_{\boldsymbol{k}}\frac{1+\cos(2\phi)}{2}\left(e^{(\lambda_{\boldsymbol{k}\alpha}-\mu)/T} + 1\right)^{-1} + \sum_{\boldsymbol{k}}\frac{1-\cos(2\phi)}{2}\left(e^{(\lambda_{\boldsymbol{k}\beta}-\mu)/T} + 1\right)^{-1}, \quad (9)$$

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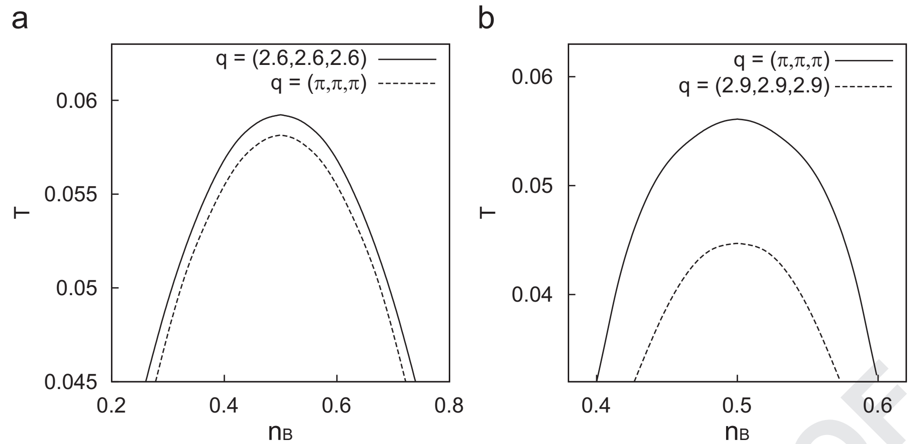

Fig. 1. Lines of divergence of the static density–density correlator for $W=1$, $g=-0.4$, $J=0.05$, $n_f=0.3$, $\Omega=0$ (a, nonsuperfluid phase) and $n_f=0.45$, $\Omega=0.2$ (b, superfluid phase).

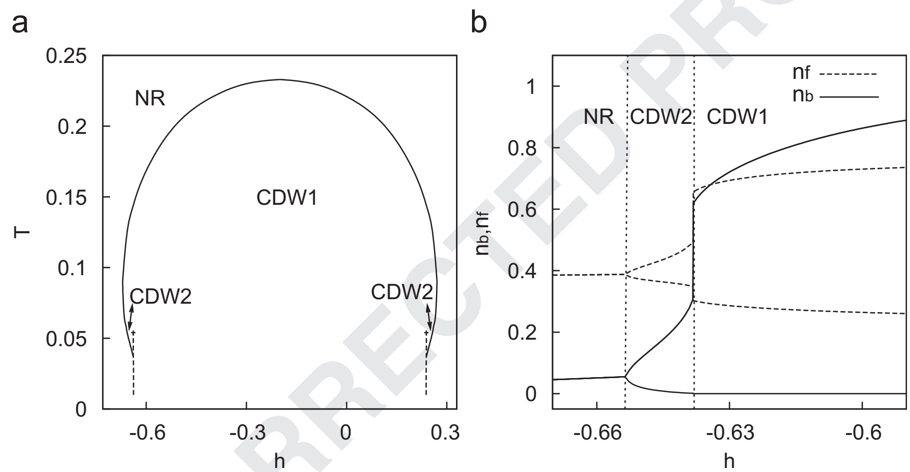

Fig. 2. (a) Phase transition lines of the second (solid line) and first (dashed line) order for $W=1$, $g=-0.4$, $\mu=0$, $\Omega=0$, $J=0.4$. (b) Bosonic and fermionic concentrations as functions of the bosonic chemical potential for $T=0.05$.

$$\langle S^z_\alpha\rangle = \frac{h-gn_\alpha-2J\langle S^z_\beta\rangle}{2\tilde{\lambda}_\alpha}\tanh\left(\frac{\beta\tilde{\lambda}_\alpha}{2}\right), \qquad (10)$$

$$\langle S^x_\alpha\rangle = \frac{2\Omega\langle S^x_\beta\rangle}{2\tilde{\lambda}_\alpha}\tanh\left(\frac{\beta\tilde{\lambda}_\alpha}{2}\right) \qquad (11)$$

with

$$\lambda_{\mathbf{k}\alpha} = g\frac{\langle S^z_1\rangle+\langle S^z_2\rangle}{2}+(-1)^\alpha\sqrt{\left(g\frac{\langle S^z_1\rangle-\langle S^z_2\rangle}{2}\right)^2+t^2_{\mathbf{k}}},$$

$$\sin 2\phi = \frac{-t_{\mathbf{k}}}{\sqrt{\left(g\frac{\langle S^z_1\rangle-\langle S^z_2\rangle}{2}\right)^2+t^2_{\mathbf{k}}}},$$

$$\tilde{\lambda}_\alpha = \sqrt{(gn_\alpha-h+2J\langle S^z_\beta\rangle)^2+\left(2\Omega\langle S^x_\beta\rangle\right)^2}, \quad \alpha\neq\beta. \qquad (12)$$

Next we derive an analytic formula for the grand canonical potential to find thermodynamically stable states:

$$\frac{\Phi}{\frac{N}{2}} = -\frac{T}{N}\sum_{\mathbf{k}}\ln\left[\left(1+e^{(\mu-\lambda_{\mathbf{k}1})/T}\right)\left(1+e^{(\mu-\lambda_{\mathbf{k}2})/T}\right)\right]$$
$$-T\ln\left[4\cosh\left(\frac{\beta\tilde{\lambda}_1}{2}\right)\cosh\left(\frac{\beta\tilde{\lambda}_2}{2}\right)\right]$$
$$-g(n_1\langle S^z_1\rangle+n_2\langle S^z_2\rangle)+2\Omega\langle S^x_1\rangle\langle S^x_2\rangle-2J\langle S^z_1\rangle\langle S^z_2\rangle. \qquad (13)$$

As it was shown in Ref. [11], our scheme for the calculation of the density–density correlator in the RPA and the corresponding averages $\langle n\rangle$, $\langle S^z\rangle$, and $\langle S^x\rangle$ in the MFA is a self-consistent scheme. The phase transition lines are shown in Fig. 2. The phase transition from the normal uniform nonsuperfluid to CDW phase can be of the second or first order (the above-mentioned lines of the instability shown in Fig. 1 allow us to investigate the phase transitions of the second order only). From Fig. 2, we observe that there exists a possibility of the first-order phase transition between two CDW phases (we identify two CDW phases denoted by CDW1 and CDW2 which differ by the average values of the fermionic and bosonic concentrations).

In Fig. 3, we show the phase diagrams in the plane (h–Ω). The presence of the direct boson–boson interaction leads to the shift of the supersolid phase into the region with the higher values of the bosonic hopping parameter. With increasing temperature, the regions of the existence of the CDW and supersolid phases are possible for smaller parameter space and the first-order phase transition transforms into the second one.

The existence of the first-order phase transition leads to phase separation in the regime of the fixed concentrations. It is illustrated in Fig. 4. In the regime of the fixed value of the fermionic concentration the system can separate into the uniform and CDW phases (CDW+NR) or into two CDW phases (CDW+CDW), the phase separation takes place at the intermediate values of the

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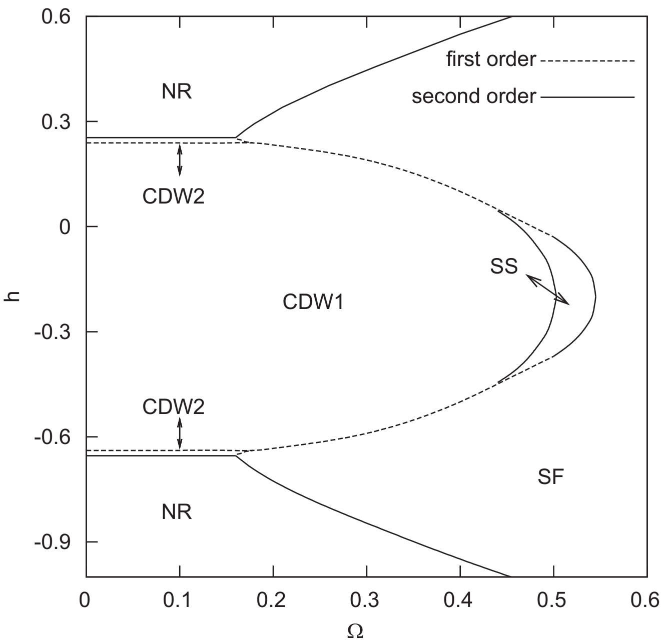

Fig. 3. Phase diagram in the $(h-\Omega)$ plane for $W=1$, $g=-0.4$, $\mu=0$, $T=0.05$, $J=0.4$.

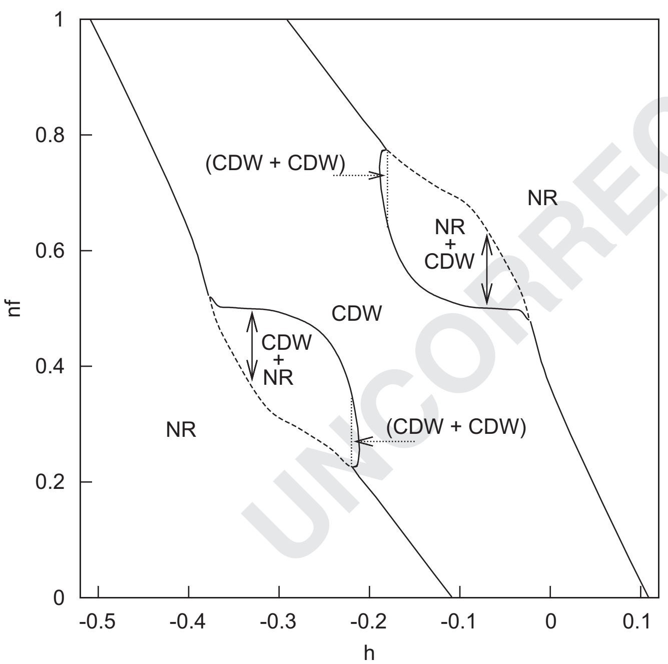

Fig. 4. Phase diagram in the (n_f-h) plane for $W=1$, $g=-0.4$, $T=0.03$, $J=0.1$, $\Omega=0$.

fermionic concentration, at high or low fermionic concentration the system is in the uniform or CDW phases. It should be noted that when the direct boson interaction is not taken into account the phase transition of the first order between two uniform phases and phase separation into two uniform phases with different concentrations is possible [3].

3. Conclusions

The phase transitions in the Bose–Fermi–Hubbard model with direct interaction between bosons have been considered in this work at finite temperature. Examples of the real systems where this model can be applied are intercalated by ions crystals and atoms in optical lattices. The density–density correlator has been calculated in the random phase approximation. The thermodynamical properties of the model are defined by the effective interaction between bosons via fermions and the direct boson–boson interaction. At finite temperature and small values of the bosonic hopping parameter the system can undergoes the phase transition from the uniform nonsuperfluid phase to the chessboard phase. At certain values of the bosonic hopping parameter the phase transition from the superfluid phase to the supersolid phase with a doubly modulated lattice period takes place at the decrease of the temperature. In the regime of the fixed concentration the phase separation into modulated and uniform phases takes place. Phase separation into two phases with different concentrations is important for the intercalated by ion crystals because the chemical potential is constant at the change of the concentrations and this peculiarity is used when constructing batteries.

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