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Модель Бозе-Фермі-Хаббарда: вихід за рамки наближення середнього поля

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T.S.Mysakovych

BOSE-FERMI-HUBBARD MODEL BEYOND MEAN FIELD APPROXIMATION

ЛЬВІВ

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Модель Бозе-Фермі-Хаббарда: вихід за рамки наближення середнього поля

Т.С.Мисакович

Анотація. Розвинуто аналітичний підхід, за допомогою якого можна досліджувати фазові переходи в моделі Бозе-Фермі-Хаббарда виходячи за рамки наближення середнього поля. Розглянуто випадок жорстких бозонів та слабкого бозон-ферміонного зв'язку. Термодинамічний потенціал системи розраховано беручи до уваги поправки петлевого типу (в наближенні хаотичних фаз) до виразу для цього потенціалу, отриманого в наближенні середнього поля.

Bose-Fermi-Hubbard model beyond mean field approximation

T.S.Mysakovych

Abstract. We develop the approach which allows us to investigate the phase transitions in the Bose-Fermi-Hubbard model beyond the mean-field approximation. We consider the case of hard-core bosons and weak boson-fermion interaction. We calculate the thermodynamical potential of the system taking into account loop-like corrections (in the random phase approximation) to the mean-field expression for this potential.

1. Introduction

Mixtures of boson and fermion atoms (e.g., ^{6}Li- ^{7}Li, ^{40}K- ^{87}Rb, ^{6}Li-^{87}Rb atoms) in optical lattices are investigated both theoretically and experimentally, such lattices were successfully realized in one, two and three dimensions. Such systems can be described by the the Bose-Fermi-Hubbard model (BFHM), the Hamiltonian of this model was introduced in [1] and since this different theoretical approaches have been used to study this model [2–11]. A Mott insulator phase is realized in such systems when a kinetic energy term (which allows for the tunneling of the particles between neighbour sites) is much smaller than a potential energy term, otherwise a superfluid phase takes place. Due to the remarkable control of model parameters the transition between these two phases was observed experimentally [12]. The bosonic kinetic energy term in this model is usually considered in the mean-field approximation, while the fermionic part of the Hamiltonian can be treated at the dynamical mean field theory level [9]. The case of weak boson-fermion coupling was considered in [11] and the susceptibility of the system was calculated in the framework of the random phase approximation. In addition to the superfluid and Mott insulator states [13,14] the BFHM possesses of more complicated phase diagram in comparison with the Bose-Hubbard model. For example, one of such peculiarities is a supersolid (SS) phase which appears due to the effective interaction between bosons via fermions, in supersolid phases both diagonal (crystalline) and off-diagonal (superfluid) long-range orders coexist. There are also many generalizations of the Bose-Hubbard and Bose-Fermi-Hubbard models, for example, extended models with long-range direct interaction between nearest (next-nearest) particles [15] (this interaction may arise, in particular, due the the presence of excited states or due to dipole-dipole interactions), models on superlattices [16–19], two-state Bose-Hubbard models [20]. A confining potential is present in experiments with optical lattices and this leads to inhomogeneous version of the model [4, 21].

Besides optical lattices the Bose-Fermi-Hubbard-type models can also be applied for the description of intercalation of ions in crystals (for example, lithium intercalation in TiO_2 crystals). In such systems ion-electron interaction can play a significant role because Li is almost fully ionized once intercalated and reconstruction of electron spectrum at intercalation takes place [22–24].

In our previous work [11] we calculated the density-density correlator of the BFHM in the framework of the random phase approximation and the thermodynamical potential of the system was calculated in the mean-

field approximation. In this paper we develop an approach which allows us to calculate the thermodynamical potential of the system beyond the mean field approximation and compare the obtained phase diagrams with that calculated in the mean field approximation.

2. Calculation of the thermodynamical potential

Using the pseudospin formalism the Hamiltonian of the BFHM in the hard core limit is

$$\begin{aligned} H &= \sum_{ij}\Omega_{ij}S_i^+S_j^- + \sum_{ij}t_{ij}c_i^+c_j \\ &\quad + \sum_i(gS_i^zn_i - \mu n_i) - \sum_i hS_i^z. \end{aligned} \tag{2.1}$$

The bosonic concentration n_B can be written as $n_B = S^z + 1/2$, c_i^+ and c_i are fermion creation and annihilation operators, respectively. Ω and t-terms in Eq. (2.1)) are responsible for nearest neighbour boson and fermion hopping, respectively; g-term accounts for the boson-fermion interaction energy. The bosonic and fermionic chemical potentials h and μ are introduced to control the number of bosons and fermions.

In our previous work [11] we obtained the mean-field Hamiltonian H_0 using the following simplification

$$\begin{aligned} &gn_iS_i^z \to g\langle n_i\rangle S_i^z + gn_i\langle S_i^z\rangle - g\langle n_i\rangle\langle S_i^z\rangle \\ &\Omega S_i^+S_j^- \to \Omega\langle S_i^+\rangle S_j^- + \Omega S_i^+\langle S_j^-\rangle - \Omega\langle S_i^+\rangle\langle S_j^-\rangle, \end{aligned} \tag{2.2}$$

the application of such a mean-field approximation to the strongly correlated systems allows one to satisfactorily describe their properties at the weak on-site correlation. The Hamiltonain therefore is written as

$$\begin{aligned} H &= H_0 + H_{int}, \\ H_0 &= \sum_{ij}t_{ij}c_i^+c_j + \sum_i(g\langle S^z\rangle n_i + gS_i^z\langle n\rangle - g\langle S^z\rangle\langle n\rangle) \\ &\quad - \sum_i hS_i^z - \sum_i\mu n_i \\ &\quad + 2\sum_{ij}\Omega_{ij}S_i^x\langle S^x\rangle - \sum_{ij}\Omega_{ij}\langle S^x\rangle^2, \end{aligned} \tag{2.3}$$

$$\begin{aligned} H_{int} &= \sum_i g(S_i^z - \langle S^z\rangle)(n_i - \langle n\rangle) \\ &\quad + \sum_{ij}\Omega_{ij}((S_i^x - \langle S^x\rangle)(S_j^x - \langle S^x\rangle) + S_i^yS_j^y). \end{aligned} \tag{2.4}$$

We consider the case of the weak on-site boson-fermion correlation. To diagonalize the Hamiltonian H_0 we pass to $\boldsymbol{k}$-representation and perform the transformations

$$\begin{aligned} S_i^z &= \sigma_i^z\cos\theta + \sigma_i^x\sin\theta, \\ S_i^x &= \sigma_i^x\cos\theta - \sigma_i^z\sin\theta, \\ \sin\theta &= \frac{2\Omega\langle S^x\rangle}{\lambda}, \quad \cos\theta = \frac{h-gn}{\lambda}, \\ \lambda &= \sqrt{(gn-h)^2 + (2\Omega\langle S^x\rangle)^2}, \quad \Omega \equiv \Omega_{\boldsymbol{q}=0} \\ H_0 &= \sum_{\boldsymbol{k}}(t_{\boldsymbol{k}} - \mu - g\langle S^z\rangle)c_{\boldsymbol{k}}^+c_{\boldsymbol{k}} - \sum_i\lambda\sigma_i \\ &\quad - Ng\langle S^z\rangle\langle n\rangle - N\Omega\langle S^x\rangle^2, \end{aligned} \tag{2.5}$$

here N is a number of lattice sites.

In the present article we want to go beyond the mean field approximation and for this purpose we develop the following approach. To calculate the thermodynamical potential of the system

$$\Phi = -T\ln Z, \quad Z = Tr\exp(-\beta H), \tag{2.6}$$

we perform an expansion in powers of H_{int}

$$\exp(-\beta H) = \exp(-\beta H_0)\sigma(\beta), \tag{2.7}$$

$$\begin{aligned} \sigma(\beta) &= T_\tau\exp(-\int_0^\beta H_{int}(\tau)d\tau), \\ Z &= Z_0\langle\sigma(\beta)\rangle_0, \end{aligned} \tag{2.8}$$

$$\begin{aligned} \Phi &= -T\ln Z = -T\ln Z_0 - T\ln\langle\sigma(\beta)\rangle_0 \\ &= \Phi_{MFA} + \Delta\Phi, \end{aligned} \tag{2.9}$$

where T_τ is the imaginary time ordering operator and $\beta = 1/T$ is the inverse temperature, Tr denotes the trace.

We restrict ourselves to loop-like diagrams in the spirit of a random phase approximation (RPA) when we perform an expansion in powers of H_{int}.

$$\begin{aligned} \langle\sigma(\beta)\rangle_0 &= 1 - \int_0^\beta T_\tau\langle H_{int}(\tau)\rangle d\tau \\ &\quad + \frac{1}{2!}\int_0^\beta\int_0^\beta T_\tau\langle H_{int}(\tau_1)H_{int}(\tau_2)\rangle d\tau_1 d\tau_1 \\ &\quad + \dots \end{aligned} \tag{2.10}$$

Typical RPA diagrams are shown in figure 1 (it should be noted that in the case of the Bose-Hubbard model similar scheme was used in [25]). We use the diagrammatic teqnique based on Wick's theorem for the spin operators and the usual procedure for Fermi operators. To calculate the remaining product of the diagonal σ^z operators we perform the semi-invariant expansion. Here we have introduced the unperturbed bosonic Green's function $\langle T_\tau \sigma^+(\tau)\sigma^-\rangle_0 = -2\langle\sigma^z\rangle K(\tau)$,

$$K(\omega_n) = \frac{1}{i\omega_n - \lambda}, \tag{2.11}$$

with imaginary discrete Matsubara frequency $i\omega_n = i2n\pi T$ ($n = 0, \pm1, ...$), the fermionic loop

$$\Pi_{\boldsymbol{q}}(\omega_n) = \frac{1}{N}\sum_{\boldsymbol{k}} \frac{n(t_{\boldsymbol{k}}) - n(t_{\boldsymbol{k}-\boldsymbol{q}})}{i\omega_n + t_{\boldsymbol{k}} - t_{\boldsymbol{k}-\boldsymbol{q}}}, \tag{2.12}$$

semi-invariant $\langle T_\tau \sigma^z(\tau)\sigma^z\rangle_0 = \langle\sigma^z\rangle^2 + M(\tau)$, $M(\omega_n) = \beta\delta_{\omega_n,0}(\frac{1}{4} - \langle\sigma^z\rangle^2)$, and $\langle\sigma^z\rangle = \frac{1}{2}\tanh(\frac{\beta\lambda}{2})$.

In our approximation we can write the following expression for the $\langle\sigma(\beta)\rangle_0$:

$$\langle\sigma(\beta)\rangle_0 = 1 + A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + ... = \exp(A), \tag{2.13}$$

$$\begin{aligned} A &= \frac{1}{2}\frac{1}{N}\sum_{\boldsymbol{q},\omega_n,\alpha,\beta} J^{\alpha\beta}(\boldsymbol{q},\omega_n)G^{\beta\alpha}(\omega_n) \\ &+ \frac{1}{2}\frac{1}{2N}\sum_{\boldsymbol{q},\omega_n} Tr\left[\hat{J}(\boldsymbol{q},\omega_n)\hat{G}(\omega_n)\hat{J}(\boldsymbol{q},\omega_n)\hat{G}(\omega_n)\right] \\ &+ \ldots \end{aligned} \tag{2.14}$$

Here we have introduced matrices $\hat{J}$ and $\hat{G}$, this matrices are as follows

$$\begin{aligned} G^{zz}(\omega_n) &= \beta\delta(\omega_n)(\frac{1}{4} - \langle\sigma^z\rangle^2), \\ G^{+-}(\omega_n) &= \frac{-2\langle\sigma^z\rangle}{i\omega_n - \lambda}, \\ G^{-+}(\omega_n) &= \frac{2\langle\sigma^z\rangle}{i\omega_n - \lambda}, \\ J^{zz}(\boldsymbol{q},\omega_n) &= -\Pi_{\boldsymbol{q}}(\omega_n)g^2\cos^2\theta - 2\Omega_{\boldsymbol{q}}\sin^2\theta, \\ J^{--}(\boldsymbol{q},\omega_n) &= \frac{-\Pi_{\boldsymbol{q}}(\omega_n)g^2\sin^2\theta - 2\Omega_{\boldsymbol{q}}(\cos^2\theta - 1)}{4}, \end{aligned} \tag{2.15}$$

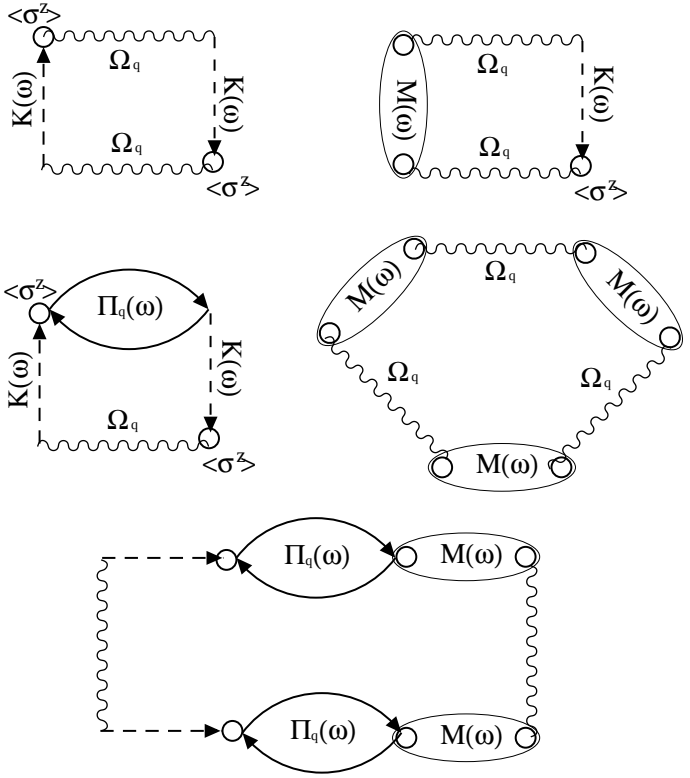

Figure 1. Typical RPA diagrams for thermodynamical potential. Solid and dashed lines with arrows denote the unperturbed bosonic and fermionic Green's functions, respectively. Wavy lines indicate the boson energy dispersion, circles and ovals denote the average value of $\langle s^z\rangle$ and semi-invariants, respectively.

$$
\begin{aligned}
J^{+-}(\boldsymbol{q},\omega_n) &= \frac{-\Pi_{\boldsymbol{q}}(\omega_n)g^2\sin^2\theta - 2\Omega_{\boldsymbol{q}}(\cos^2\theta - 1)}{4},\\
J^{+z}(\boldsymbol{q},\omega_n) &= \frac{-\Pi_{\boldsymbol{q}}(\omega_n)g^2 + 2\Omega_{\boldsymbol{q}}}{2}\cos\theta\sin\theta,\\
J^{+z}(\boldsymbol{q},\omega_n) &= J^{-z}(\boldsymbol{q},\omega_n) = J^{z+}(\boldsymbol{q},\omega_n) = J^{z-}(\boldsymbol{q},\omega_n)\\
J^{+-}(\boldsymbol{q},\omega_n) &= J^{-+}(\boldsymbol{q},\omega_n),\\
J^{++}(\boldsymbol{q},\omega_n) &= J^{--}(\boldsymbol{q},\omega_n),
\end{aligned}
\tag{2.16}
$$

here we take into account unperturbed bosonic Green's functions $G^{\alpha\beta}$ and semi-invariants (in general, we could consider the bosonic Green's functions in the random phase approximation [11], but in this work we limit ourselves to unperturbed functions).

The expression for A can be written in the following compact form

$$
\begin{aligned}
A &= -\frac{1}{2N}\sum_{\boldsymbol{q},\omega_n} Tr\ln\left[1 - \hat{J}(\boldsymbol{q},\omega_n)\hat{G}(\omega_n)\right]\\
&= -\frac{1}{2N}\sum_{\boldsymbol{q},\omega_n}\ln\det[1 - \hat{J}(\boldsymbol{q},\omega_n)\hat{G}(\omega_n)].
\end{aligned}
\tag{2.17}
$$

As a result the thermodynamical potential (2.6) of the system is

$$
\begin{aligned}
\Phi &= \Phi_{MFA} + \Delta\Phi,\\
\Delta\Phi &= \frac{1}{2\beta N}\sum_{\boldsymbol{q},\omega_n}\ln\det[1 - \hat{J}(\boldsymbol{q},\omega_n)\hat{G}(\omega_n)].
\end{aligned}
\tag{2.18}
$$

Here $\Delta\Phi$ is a correction to the mean-field expression for the thermodynamical potential. Using the conditions

$$
\frac{\partial\Phi}{\partial n} = \frac{\partial\Phi}{\partial\langle S^z\rangle} = \frac{\partial\Phi}{\partial\langle S^x\rangle} = 0
\tag{2.19}
$$

(the partial differentiation is taken at the fixed values of h, μ, T) we can write the equations for the average value of the bosonic concentration $n_b = \langle S^z\rangle + 1/2$, fermionic concentration n_F and average value $\langle S^x\rangle$ (the nonzero value of $\langle S^x\rangle$ indicates the presence of bose-condensate and is a signature of a superfluid or supersolid phase):

$$
\langle S^z\rangle = \frac{1}{2}\cos\theta\tanh(\frac{\beta\lambda}{2}) + \frac{1}{Ng}\frac{\partial\Delta\Phi}{\partial n},
\tag{2.20}
$$

$$
n = \frac{1}{N}\sum_{\boldsymbol{k}}\frac{1}{e^{\beta(g\langle S^z\rangle - t_{\boldsymbol{k}} - \mu)} + 1} + \frac{1}{Ng}\frac{\partial\Delta\Phi}{\partial\langle S^z\rangle},
\tag{2.21}
$$

$$
\langle S^x\rangle = -\frac{1}{2}\sin\theta\tanh(\frac{\beta\lambda}{2}) + \frac{1}{2N\Omega}\frac{\partial\Delta\Phi}{\partial\langle S^x\rangle}.
\tag{2.22}
$$

After some tedious algebra we can obtain the expression for the determinant $\det[1 - \hat{J}(\boldsymbol{q},\omega_n)\hat{G}(\omega_n)]$:

$$
\det[1 - \hat{J}(\boldsymbol{q},\omega_n)\hat{G}(\omega_n)] = \frac{(i\omega_n)^2 - a_{\boldsymbol{q}}b_{\boldsymbol{q}}(\omega_n)}{(i\omega_n)^2 - \lambda^2}
\tag{2.23}
$$

where

$$
a_{\boldsymbol{q}} = \lambda + 2\Omega_{\boldsymbol{q}}\langle\sigma^z\rangle
\tag{2.24}
$$

$$
\begin{aligned}
b_{\boldsymbol{q}}(\omega_n) &= \lambda + \langle\sigma^z\rangle\left(2\Omega_{\boldsymbol{q}}\cos^2\theta + g^2\sin^2\theta\Pi_{\boldsymbol{q}}(\omega_n)\right)\\
&+ M\lambda\left(2\Omega_{\boldsymbol{q}}\sin^2\theta + g^2\Pi_{\boldsymbol{q}}(\omega_n)\cos^2\theta\right)\\
&+ 2\langle\sigma^z\rangle\Omega_{\boldsymbol{q}}Mg^2\Pi_{\boldsymbol{q}}(\omega_n).
\end{aligned}
\tag{2.25}
$$

Unfortunately, we can not perform analytical summation over Matsubara frequencies to simplify the expression for this determinant because $b_{\boldsymbol{q}}(\omega_n)$ nontrivially depends on ω_n. The terms in (2.25) which arise due to the semi-invariant $M(\omega_n)$ are nonergodic ones. As it was noted in [11] the equation of motion method for Green's functions does not allow us to calculate such terms and we should use the presented above diagrammatic teqnique.

Numerical calculations of this corrections are not simple, we should perform summation over Matsubara frequencies and take into account nonergodic terms $\sum_{n=-\infty}^{+\infty} f(\omega_n) = f(0) + 2\sum_{n=1}^{+\infty}\mathrm{Re}\,(f(\omega_n))$. This is the task for future investigations.

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