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Ігор Васильович Стасюк
Володимир Олександрович Краснов

ФЕРМІОННИЙ СПЕКТР МОДЕЛІ БОЗЕ-ФЕРМІ-ХАВБАРДА У ФАЗІ З
БОЗЕ-КОНДЕНСАТОМ

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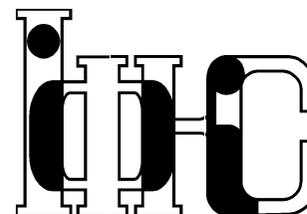
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ІНСТИТУТ
ФІЗИКИ
КОНДЕНСОВАНИХ
СИСТЕМ

ICMP-13-13U

I.V. Stasyuk, V.O. Krasnov

FERMION SPECTRUM OF BOSE-FERMI-HUBBARD MODEL
IN THE PHASE WITH BOSE-EINSTEIN CONDENSATE

ЛЬВІВ

УДК: 538.945

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Ферміонний спектр моделі Бозе-Фермі-Хаббарда у фазі з бозе-конденсатом

І.В. Стасюк, В.О. Краснов

Анотація. Досліджено ферміонний енергетичний спектр бозон-ферміонних сумішей ультрахолодних атомів у оптичних ґратках. Використано підхід, що ґрунтується на формалізмі операторів Хаббарда, які діють на базисі одновузлових станів. Побудовано рівняння для ферміонної функції Гріна в моделі Бозе-Фермі-Хаббарда; функції Гріна вищого порядків розщеплено в дусі наближення Хаббард-I (це відповідає сильним вузловим взаємодіям). Проведено розрахунок відповідних спектральних густин. Для випадку жорстких бозонів досліджено умови появи додаткових підзон у спектрі ферміонів. Показано, що вони існують лише у стані з бозе-конденсатом та проявляються завдяки перемішуванню станів з різним числом бозонів. Ці додаткові підзони є проявом композитних збуджень (коли поява ферміона на вузлі супроводжується одночасною появою (чи зникненням) бозона).

Fermion spectrum of Bose-Fermi-Hubbard model in the phase with Bose-Einstein condensate

I.V. Stasyuk, V.O. Krasnov

Abstract. We investigated the fermion spectrum of the Bose-Fermi-Hubbard model, used for description of boson-fermion mixtures of ultra-cold atoms in optical lattices. We used the method based on Hubbard operator approach for on-site basis. The equation for fermion Green's function in the Bose-Fermi-Hubbard model was built; Green's functions of higher order were decoupled in Hubbard-I approximation approach (the case of strong on-site interaction). Appropriate spectral densities were calculated. For the case of hard-core bosons the condition of appearance of additional bands in fermion spectrum was investigated. It's shown, that these bands exist only in the state with Bose-Einstein condensate and manifest themselves because of mixing of states with different number of bosons. These additional bands are reflection of composite excitations (when appearing of fermion on a site is accompanied by simultaneous creation (or disappearing) of boson).

1. Introduction

The Bose-Fermi-Hubbard model (BFHM) in its general form has a direct relation to the ultra-cold boson-fermion mixtures in optical lattices, which are the object of an intense theoretical investigation during last years [1]. The investigation of fermion spectrum of BFHM and its transformation when the Bose-Einstein condensate (the SF-phase) appears is an interesting problem. Earlier [2] the thermodynamics of the model has been investigated in the mean-field approximation (MFA); the influence of fermion subsystem was studied and phase diagrams, illustrating the MI-SF phase transition were built. Here we are going beyond the MFA and calculate the fermion band spectrum as well as single-particle density of states using the Green's function technique and taking into account the strong on-site interactions.

2. Hamiltonian of the model and its transformation

The Hamiltonian of the Fermi-Bose-Hubbard model is:

$$\begin{aligned}\hat{H} &= \sum_{i,n} \lambda_n X_i^{nn} + \sum_{i,\tilde{n}} \lambda_{\tilde{n}} \tilde{X}_i^{\tilde{n}\tilde{n}} + \sum_{\langle i,j \rangle, \sigma} t'_{ij} a_{i\sigma}^+ a_{j\sigma} + \sum_{\langle i,j \rangle, \sigma} t_{ij} b_{i\sigma}^+ b_{j\sigma} \\ \hat{H} &= \hat{H}_0 + \hat{H}'\end{aligned}\quad (2.1)$$

where the single-site basis is $|n\rangle = |n, 0\rangle$, $|\tilde{n}\rangle = |n, 1\rangle$; $|n_B, n_F\rangle$. Here

$$\lambda_n = \frac{U}{2}n(n-1) - n\mu, \quad \lambda_{\tilde{n}} = \frac{U}{2}\tilde{n}(\tilde{n}-1) - \mu\tilde{n} - \mu' + U'\tilde{n} \quad (2.2)$$

and

$$\begin{aligned}b_i &= \sum_n \sqrt{n+1} X_i^{n,(n+1)} + \sum_{\tilde{n}} \sqrt{\tilde{n}+1} X_i^{\tilde{n},(n+1)} \\ a_i &= \sum_n X_i^{n,\tilde{n}}\end{aligned}\quad (2.3)$$

U and U' are constants of boson-boson and boson-fermion on-site interactions; μ and μ' - are chemical potential of bosons and fermions, respectively. In general, we need to calculate the Green's function $\langle\langle a|a^+\rangle\rangle$. In our case this means that we have to find the Green's function built on Hubbard operators: $\langle\langle X^{n\tilde{n}}|X^{r\tilde{r}}\rangle\rangle$. Let us use the equation of motion

$$\hbar\omega\langle\langle A|B\rangle\rangle = \frac{\hbar}{2\pi}[A, B] + \langle\langle [A, H]|B\rangle\rangle \quad (2.4)$$

And, for this we need to find the following commutators:

$$[X_p^{m,\tilde{m}}, \hat{H}_0] = (\lambda_{\tilde{m}} - \lambda_m)X_p^{m,\tilde{m}} = (U'\tilde{m} - \mu')X_p^{m,\tilde{m}} \quad (2.5)$$

$$\begin{aligned} [X_p^{m,\tilde{m}}, b_i^+ b_j] &= [X_p^{m,\tilde{m}}, b_i^+] b_j + b_i^+ [X_p^{m,\tilde{m}}, b_j] = \\ &= \delta_{pi}(-\sqrt{m+1}X_p^{m+1,\tilde{m}} + \sqrt{\tilde{m}}X_p^{m,\tilde{m}-1})b_j + \\ &+ \delta_{pj}b_i^+(-\sqrt{m}X_p^{m-1,\tilde{m}} + \sqrt{\tilde{m}+1}X_p^{m,\tilde{m}+1}) \end{aligned} \quad (2.6)$$

$$[X_p^{m,\tilde{m}}, a_i^+ a_j] = \delta_{pi}(X_p^{mm} + X_p^{\tilde{m}\tilde{m}})a_j \quad (2.7)$$

$$\begin{aligned} [X_p^{m,\tilde{m}}, \hat{H}'] &= \sum_j t_{pj}(-\sqrt{m+1}X_p^{m+1,\tilde{m}} + \sqrt{\tilde{m}}X_p^{m,\tilde{m}-1})b_j + \\ &+ \sum_i t_{ip}b_i^+(-\sqrt{m}X_p^{m-1,\tilde{m}} + \sqrt{\tilde{m}+1}X_p^{m,\tilde{m}+1}) + \\ &+ \sum_j t'_{ij}(X_p^{mm} + X_p^{\tilde{m}\tilde{m}})a_j \end{aligned} \quad (2.8)$$

In the following, we will use the decouplings which are equivalent to the mean field approximation in the case of bosons and to the Hubbard-I approximation for fermions:

$$b_j \rightarrow \langle b_j \rangle, \quad b_i^+ \rightarrow \langle b_i^+ \rangle, \quad (X_p^{mm} + X_p^{\tilde{m}\tilde{m}}) \rightarrow \langle X^{mm} + X^{\tilde{m}\tilde{m}} \rangle \quad (2.9)$$

We will suppose that our system is already in the state with Bose-Einstein condensate, and the order parameter for this uniform condensate is:

$$\langle b_j \rangle = \varphi, \quad \langle b_j^+ \rangle = \varphi^* = \varphi \quad (2.10)$$

Then

$$\begin{aligned} [X_p^{m,\tilde{m}}, \hat{H}'] &= t_0\varphi(-\sqrt{m+1}X_p^{m+1,\tilde{m}} + \sqrt{\tilde{m}}X_p^{m,\tilde{m}-1}) + \\ &+ t_0\varphi_i^*(-\sqrt{m}X_p^{m-1,\tilde{m}} + \sqrt{\tilde{m}+1}X_p^{m,\tilde{m}+1}) + \\ &+ \sum_j t'_{ij}\langle X^{mm} + X^{\tilde{m}\tilde{m}} \rangle a_j \end{aligned} \quad (2.11)$$

Finally, for the Greens's function $\langle\langle X^{m\tilde{m}}|X^{\tilde{n}n} \rangle\rangle$ we have the equation:

$$\begin{aligned} \cdot \quad \hbar\omega\langle\langle X^{m\tilde{m}}|X^{\tilde{n}n} \rangle\rangle &= \frac{\hbar}{2\pi}\delta_{pr}\delta_{mn}\delta_{\tilde{m}\tilde{n}}\langle X^{mm} + X^{\tilde{m}\tilde{m}} \rangle + \\ &+ (U'\tilde{m} - \mu')\langle\langle X^{m\tilde{m}}|X^{\tilde{n}n} \rangle\rangle + t_0\varphi\sqrt{\tilde{m}}\langle\langle X_p^{m\tilde{m}-1}|X_r^{\tilde{n}n} \rangle\rangle + \\ &+ \sum_j t_{ij}\langle X^{mm} + X^{\tilde{m}\tilde{m}} \rangle\langle\langle a_j|X^{\tilde{n}n} \rangle\rangle \end{aligned} \quad (2.12)$$

One can see that to obtain the closed system of equations we need to find the Green's function $\langle\langle X^{m\tilde{m}-1}|X^{\tilde{n}n} \rangle\rangle$. To find it we use the similar steps and approximations done before for function $\langle\langle X^{m\tilde{m}}|X^{\tilde{n}n} \rangle\rangle$. Finally we will have:

$$\begin{aligned} \cdot \quad \hbar\omega\langle\langle X^{m\tilde{m}-1}|X^{\tilde{n}n} \rangle\rangle &= \frac{\hbar}{2\pi}\delta_{pr}\left(\delta_{mn}\langle X^{\tilde{n}\tilde{m}-1} \rangle + \delta_{\tilde{m}-1,\tilde{n}}\langle X^{mn} \rangle\right) + \\ &+ (\lambda_{\tilde{m}-1} - \lambda_m)\langle\langle X^{m\tilde{m}-1}|X^{\tilde{n}n} \rangle\rangle + \frac{t_0\varphi^*}{\sqrt{\tilde{m}}}\langle\langle X_p^{m\tilde{m}}|X_r^{\tilde{n}n} \rangle\rangle + \\ &+ \sum_j t_{ij}\frac{\varphi^*}{\sqrt{\tilde{m}}}\langle\langle a_j|X^{\tilde{n}n} \rangle\rangle \end{aligned} \quad (2.13)$$

The final system of equations, after passing to Fourier transforms, is:

$$\begin{aligned} (\hbar\omega - U'm + \mu')G^{m\tilde{m},\tilde{n}n}(\omega, q) &= \\ &= \frac{\hbar}{2\pi}\delta_{mn}\delta_{\tilde{m}\tilde{n}}\langle X^{mm} + X^{\tilde{m}\tilde{m}} \rangle + \\ &+ t_0\varphi\sqrt{\tilde{m}}G^{m\tilde{m}-1,\tilde{n}n}(\omega, q) + t'_q\langle X^{mm} + X^{\tilde{m}\tilde{m}} \rangle\langle\langle a|X^{\tilde{n}n} \rangle\rangle_{\omega,q} \\ (\hbar\omega - \lambda_{\tilde{m}-1} + \lambda_m)G^{m\tilde{m}-1,\tilde{n}n}(\omega, q) &= \\ &= \frac{\hbar}{2\pi}\left(\delta_{mn}\langle X^{\tilde{n}\tilde{m}-1} \rangle + \delta_{\tilde{m}-1,\tilde{n}}\langle X^{mn} \rangle\right) \\ &+ t_0\varphi\sqrt{\tilde{m}}G^{m\tilde{m}-1,\tilde{n}n}(\omega, q) + t'_q\langle X^{mm} + X^{\tilde{m}\tilde{m}} \rangle\langle\langle a|X^{\tilde{n}n} \rangle\rangle_{\omega,q} \end{aligned} \quad (2.14)$$

3. Four states approximation

In our earlier paper [2] we investigated the ground state diagrams for the Bose-Fermi-Hubbard model. In Fig.1 we show one of them when $0 < U' < U$:

Supposing that $U \rightarrow \infty$ (the hard-core boson limit) and $U' \gg t'_{ij}$, we restrict ourselves to the case, when only four states can be considered: $|0\rangle$ - neither bosons or fermions on site.

behaviour of single-site energy levels of our system given by formulae (3.5).

In this connection we have to consider the equation for order parameter in the case of different ground states. For the ground state $|\tilde{1}'\rangle$ we have:

$$\varphi = -\frac{1}{2} \sin(2\tilde{\psi}) = \frac{|t_0|\varphi}{\sqrt{\frac{(U'-\mu)^2}{4} + t_0^2\varphi^2}} \quad (4.1)$$

Solution $\varphi = 0$ corresponds to the normal (Mott insulator) phase; $\varphi \neq 0$ describes the phase with BEC. For this the phase, from (4.1) we have:

$$\varphi = \frac{1}{2} \sqrt{1 - \frac{(U' - \mu)^2}{t_0^2}} \quad (4.2)$$

In the same way, when the ground state is $|1'\rangle$, for the order parameter we have:

$$\varphi = \frac{1}{2} \sqrt{1 - \frac{\mu^2}{t_0^2}} \quad (4.3)$$

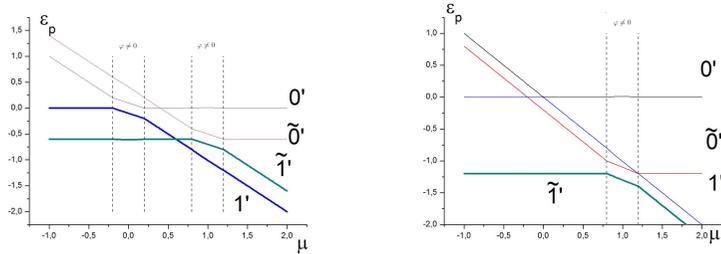


Fig.2 On-site energies ε_p for $\mu' = 0.6$ (left) and $\mu' = 1.2$ (right)

Here (see Fig. 2) two possibilities are possible: with- or without the change of ground state. On the left figure the situation is shown when we have the ground state $|\tilde{1}'\rangle$ at $\mu < \mu'$ and the $|1'\rangle$ one at $\mu > \mu'$. On the right figure the case is presented when only the ground state $|\tilde{1}'\rangle$ is realized (here the states $|\tilde{1}'\rangle$ and $|1'\rangle$ belong to the transformed basis).

In the case $T = 0$, only non-zero averages of Hubbard operators should be taken in (3.8) into consideration. For example, if the ground

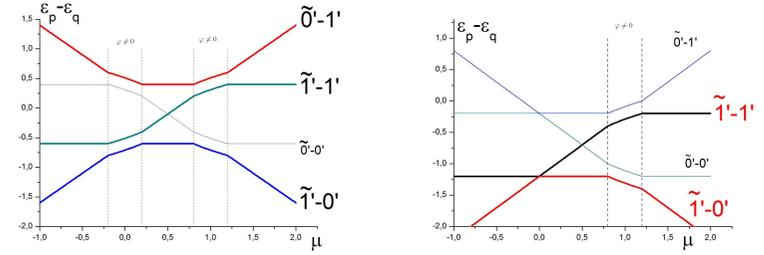


Fig.3 Energy transitions $\varepsilon_p - \varepsilon_q$ for $\mu' = 0.6$ (left) and $\mu' = 1.2$ (right)

state is $|\tilde{1}'\rangle$, only $\langle X^{\tilde{1}'\tilde{1}'} \rangle = 1$ and for others states we have $\langle X^{p'p'} \rangle = 0$. This means that in this case we will have from (3.8).

$$\begin{aligned} g_0(\omega) &= \cos^2(\tilde{\psi} - \psi) \frac{\langle X^{1'1'} + X^{\tilde{1}'\tilde{1}'} \rangle}{\hbar\omega - \varepsilon_{\tilde{1}'} + \varepsilon_{1'}} + \sin^2(\tilde{\psi} - \psi) \frac{\langle X^{0'0'} + X^{\tilde{1}'\tilde{1}'} \rangle}{\hbar\omega - \varepsilon_{\tilde{1}'} + \varepsilon_{0'}} \equiv \\ &\equiv \frac{\cos^2(\tilde{\psi} - \psi)}{\hbar\omega - \varepsilon_{\tilde{1}'} + \varepsilon_{1'}} + \frac{\sin^2(\tilde{\psi} - \psi)}{\hbar\omega - \varepsilon_{\tilde{1}'} + \varepsilon_{0'}} \end{aligned} \quad (4.4)$$

Here the energy transitions involving the ground state $|\tilde{1}'\rangle$ are present only (see Fig. 3)

Then we will obtain the following expression for fermion Green's function:

$$\begin{aligned} \langle\langle a|a^+ \rangle\rangle &= \frac{1}{2\pi} \frac{1}{g_0^{-1}(\omega) - t_k} = \\ &= \frac{1}{2\pi} \frac{(\hbar\omega - \Delta_{\tilde{1}'0'}) \cos^2(\tilde{\psi} - \psi) + (\hbar\omega - \Delta_{\tilde{1}'1'}) \sin^2(\tilde{\psi} - \psi)}{\det} \end{aligned} \quad (4.5)$$

where

$$\begin{aligned} \det &= (\hbar\omega - \Delta_{\tilde{1}'0'}) (\hbar\omega - \Delta_{\tilde{1}'1'}) + t_q (\hbar\omega - \Delta_{\tilde{1}'0'}) \cos^2(\tilde{\psi} - \psi) + \\ &+ t_q (\hbar\omega - \Delta_{\tilde{1}'1'}) \sin^2(\tilde{\psi} - \psi) \end{aligned}$$

and $\Delta_{mn} = \varepsilon_m - \varepsilon_n$.

This expression can be rewritten as decomposition into simple fractions:

$$\langle\langle a|a^+ \rangle\rangle = \frac{1}{2\pi} \left[\frac{A_1}{\hbar\omega - X_1} + \frac{A_2}{\hbar\omega - X_2} \right] \quad (4.6)$$

where X_1, X_2 - are solutions of quadratic (with respect to the variable $\hbar\omega$) equation, which determines the poles of function (4.5) (functions $\varepsilon_{1,2}(q) = X_{1,2}$ describe the dispersion laws for fermion band spectrum). A_1, A_2 are constants in the fraction decomposition.

Finally, for density of fermion states in this case we have:

$$\rho(\hbar\omega) = \frac{1}{\hbar N} \sum_q -2\text{Im}(G_q(\omega + i\epsilon))_{\epsilon \rightarrow 0} \quad (4.7)$$

$$\rho(\hbar\omega) = \int_{-W}^W dx \rho_0(x) \text{Big}(A_1(x)\delta(x - X_1) + A_2(x)\delta(x - X_2)), \quad (4.8)$$

where $\rho_0(x) = \frac{1}{N} \sum_q \delta(x - t_q)$ is the unperturbed density of states.

The similar expressions as (4.5), (4.6) and (4.8) can be obtained for the case with ground state [1'].

5. Results

The results of calculations of density of states $\rho(\hbar\omega)$ according to (4.8) are presented in Figs. 4,5 and 6

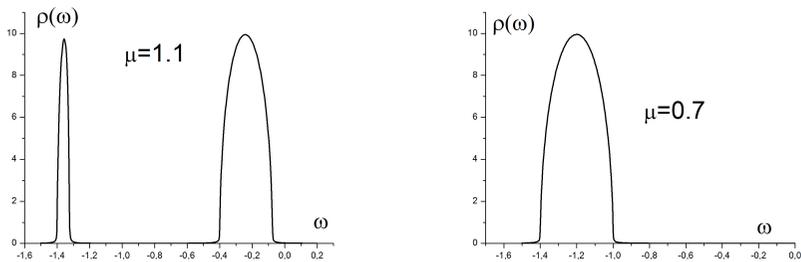


Fig.4 Density of states for different μ when $\mu' = 1.2$

6. Conclusions

Interaction between Bose- and Fermi particles in BFHM leads to changes in fermion spectrum. Besides the shift of fermion bands that depends on boson concentration, the splitting of spectrum and appearance the of

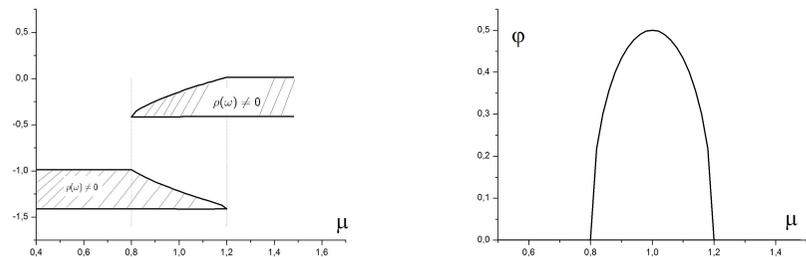


Fig.5 Single-site energy levels and order parameter for $\mu' = 1.2$

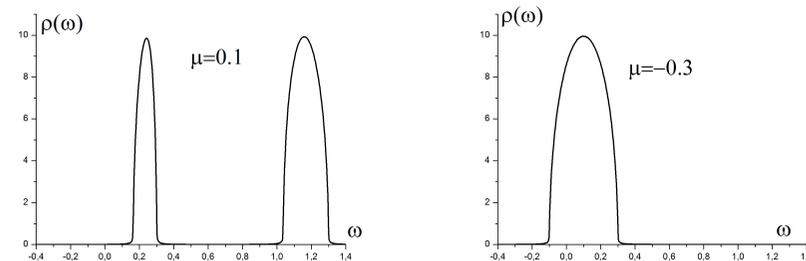


Fig.6 Density of states for different μ when $\mu' = -0.1$

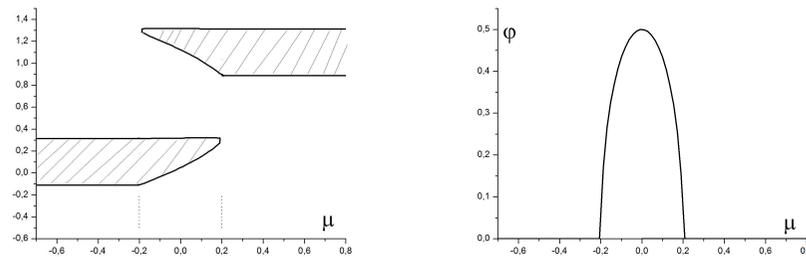
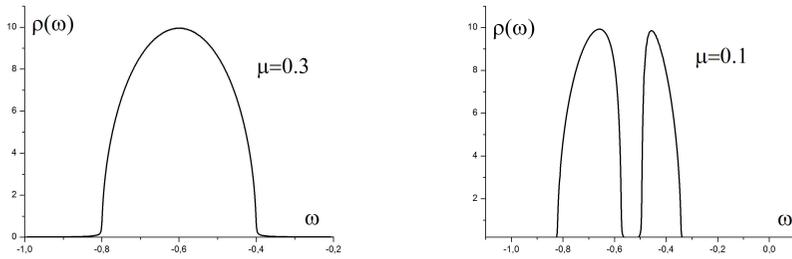
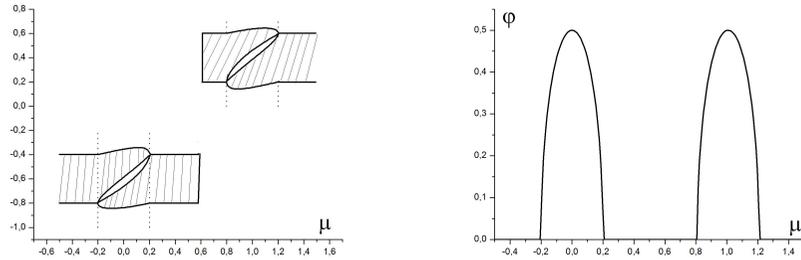


Fig.7 Single-site energy levels and order parameter for $\mu' = -0.1$

new fermion subbands in the SF-phase (the phase with BE-condensate, where $\varphi \neq 0$) takes place. The physical background of effect consists in mixing of states with different number of bosons and possibility of new fermion transitions, which are accompanied by creating or destruction

Fig.8 Density of states for different μ when $\mu' = 0.6$ Fig.9 Single-site energy levels and order parameter for $\mu' = 0.6$

of bosons. Such excitations are called “composite fermions” [4,5]. We see here their manifestation in fermion spectrum.

The presented results are restricted to the $T = 0$ limit. At finite temperatures the new subbands will appear (four subbands in the case of 4-state model). Similar effect of the fermion spectrum splitting was obtained previously for pseudospin-electron model [3] where calculations were performed in the DMFT approach. The more complete analysis of reconstruction of energy spectrum will be a subject of our subsequent consideration.

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CONTACT INFORMATION:

Institute for Condensed Matter Physics
of the National Academy of Sciences of Ukraine
1 Svientsitskii Str., 79011 Lviv, Ukraine
Tel: +38(032)2761978; Fax: +38(032)2761158
E-mail: cmp@icmp.lviv.ua <http://www.icmp.lviv.ua>