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Nature of correlations in the atomic limit of the boson fermion model

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Abstract. Using the equation of motion technique for Green's functions we derive the exact solution of the boson fermion model in the atomic limit. Both (fermion and boson) subsystems are characterised by the effective three level excitation spectra. We compute the spectral weights of these states and analyse them in detail with respect to all possible parameters. Although in the atomic limit there is no true phase transition, we notice that upon decreasing temperature some pairing correlations start to appear. Their intensity is found to be proportional to the depleted amount of the fermion nonbonding state. We notice that pairing correlations behave in a fashion observed for the optimally doped and underdoped high T_c superconductors. We try to identify which parameter of the boson fermion model can possibly correspond to the actual doping level. This study clarifies the origin of pairing correlations within the boson fermion model and may elucidate how to apply it for interpretation of experimental data.

PACS. 74.20.Mn Nonconventional mechanisms (spin fluctuations, polarons and bipolarons, resonating valence bond model, anyon mechanism, marginal Fermi liquid, Luttinger liquid, etc.) – 74.25.Bt Thermodynamic properties – 71.10.Li Excited states and pairing interactions in model systems

Boson fermion (BF) model describes a system composed of the narrow band electrons or holes (fermions) which coexist and interact with the local pairs (hard-core bosons) of, for example, bipolaronic origin [1]. The BF model has been recently intensively studied by various methods, such as: the standard mean field theory [1], the perturbative procedure with respect to the boson fermion coupling [2], perturbative expansion with respect to the kinetic hopping [3], the dynamical mean field procedure [4], the continuous canonical transformation [5], etc. Apart of studying the mechanism responsible for superconductivity, there have been also investigated the many-body effects which, above T_c, lead to an appearance of fermion pairs without their long range coherence. Indeed, three independent procedures [2,4,5] gave unambiguous arguments for the precursor effects, out of which a pseudogap is the most transparent one.

The pseudogap feature gradually builds up upon lowering temperature. It is observed in a temperature regime $T^* > T > T_c$, with both characteristic temperatures T^* and T_c depending on the BF model parameters. Absence of the long range coherence between pairs is caused by quantum fluctuations of the order parameter $\langle c_{i\downarrow} c_{i\uparrow} \rangle \equiv \chi_i e^{i\phi_i}$. In general, it is hard to distinguish between the amplitude χ_i and phase ϕ_i fluctuations because they are convoluted. Intuitively one may expect that phase fluctuations would dominate for a dilute concentration of paired fermions, while in the opposite limit the amplitude fluctuations take over. Some analysis along this line was recently discussed in reference [6]. Fluctuation effects were also studied for the 2 dimensional (isotropic and anisotropic) BF model by Micnas *et al.* [7] using the Kosterlitz Thouless theory. Authors reported a noticeable splitting between T^* and T_c which considerably increased for increasing population of the paired fermions. This result supports the above mentioned reasoning.

In this brief report we show that already on a level of the zero-dimensional (atomic limit) physics there is some evidence for pairing correlations which gradually increase in strength upon lowering temperature. We study such effect on a basis of the rigorous solution of the BF model in the atomic limit.

In our previous paper [3] we have investigated some aspects of the atomic limit solution. The effective fermion spectrum was determined there by a direct diagonalisation of the Hilbert space. In a current work we rederive the exact solution using the equation of motion technique [8] for Green's functions. Advantage of this method is that it gives the spectral weights for the eigenstates expressed in terms of the corresponding correlation functions. Of course, diagonalisation and Green's function method are equivalent and complementary to each other.

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Hamiltonian of the boson fermion model can be written as $H = \sum_{i,j,\sigma} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \sum_i H_i$ where t_{ij} stands for the hopping integral and the local part H_i is given by [1]

$$H_i = \varepsilon_0 \sum_{\sigma} c^{\dagger}_{i,\sigma} c_{i,\sigma} + E_0 b^{\dagger}_i b_i + g \left(b_i c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow} + b^{\dagger}_i c_{i,\downarrow} c_{i,\uparrow} \right). \tag{1}$$

We use here standard notations for the second quantisation operators of fermion $c_{i,\sigma}$, $c^{\dagger}_{i,\sigma}$ and hard core boson b_i, $b^{\dagger}_i$ fields. Site energies are correspondingly expressed as $\varepsilon_0 = \varepsilon_f - \mu$ and $E_0 = \Delta_B - 2\mu$ where a common chemical potential μ ensures conservation of the total charge concentration $n_{tot} = \left\langle 2 b^{\dagger}_i b_i + \sum_{\sigma} c^{\dagger}_{i,\sigma} c_{i,\sigma} \right\rangle$. Fermion and boson fields are coupled through the exchange interaction $g b_i c^{\dagger}_{i,\uparrow} c^{\dagger}_{i,\downarrow}$ + h.c. which can transform a fermion pair into a hard core boson and *vice versa*.

In the strict atomic limit $t_{ij} = 0$ one needs a solution of only the local part (1). Let us notice that the hard core boson operators obey, in general, the spin $\frac{1}{2}$ algebra, characterised by the following commutation rules $[b_i, b^{\dagger}_i] = \delta_{ij}(1 - 2 b^{\dagger}_i b_i)$ and $[b_i, b_j] = 0 = [b^{\dagger}_i, b^{\dagger}_j]$. For the same site $i = j$ (which is relevant in the atomic limit) they simply reduce to the anticommutation relations [9]. We can thus construct the fermionic Green's function $\langle\langle A_i; A^{\dagger}_i \rangle\rangle_{\omega}$ both for fermions $A_i = c_{i\sigma}$ and for hard-core bosons $A_i = b_i$, where we introduced the Fourier transform of the retarded Green's function $-\mathrm{i}\Theta(t) \left\langle \left[A_i(t), A^{\dagger}_i(0) \right] \right\rangle \equiv \int \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega t} \langle\langle A_i; A^{\dagger}_i \rangle\rangle_{\omega}$.

According to the equation of motion [8] $\omega \langle\langle A; B \rangle\rangle_{\omega} = \langle \{A, B\} \rangle + \langle\langle [A, H]\, ; B \rangle\rangle_{\omega}$ we find the following set of coupled equations

$$(\omega - \varepsilon_0) \left\langle\left\langle c_{i,\uparrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega} = 1 + g \left\langle\left\langle b_i c^{\dagger}_{i,\downarrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega}, \tag{2}$$

$$(\omega + \varepsilon_0 - E_0) \left\langle\left\langle b_i c^{\dagger}_{i,\downarrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega} = g \left\langle\left\langle (n^F_{i,\downarrow} - n^B_i)^2 c_{i,\uparrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega}, \tag{3}$$

$$(\omega - E_0) \left\langle\left\langle (n^F_{i,\downarrow} - n^B_i)^2 c_{i,\uparrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega} = \left\langle (n^F_{i,\downarrow} - n^B_i)^2 \right\rangle + g \left\langle\left\langle b_i c^{\dagger}_{i,\downarrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega}, \tag{4}$$

where $n^F_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ and $n^B_i = b^{\dagger}_i b_i$. After some algebraic calculations we determine that these three functions read

$$\left\langle\left\langle c_{i,\uparrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega} = \frac{1 - \langle (n^F_{i,\downarrow} - n^B_i)^2 \rangle}{\omega - \varepsilon_0} + \frac{\langle (n^F_{i,\downarrow} - n^B_i)^2 \rangle (\omega + \varepsilon_0 - E_0)}{(\omega - \varepsilon_0)(\omega + \varepsilon_0 - E_0) - g^2}, \tag{5}$$

$$\left\langle\left\langle b_i c^{\dagger}_{i,\downarrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega} = \langle (n^F_{i,\downarrow} - n^B_i)^2 \rangle \times \frac{g}{(\omega - \varepsilon_0)(\omega + \varepsilon_0 - E_0) - g^2}, \tag{6}$$

$$\left\langle\left\langle (n^F_{i,\downarrow} - n^B_i)^2 c_{i,\uparrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega} = \langle (n^F_{i,\downarrow} - n^B_i)^2 \rangle \frac{\omega + \varepsilon_0 - E_0}{(\omega - \varepsilon_0)(\omega + \varepsilon_0 - E_0) - g^2} \cdot \tag{7}$$

It is convenient to rewrite the single particle Green's function in the following way

$$\left\langle\left\langle c_{i,\uparrow}; c^{\dagger}_{i,\uparrow} \right\rangle\right\rangle_{\omega} = \frac{Z^F}{\omega - \varepsilon_0} + \left(1 - Z^F\right) \left[\frac{v^2}{\omega - \varepsilon_+} + \frac{u^2}{\omega - \varepsilon_-} \right], \tag{8}$$

$$Z^F = 1 - \left\langle (n^F_{i,\downarrow} - n^B_i)^2 \right\rangle, \tag{9}$$

$$\varepsilon_{\pm} = \frac{E_0}{2} \pm \sqrt{\left(\varepsilon_0 - \frac{E_0}{2} \right)^2 + g^2}, \tag{10}$$

$$v^2 = 1 - u^2 = \frac{1}{2} \left[1 + \frac{\varepsilon_0 - \frac{E_0}{2}}{\sqrt{\left(\varepsilon_0 - \frac{E_0}{2} \right)^2 + g^2}} \right] \cdot \tag{11}$$

Another set of coupled equations to determine the hard core boson propagator $\langle\langle b_i; b^{\dagger}_i \rangle\rangle_{\omega}$ involves the following Green's functions

$$(\omega - E_0) \left\langle\left\langle b_i; b^{\dagger}_i \right\rangle\right\rangle_{\omega} = 1 + g \left\langle\left\langle c_{i,\downarrow} c_{i,\uparrow}; b^{\dagger}_i \right\rangle\right\rangle_{\omega}, \tag{12}$$

$$(\omega - 2\varepsilon_0) \left\langle\left\langle c_{i,\downarrow} c_{i,\uparrow}; b^{\dagger}_i \right\rangle\right\rangle_{\omega} = 2 \left\langle c_{i,\downarrow} c_{i,\uparrow} b^{\dagger}_i \right\rangle + g \left\langle\left\langle b_i; b^{\dagger}_i \right\rangle\right\rangle_{\omega} - g \sum_{\sigma} \left\langle\left\langle c^{\dagger}_{i,\sigma} c_{i,\sigma} b_i; b^{\dagger}_i \right\rangle\right\rangle_{\omega}, \tag{13}$$

$$(\omega - E_0) \sum_{\sigma} \left\langle\left\langle c^{\dagger}_{i,\sigma} c_{i,\sigma} b_i; b^{\dagger}_i \right\rangle\right\rangle_{\omega} = \left\langle n^F_{i,\uparrow} + n^F_{i,\downarrow} \right\rangle \cdot \tag{14}$$

In analogy to (8) we present the explicit form of the single particle Green's function as

$$\left\langle\left\langle b_i; b^{\dagger}_i \right\rangle\right\rangle_{\omega} = \frac{Z^B}{\omega - E_0} + \left(1 - Z^B\right) \left[\frac{u^2}{\omega - E_+} + \frac{v^2}{\omega - E_-} \right], \tag{15}$$

$$Z^B = \left\langle (n^F_{i,\uparrow} - n^F_{i,\downarrow})^2 \right\rangle, \tag{16}$$

$$E_{\pm} = \varepsilon_{\pm} + \varepsilon_0. \tag{17}$$

The single particle propagators (8) and (15) are both characterised by a three pole structure. One of the poles is a remnant of the free nonbonding state (ε_0 for fermions and E_0 for hard core bosons). The other two poles ($\varepsilon_\pm$ and $E_\pm$) correspond to the bonding and antibonding states which arise due to the boson fermion interaction. Hamiltonian (1) is no longer diagonal in the occupation representation $|n^F_\uparrow, n^F_\downarrow; n^B\rangle$ because two eigenvectors contain admixture of $|\uparrow,\downarrow;0\rangle$ and $|0,0;1\rangle$ [3]. Loosely speaking, an ability of the system to fluctuate between these two states is a measure of pairing correlations (we mean the correlations in time, because in the atomic limit there exist no spatial correlations).

Let us inspect in some detail the spectral weight Z_F of the nonbonding fermions' state. From (9) we see that Z^F is depleted from unity by $\langle (n^F_{i,\downarrow} - n^B_i)^2\rangle = \langle n^F_{i,\downarrow}\rangle + \langle n^B_i\rangle - \langle 2n^F_{i,\downarrow} n^B_i\rangle$. It means that propagation (in time) of the free fermion (with spin $\sigma = \uparrow$) occurs unless: (a) there exists another fermion on the same site with the opposite spin and simultaneously no hard-core boson is present there, (b) there is boson while $\downarrow$ fermion is absent. Disappearance of the nonbonding state depends thus on fermion and boson concentrations. Role of other factors, such as for example temperature, is less evident at this point.

Spectral weight of hard core boson nonbonding state is given by

$$Z^B = \left\langle (n^F_{i,\uparrow} - n^F_{i,\downarrow})^2\right\rangle = \left\langle n^F_i\right\rangle - 2\left\langle n^{pair}_i\right\rangle, \tag{18}$$

where $n^F_i = n^F_{i,\uparrow} + n^F_{i,\downarrow}$ counts the total number of fermions on site i, while n^{pair}_i counts only the doubly occupied fermion states $n^{pair}_i \equiv c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow}$. The hard core boson can safely exist in a free (nonbonding) state when there are only single fermions present on the same site. The more fermions are paired, the less spectral weight is left for a free hard core boson.

We can express the spectral weights Z^F and Z^B explicitly *via* the concentrations $n^F \equiv \sum_\sigma \langle c^\dagger_{i,\sigma} c_{i,\sigma}\rangle$, $n^B \equiv \langle b^\dagger_i b_i\rangle$ and through such parameters as temperature T and Δ_B. From a general relation [8] $\langle AB\rangle = -\frac{1}{\pi}\int \mathrm{d}\omega f(\omega)\mathrm{Imag}\langle\langle B;A\rangle\rangle_{\omega+i\eta}$ we obtain

$$Z^F = \frac{n^F - \left[v^2 f(\varepsilon_+) + u^2 f(\varepsilon_-)\right]}{f(\varepsilon_0) - \left[v^2 f(\varepsilon_+) + u^2 f(\varepsilon_-)\right]}\,, \tag{19}$$

$$Z^B = \frac{n^B - \left[u^2 f(E_+) + v^2 f(E_-)\right]}{f(E_0) - \left[u^2 f(E_+) + v^2 f(E_-)\right]}\,, \tag{20}$$

where $f(x) = \left[\mathrm{e}^{x\beta} + 1\right]^{-1}$ is the Fermi Dirac distribution and $\beta = 1/k_B T$. These quantities can be computed also from the diagonalized Hamiltonian using the Lehmann representation. They are found to be [3] $Z^F = \left[1 + \mathrm{e}^{-\beta\varepsilon_0} + \mathrm{e}^{-\beta(\varepsilon_0+E_0)} + \mathrm{e}^{-\beta(2\varepsilon_0+E_0)}\right]/\Theta$ ($\Theta = 1 + 2\mathrm{e}^{-\beta\varepsilon_0} + 2\mathrm{e}^{-\beta(\varepsilon_0+E_0)} + \mathrm{e}^{-\beta(2\varepsilon_0+E_0)} + \mathrm{e}^{-\beta E_+} + \mathrm{e}^{-\beta E_-}$ is the partition function) and $Z^B = \left[2\mathrm{e}^{-\beta\varepsilon_0} + 2\mathrm{e}^{-\beta(\varepsilon_0+E_0)}\right]/\Theta$. These expressions are of course identical with (19, 20).

We explored numerically variation of the spectral weights Z^F, Z^B *versus* temperature T and Δ_B for several

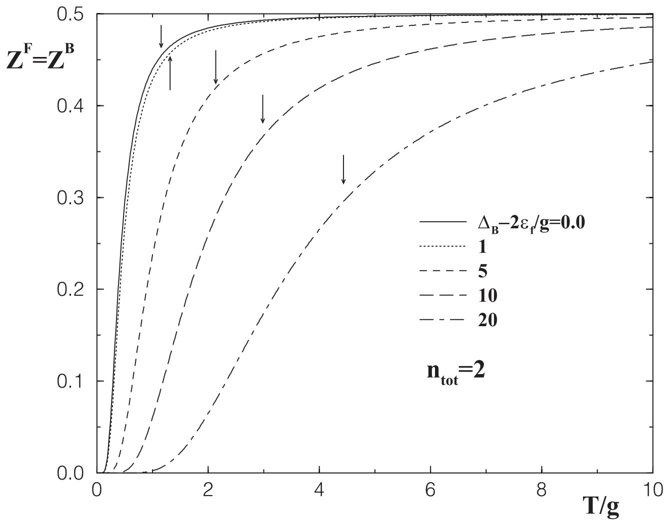


Fig. 1. Spectral weight of the nonbonding state of the fermion and hard core boson subsystems for total charge concentration $n_{tot} = 2$. Main suppression of the spectral weight of the nonbonding state occurs near T^* (pointed by the arrows) and depends on the parameter Δ_B.

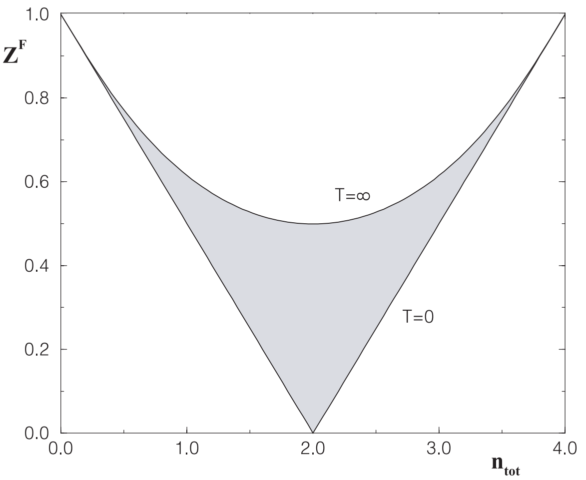
fixed charge concentrations $n_{tot} = n^F + 2n^B$. From our analysis it turns out that the most sensitive T-dependence of these quantities occurs for $\varepsilon_0 + E_0 = 0$ when $n_{tot} = 2$. One can show that

$$Z^F_{|n_{tot}=2} = \frac{2}{3 + \frac{\cosh \beta\sqrt{(\Delta_B/2)^2 + g^2}}{\cosh(\beta\Delta_B/6)}} = Z^B_{|n_{tot}=2} \tag{21}$$

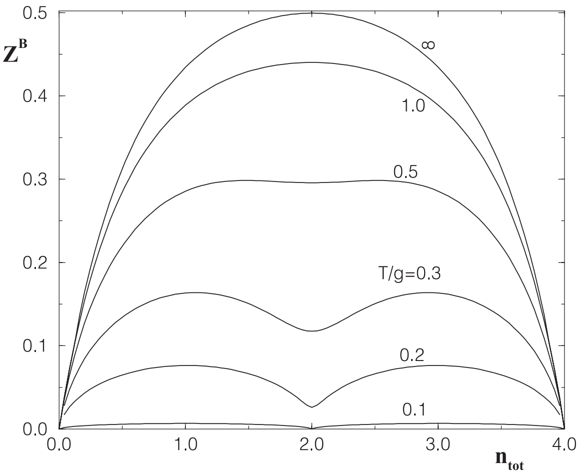
which at high temperature approach the asymptotic value $\lim_{T\to\infty} Z^{F,B}_{|n_{tot}=2} = 0.5$, while for $T \longrightarrow 0$ diminish to zero. Figure 1 illustrates this behaviour.

In any other case the spectral weights Z^F, Z^B may not vanish in the ground state. They vary within a narrower regime signaling that interaction effect is then less efficient as compared to the case $n_{tot} = 2$. Figure 2 shows the spectral weights $Z^{F,B}$ as functions of n_{tot} for $\Delta_B/2 = \varepsilon_f$. For fermions we notice that away of $n_{tot} = 2$ the spectral weight Z^F increases and becomes less dependent on temperature. In the extreme dilute region $Z^F \longrightarrow 1$. As far as Z^B is concerned it follows the behaviour of Z^F only in a close vicinity of $n_{tot} = 2$. Going away from such case the nonbonding spectral weight Z^B decreases as a direct consequence of the relations (16, 18).

Parameter Δ_B has rather a minor effect on both spectral weights, it mainly affects their temperature variation similarly to what is shown in Figure 1. In order to characterise the temperature dependence of Z^F we define characteristic temperature $T^*(n_{tot}, \Delta_B)$ [3] which is an inflexion point $\mathrm{d}^2 Z^F(T^*)/\mathrm{d}T^2 = 0$. Roughly speaking, the spectral weight Z^F starts to decrease when temperature drops below T^*. From higher dimensional studies of the BF model in the symmetric case ($n_{tot} = 2$, $\Delta_B = 2\varepsilon_f$) [3,4] it is known that suppression of the nonbonding state below



(a)



(b)

Fig. 2. (a) Spectral weight of the nonbonding fermion state as a function of total charge concentration n_{tot} per site. All finite temperature values are situated within the shaded area in the figure. (b) Spectral weight of the nonbonding state in the hard core boson subsystem for several temperatures as indicated. Both figures (a) and (b) are obtained for $\Delta_B/2 = \varepsilon_f$.

T^* is accompanied by an appearance of the pseudogap structure. Apart of the symmetric case there is not enough evidence that such relation remains valid.

Reduction of the nonbonding state spectral weight Z^F for temperatures near and below T^* is closely related to appearance of the pairing-type correlations. To prove this let us consider the Green's function $\langle\langle b_i c_{i,\downarrow}^\dagger; c_{i,\uparrow}^\dagger \rangle\rangle_\omega$ given in equation (6) which yields the following correlation function

$$\langle c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger b_i \rangle = g\left(1 - Z^F\right) \frac{f(\varepsilon_+) - f(\varepsilon_-)}{\varepsilon_+ - \varepsilon_-}. \tag{22}$$

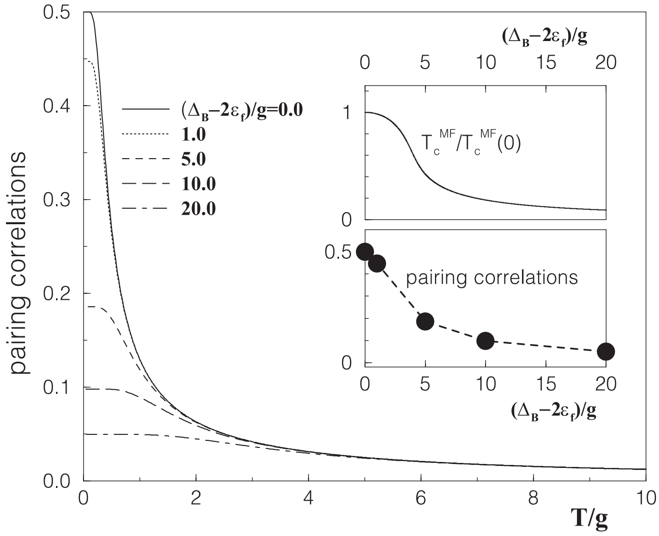


Fig. 3. The pairing correlation function $\langle c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger b_i \rangle$ induced in the atomic limit by the boson fermion coupling g. The upper inset shows a mean field value T_c^{MF} for a fixed ratio $g/D = 0.1$, where D denotes the fermion bandwidth. The lower inset is the ground state value of the correlation function. The main figure and the insets were obtained for $n_{tot} = 2$.

Let us recall that on a level of the mean field theory [1,7] the superconducting order parameter is given as

$$\langle c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger \rangle = -g \langle b_i \rangle \sum_{\mathbf{k}} \frac{1}{2\tilde{\varepsilon}_{\mathbf{k}}} \tanh\left(\frac{\tilde{\varepsilon}_{\mathbf{k}}}{2k_B T}\right), \tag{23}$$

where $\tilde{\varepsilon}_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + |g\langle b_i \rangle|^2}$ and $\varepsilon_{\mathbf{k}}$ denotes a dispersion of itinerant fermions. In the atomic limit the order parameters are on average equal zero $\langle c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger \rangle = 0 = \langle b_i \rangle$. We can think of a finite value (22) as a result of fluctuating pairing correlations. Magnitude of pairing correlations vanishes at high temperatures while, for temperatures $T \le T^*$, achieves the finite value proportional to the spectral weight depleted from the nonbonding state $(1 - Z^F)$. Figure 3 illustrates the temperature dependence of pairing correlations for several values of Δ_B at the fixed charge concentration $n_{tot} = 2$. Magnitude of $\langle c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger b_i \rangle$ turns out to be proportional to the mean field value of T_c^{MF} which proves their close relation.

The boson fermion model is claimed by some authors [1,6,7,10] to capture key aspects of the theory for high temperature superconductors (HTSC). In realistic description of the HTSC materials one must however consider their anisotropic $dim = 2 + \delta$ structure. Pairing correlations discussed here for the atomic limit would in higher dimensions lead to: (a) formation of fermion pairs at T_p, and (b) at $T_c \le T_p$ to their long range coherence, establishing the superconductivity (with $T_c \ne 0$). What remains to be studied for the realistic $dim = 2 + \delta$ systems is a pseudogap region of the incoherent fermion pairs $T_c \le T \le T_p$. We hope that the exact solution of the BF model discussed here for the atomic limit may help in such future investigations.

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