

# The Luttinger sum rule in the slave-particle theories

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**Abstract.** The usual mean field decoupling procedure applied to the slave-particle representations of the problems with strong local interaction produces a resonant band, but violates the Luttinger sum rule for the physical single-electron propagator. The number of occupied resonant states is small and equal to the deviation from the sum rule, shedding doubt on the overall results. It is therefore argued and illustrated on the example of the Emery model for the high- $T_c$  superconductors that, through the consistent application of the mean field procedure to the Hamiltonian and the propagators, the sum rule is restored and the resonant band conserved. In addition to the resonant band, the electron spectrum contains large number of occupied states close to the bare site-energy of the site with strong repulsion. These results are also related here to the other similar decoupling problems, which also lead to the breakdown of the Luttinger sum rule.

**PACS.** 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 71.27.+a Strongly correlated electron systems; heavy fermions

## 1 Introduction

The study of strongly interacting electron systems has been one of the most active research fields of solid state physics for a long time. In the present context, it is appropriate to mention Friedel/Anderson and Kondo impurity problems, extended to the case of Anderson lattice, the (extended) Hubbard models and their t-J derivatives and the Emery model of the  $\text{CuO}_2$  conducting planes for the high- $T_c$  rare-earth oxides with its t-J limit.

The general feature of many approaches to the above lattice problems is the appearance of the resonant band at the Fermi level. This includes the non-crossing approximation (NCA) of the perturbation theory in terms of inter-site hybridization [1–5], the dynamical mean field theory (DMFT) [6–8], the singlet and triplet bands in t-J models [9]. The simplest (and the earliest [10]) approach which, after the inclusion of the Gaussian fluctuations around the saddle point [2, 11–13], results in the resonant band [14–16] is the mean field slave boson (MFSB) approximation. The problem with this approximation is however, that the error in the Luttinger sum rule, giving the total number of the occupied states, is strictly equal to the number of states in the resonant band, shedding doubt on its results. Similar error occurs in some other decoupling schemes [17]. Nevertheless, the concept of the resonance is quite appealing because it appears also in the methods which obey the Luttinger sum rule by construction. In particular, it is interesting to note in this respect that singlet and triplet

bands in the t-J models have the site energy similar to the one of the corresponding MFSB resonant band.

Here, it will be argued that it is possible to deal with the error in the Luttinger sum rule, conserving simultaneously the concept of the resonant band. In contrast to the band structure, the Luttinger sum rule corresponds to the average numbers of fermions on various lattice sites, *i.e.* it is a local, static property, involving averaging over wave-vectors and frequencies. The related static and dynamic properties are therefore discussed consecutively here.

After the short introduction concerning the slave boson approach, Section 2 defines general static and dynamic aspects of the problem and sets the MFSB theory in this context. Section 3 is devoted to the description of the MFSB approach and suggests how to deal with static and dynamic problems behind the breakdown of the Luttinger sum rule in this approach. Section 4 illustrates the mechanism of the MFSB theory on the specific case of the Emery model for the  $\text{CuO}_2$  planes for high- $T_c$  superconductors, discussing time and space scales involved. In Section 5 the Luttinger sum rule is reestablished by the correction of the overall weight of the terms corresponding to various MF time and space scales, without changing the scales themselves. In this section the behavior of the resonant band and the dispersionless background is also briefly discussed. Section 6 compares the MFSB results to the perturbation approach in absence of the long-range order, relating the long-range ordering of the former to the long-time ordering of the latter. In this section some similar previous results

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are discussed in this spirit. Finally, the present results are briefly summarized in Section 7.

## 2 Slave-boson approach – General

Many methods used in the treatment of strongly correlated systems with local interaction  $U_d$  between physical fermions introduce auxiliary fermions and bosons [3,10,18–22] on the interaction sites. Although the transformation of the underlying Hamiltonian  $h = h_0 + U_d \sum_R n_{R,\uparrow}^d n_{R,\downarrow}^d$  to new particles is exact at the outset, it actually becomes useful in methods and approximations applied to the coupled fermion-boson system. Especially simple situation, considered also here, occurs when only the on-site interaction  $U_d$  is taken to infinity, because then only one fermion field  $f_R$  and one boson field  $b_R$  are sufficient: these fields are introduced by expressing the creation operator of the physical fermion  $c_R^{d\dagger}$  on the interaction site  $R$  as a composite, gauge-invariant fermion-boson entity

$$c_R^{d\dagger} = f_R^\dagger b_R. \quad (1)$$

An important role in such approach plays the resulting local gauge invariance of the slave boson Hamiltonian  $h$ , which implies the conservation of the “local charge”

$$Q_R = b_R^\dagger b_R + n_R^f = 1, \quad (2)$$

where  $n_R^f$  is the number of  $f$ -fermions of both spins.  $Q_R = 1$  means in particular that breaking of local gauge symmetry, either towards  $Q_R = 0$  or  $Q_R > 1$  subspaces is forbidden.

The first immediate consequence of the requirement (2) is the vanishing of the expectation value of  $b_R^\dagger$  and  $b_R$  in the ground state  $|G\rangle$  of the  $Q_R = 1$  subspace,  $\langle G|b_R^\dagger|G\rangle = \langle G|b_R|G\rangle = 0$  (and, of course,  $\langle G|f_R^\dagger|G\rangle = \langle G|f_R|G\rangle = 0$ ).

The second consequence is what is usually called the Luttinger sum rule for the reasons which will become clear later. According to equation (1) the number operator is

$$n_R^d = n_R^f b_R b_R^\dagger. \quad (3)$$

Realizing that the operator  $n_R^f b_R^\dagger b_R$  vanishes in the  $Q_R = 1$  subspace, it follows that

$$\langle n_R^d \rangle = \langle G|n_R^f b_R b_R^\dagger|G\rangle = \langle n_R^f \rangle. \quad (4)$$

This relation generates the Luttinger sum rule. For later convenience, it is interesting to note that this equality is however violated when the decoupling approximation is applied to equation (4),

$$\langle n_R^d \rangle \approx \langle G|n_R^f|G\rangle \langle G|b_R b_R^\dagger|G\rangle = \langle n_R^f \rangle (1 + \langle b_R^\dagger b_R \rangle). \quad (5)$$

The error occurs after the  $f_R^\dagger b_R$  interaction and/or doping of the interaction-sites are turned on, leading to  $\langle b_R^\dagger b_R \rangle > 0$ . It is obviously removed when transitions to

the intermediate excited states in the  $Q_R = 1$  subspace, omitted in equation (5), are also included.

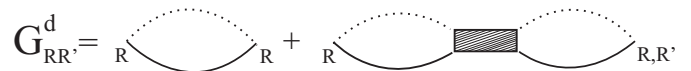
While equations (2–5) are based only on the local gauge invariance of  $h$ , associated with equation (1), in the following text the class of Hamiltonians  $h_0$  under consideration will be restricted to those with intersite hybridization term (bi)linear in fermion operators  $c_R^{d\dagger}$  or  $c_R^d$ , members of which are *e.g.* Hubbard’s, Emery’s and Anderson’s lattice Hamiltonian.

The  $U_d = \infty$  slave boson approaches [23–27] do not usually work with the restriction to  $Q_R = 1$  and the slave boson Hamiltonian  $h_0$  of  $h = h_0 + U_d \sum_R n_{R,\uparrow}^d n_{R,\downarrow}^d$ , but rather use the Lagrange multipliers  $\lambda_R$  to construct  $H = h_0 + \sum_R \lambda_R (Q_R - 1)$ , allowing fluctuations of  $Q_R$ , and searching for the ground state and the excited states of  $H$ . This introduces the usual many-body techniques into the problem, the perturbation schemes in particular.

Since  $H$  is itself locally gauge invariant, particularly instructive are the approaches perturbative in intersite hybridization, which start from the ground state  $|G_0\rangle$  of the unperturbed (non-hybridized) system is in the  $Q_R = 1$  subspace, thus with vanishing average values of  $b_R^\dagger$ ,  $b_R$ ,  $f_R^\dagger$  and  $f_R$ . It is then possible to show [13] that the single particle propagators of  $f$ -fermions and  $b$ -bosons remain local to all orders of the perturbation theory. The physical particle propagator between two interaction sites is

$$G_{RR'}^d(\tau) = -i \langle G|T f_R^\dagger(\tau) b_R(\tau) f_{R'} b_{R'}^\dagger|G\rangle, \quad (6)$$

satisfying the two-particle Bethe-Salpeter equation shown in Figure 1, which is however non-local when four-leg hybridization vertex is nonlocal, as it is in problems with the lattice of interacting sites, discussed here.



**Fig. 1.** Bethe-Salpeter representation of the physical single particle propagator in the slave boson theory. Dotted line: exact single boson propagator, solid line: exact single fermion propagator, square: exact four-leg vertex, hybridizing interaction sites at  $R, R'$ .

The first local term in Figure 1 corresponds at  $\tau = 0_+$  to the approximation of equation (5), *i.e.* it violates the Luttinger sum rule, independently on the dynamics involved in the fermion and boson single-particle propagators building it up. The correction to equation (5), which comes from the excited states, is related then to the second term of Figure 1, taken at  $\tau = 0_+$  and  $R = R'$ . With this term the Luttinger sum rule is obeyed through equation (4), since  $|G\rangle$ , generated by the exact perturbation theory with gauge-invariant Hamiltonian from  $|G_0\rangle$ , belongs itself to the  $Q_R = 1$  space. This, however is not necessarily true in approximate perturbative approaches, which start from  $|G_0\rangle$ .

The dynamical analysis of Figure 1 carried out in non-crossing approximation (NCA), starting from  $|G_0\rangle$

for  $\lambda_R = \lambda$ , suggests [13] that the single boson propagator develops a central peak by the transfer of the spectral weight from the frequency  $\lambda$ . This peak is responsible for the formation of the resonant band in  $G^d$ . The situation is relatively simple when the transfer of the boson spectral weight is complete, and the width of the central peak smaller than the  $f$ -fermion propagation scale:  $f$ -fermions respond adiabatically to the soft b-boson. In this sense (only) slow boson field acts as a static mean field  $\langle b_R^\dagger \rangle = \langle b_R \rangle \neq 0$  and its quantum fluctuations can be restored requiring finally  $[b_R, b_R^\dagger] = 1$ . Even when the transfer of the spectral weight is incomplete, an attempt to separate the slow and the fast component of the boson field can be made, associating the slow component with finite static  $\langle b_R^\dagger \rangle = \langle b_R \rangle = b_0$  and the fast component with the boson  $b'_R$ . Neglecting thus the width of the boson central peak, the resonant band in  $G^d$  is obtained with the dispersion in the reciprocal  $\mathbf{k}$  space emphasized at the expense of the “lifetime” effects. Such a view of MFSB will prove useful here. This line of thinking appeared also more or less explicitly and consistently in some earlier slave boson works [13, 15, 28].

### 3 MFSB local statics and dynamics

In the MFSB approximation the ground state is approximated by the direct product of fermion and boson states

$$|G\rangle \approx |G_{MF}\rangle = |G_0(b)\rangle \times |G_0(f)\rangle. \quad (7)$$

With the ansatz (7) in equation (4), the Luttinger sum rule is violated again

$$\langle n^d \rangle \approx \langle G_{MF} | n_R^f b_R b_R^\dagger | G_{MF} \rangle = \langle n_R^f \rangle (1 + \langle b_R^\dagger b_R \rangle). \quad (8)$$

Although the error in equation (8) looks just the same as in equation (5), its formal origin is completely different. While in equation (5) the error arises from neglecting the excited states in the  $Q_R = 1$  space, in equation (8) it is due to the component of  $|G_{MF}\rangle$  in the unphysical  $Q_R > 1$  space, where the operator  $n^f b_R^\dagger b_R$  differs from zero. Indeed, the excited states are not involved in equation (8), because the expectation value of the product of  $f$  and  $b$  operators for  $|G_{MF}\rangle$  separates exactly into the product of their expectation values.

Dealing with the error in equation (8), it is useful to realize that the choice of the SB Hamiltonian  $h_0$  and the particle number  $n$ , representing the physical problem, is not unique. All SB representations of the original physical problem which are the same in the  $Q_R \leq 1$  subspace are in principle equally good, even if they differ in the unphysical  $Q_R > 1$  subspace. However, when dealing with states, such as  $|G_{MF}\rangle$ , which leak into the  $Q_R > 1$  subspace, the best representation for  $h_0$  and  $n$  is the one which is the least sensitive to the component of  $|G_{MF}\rangle$  in the  $Q_R > 1$  subspace. This representation is chosen noting that  $\nu n_R^f b_R^\dagger b_R$ , with  $\nu$  scalar, can be added to any operator in the  $Q_R = 1$  space, without changing anything in

this (and  $Q_R = 0$ ) subspace, where this operator vanishes. This means in particular that  $n_R^d$  can be represented by

$$n_R^d = n_R^f (b_R b_R^\dagger + \nu b_R^\dagger b_R) \quad (9)$$

instead of equation (3). Irrelevant in the exact calculations, the choice of  $\nu$  in equation (9) is important for any approximate procedure involving the  $Q_R > 1$  space. Then the only way to keep  $n_R^d$  independent on the boson variables, *e.g.* in  $n$  and  $H$ , as it is in the exact calculations, is to choose [23–27]

$$\nu = -1, \quad n_R^d = n_R^f \quad (10)$$

in equation (9), extending this relation from the  $Q_R \leq 1$  subspace to the whole boson-fermion Hilbert space.

Of course, with equation (10), the Luttinger sum rule  $\langle n_R^d \rangle = \langle n_R^f \rangle$  is automatically satisfied. What remains is to show that it can appear in the limit  $R = R'$ ,  $\tau = 0_+$  of the physical propagator  $G_{RR'}^d(\tau)$ , which, after replacing  $|G\rangle$  by  $|G_{MF}\rangle$  in equation (6), violates, as it stands, the Luttinger sum rule, according to equation (8). The local propagation operator in equation (6) should therefore be reconstructed in order to be consistent with the representation (10) of the number operator. This is achieved by noting first that  $\nu(\tau) f_R^\dagger f_R b_R^\dagger b_R$  with  $\nu(\tau)$  a scalar function of  $\tau$  can be added to the propagation operator at  $R = R'$  in equation (6),

$$T f_R^\dagger(\tau) f_R b_R(\tau) b_R^\dagger + \nu(\tau) f_R^\dagger f_R b_R^\dagger b_R \quad (11)$$

without changing  $G_{RR'}^d(\tau)$  of equation (6). With this choice of the local propagation operator, the Luttinger sum rule is automatically obeyed again with any state instead of  $|G\rangle$  in equation (6), provided that for states which leak in the  $Q_R > 1$  space,  $|G_{MF}\rangle$  in particular,

$$\nu(\tau = 0_+) = -1. \quad (12)$$

On the other hand,  $\nu(\tau)$  is irrelevant for propagation in the  $Q_R = 1$  subspace, *i.e.* the modification (11) cannot be used straightforwardly to correct the error of equation (5):  $\nu(\tau)$  helps only in the  $Q_R > 1$  subspace. In the second step of the MFSB treatment, it should be shown that  $\nu(\tau)$  can be chosen consistently with aforementioned physical and usual formal constraints concerning the propagator of the single physical particle.

### 4 MFSB statics and dynamics: Emery model

The extension to finite times  $\tau$  requires the introduction of time and space scales generated by MFSB approximation. To some extent this is model-dependent and the  $U_d = \infty$  Emery [29] model for  $\text{CuO}_2$  lattice of high- $T_c$  cuprates will be used for illustration here. Quite rich, it contains the Hubbard-like and charge-transfer (valence fluctuation) limits [23, 27, 30, 31]. At finite  $t'$  and for the appropriate band-fillings, it is similar in many respects to the Anderson lattice model [3, 4].

The corresponding Hamiltonian  $h_0$  is

$$h_0 = \sum_{s,R} \{ \varepsilon_d n_R^f + \varepsilon_p \sum_{i=x,y} n_{R,i}^p \} \quad (13)$$

$$+ \sum_{i=x,y} [ t_0 c_{R,s}^\dagger (p_{R,i,s} + \sum_r t_0(r) p_{R+r,i,s} + \text{h.c.}) ]$$

$$- t' [ p_{R,x,s}^\dagger (p_{R,y,s} + \sum_r t'(r) p_{R+r,y,s} + \text{h.c.}) ],$$

with  $r$  denoting the nearest neighbors.  $t_0(r)$  and  $t'(r)$  are  $\pm t_0$  and  $\pm t'$ , respectively, according to the usual convention [32].  $c_R^\dagger$  of equation (1) is combined here with the fermions fields  $p_R^\dagger$  associated with the oxygen sites, and  $\nu = -1$  of equation (10) is chosen in the term describing the Cu-site energy  $\varepsilon_d n_R^d$  and the number of physical fermions in the CuO<sub>2</sub> unit cell,  $n_R = n_R^f + 2n_R^p$ .  $H$  with  $\lambda_R = \lambda$  is considered next, with  $|G_0(f)\rangle$  in equation (7) chosen spin unpolarized. The MF Hamiltonians for  $f$ -fermions and  $b$ -bosons are obtained as usual by averaging out with  $|G_0(b)\rangle$  and  $|G_0(f)\rangle$  respectively, the  $b$  and  $f$  fields. Taking  $|G_0(b)\rangle$  as a site product of wavefunctions  $|G_0^R(b_R)\rangle$  with finite, translationally invariant  $b_0 = \langle G_0(b) | b_R^\dagger | G_0(b) \rangle = \langle G_0(b) | b_R | G_0(b) \rangle$ , consistent with  $\lambda = \lambda_R$ , the MF Hamiltonian describing  $f$ -fermions is  $h_0$  of equation (13) with the effective (renormalized) parameters  $t = t_0 b_0$  and  $\varepsilon_f = \varepsilon_d + \lambda$ , while  $\varepsilon_p$  and  $t'$  remain unchanged. On the other hand, when  $f$ -field is averaged out (note that  $\langle f_R^\dagger \rangle = \langle f_R \rangle = 0$ ), the Hamiltonian of the displaced, but uncoupled harmonic oscillators  $b_R = b_0 + b'_R$  with frequency  $\lambda$  is obtained in the saddle point.  $|G_0(b)\rangle$  has thus the property  $\langle b_R^\dagger b_R \rangle = \langle b_R^\dagger \rangle^2 = \langle b_R \rangle^2 = b_0^2$  and  $\langle b'_R b'_R \rangle = \langle b'_R \rangle^2 = \langle b'_R \rangle^2 = 0$ . Here again the choice  $\nu = -1$  in equation (13) is important because it leaves  $\lambda$  to govern alone the energy  $\lambda b'_R b'_R$  of the dispersionless  $b'_R$  boson. Finally,  $\lambda$  and  $b_0$  are obtained from the minimization of the approximate ground state energy [30,31] of the physical particles  $E = \langle G_{MF} | H | G_{MF} \rangle$  at fixed number of physical particles  $n = \langle n^f \rangle + 2\langle n^p \rangle$ , or of  $\Omega = E - \mu n$  at fixed  $\mu$ .  $\mu$  and  $\langle n \rangle$  are related by

$$\langle n \rangle = \int^\mu g_c(\varepsilon) d\varepsilon, \quad (14)$$

where  $g_c(\varepsilon)$  is the density of states of the conducting band  $\varepsilon_c(\mathbf{k})$  of the  $f$ -fermions, assuming for simplicity that the Fermi level crosses only one band [30,32] at  $\mu = \varepsilon_c(\mathbf{k})$ .

Turning now to the propagation of the physical particles in time and space, as defined by MF Hamiltonians for  $f$  and  $b$  particles, it follows that

$$iG_{RR'}^d(\tau) \approx b_0^2 \langle G_0(f) | T f_R^\dagger(\tau) f_{R'} | G_0(f) \rangle, \quad R \neq R', \quad (15)$$

and

$$iG_{RR}^d(\tau) \approx \langle G_0(f) | T f_R^\dagger(\tau) f_R | G_0(f) \rangle \quad (16)$$

$$\times (b_0^2 + \langle G(b_0) | T b'_R(\tau) b'_R | G(b_0) \rangle) + \frac{1}{2} \nu(\tau) \langle n^f \rangle b_0^2.$$

Equation (15) is obtained by using  $|G_{MF}\rangle$  of equation (7) in equation (6), remembering that the boson  $b'_R = b_R - b_0$

is local and in its ground state  $\langle b'_R \rangle^2 = \langle b'_R \rangle^2 = \langle b'_R b'_R \rangle = 0$ , while equation (16) uses the propagation operator (11) concomitantly with  $|G_{MF}\rangle$  in equation (6), in agreement with the discussion leading to equation (12). The same equations are valid in the MFSB approximation for any model which generates a local boson  $b'_R$ . As will become clear now, equations (16) and (12) become the Luttinger sum rule for physical particles in the usual sense.

## 5 The Luttinger sum rule

For this purpose, the appropriate MF free-particle propagators [12, 1] of the Emery model are introduced now. The Fourier transform of fermion propagator  $G^f$  for the lowest occupied  $f$ - $p$  band projected on the occupied states with  $\mu$  from equation (14) is

$$\hat{G}^f(\omega, \mathbf{k}) = \frac{|m_f^c(\mathbf{k})|^2 \theta(\mu - \varepsilon_c(\mathbf{k}))}{\omega - \varepsilon_c(\mathbf{k}) - i\eta}, \quad (17)$$

where again  $\varepsilon_c(\mathbf{k})$  is the dispersion of  $f$ - $p$  fermion conduction band and  $|m_f^c(\mathbf{k})|^2$  is the probability of finding  $f$ - $p$  fermion on the Cu-site. This factor determines explicitly the average number of  $f$ -fermions on Cu site

$$\pi^{-1} \int \sum_{\mathbf{k}} \text{Im} \hat{G}^f(\omega, \mathbf{k}) d\omega = \sum_{\mathbf{k}} \theta(\mu - \varepsilon(\mathbf{k})) |m_f(\mathbf{k})|^2 = \frac{1}{2} \langle n^f \rangle. \quad (18)$$

On the other hand, MF boson propagator  $\langle G(b_0) | T b'(\tau) b'^\dagger | G(b_0) \rangle$  in equation (12) is given by

$$D^{b'}(\omega) = \frac{1}{\omega - \lambda + i\eta}. \quad (19)$$

As already mentioned, dynamics of the displaced boson  $b'$  is local and determined by the frequency  $\lambda$  (Cartesian gauge of the boson field is meant here [12]). Only  $+i\eta$  term appears in equation (19) because  $-i\eta$  component, associated with  $\langle b'_R b'_R \rangle \neq 0$ , vanishes for the harmonic  $b'$ -boson in its ground state.

Combining equations (15,16,17) and (19),  $G^d(\omega, \mathbf{k})$  reads

$$G^d(\omega, \mathbf{k}) = b_0^2 G^f(\omega, \mathbf{k}) + \int \frac{d\mathbf{k}}{(2\pi)^2} \hat{G}^f(\omega + \lambda, \mathbf{k}) - \frac{i\pi}{2} \langle n_f \rangle \nu(\omega) b_0^2. \quad (20)$$

Here, according to equations (15) and (16),  $G^f$  is the full free  $f$ -fermion propagator including occupied and unoccupied  $f$ -fermion states, unlike  $\hat{G}^f$ , which involves only the occupied states. The latter appears alone in the second term of equation (20), because  $D^{b'}$  of equation (19) couples in equation (16) only to the  $-i\eta$  component  $\hat{G}^f$  of  $G^f$ , given by equation (17).

The Luttinger sum rule of equation (12) sets weak requirement on the Fourier transform  $\nu(\omega)$  of  $\nu(\tau)$ . Further

restriction on  $\nu(\omega)$  comes from the requirement that the spectral density  $\pi^{-1}\text{Im}G^d(\omega, \mathbf{k})$  is positively definite. Both these requirements can be satisfied by various functions  $\nu(\omega)$ , some of which change qualitatively spectral density of d-electrons given by the first term, describing the resonant band, and the second term related to dispersionless background.  $\nu(\omega)$  will be chosen here to respect the time (“slow” and “fast”) and space scales introduced by the MF theory in the  $b$ -boson behavior, without introducing the new ones. It is thus meant to allow only the change in the respective normalization of the first (“adiabatic”) and second (“anti-adiabatic”) term in equation (20).

In order to find the appropriate  $\nu(\omega)$ , it is useful to note that equation (20) corresponds to the decomposition of  $\langle n^d \rangle$  in  $\langle n^d \rangle = b_0^2 \langle n^f \rangle + \langle n^f \rangle - b_0^2 \langle n^f \rangle$ , from equation (16) or directly from equation (20), using equations (17) and (18). Equation (20) then shows that if the third term were used to renormalize the first, resonant band term by cancelling its contribution to  $\langle n^d \rangle$ , the spectral density at a given  $\mathbf{k}$  would not be positively definite in the energy range  $\varepsilon_c(\mathbf{k}) \approx \varepsilon_d + \lambda$  of the resonant band. The third dispersionless, term therefore has to be used for the normalization of the second term, belonging to the energy range  $\varepsilon_c(\mathbf{k}) - \lambda \approx \varepsilon_d$ , which is also dispersionless (due to the local nature of slave boson  $b'$ ). This leads immediately to the final expression for the physical propagator

$$G^d(\omega, \mathbf{k}) = b_0^2 G^f(\omega, \mathbf{k}) + (1 - b_0^2) \int \frac{d\mathbf{k}}{(2\pi)^2} \hat{G}^f(\omega + \lambda, \mathbf{k}). \quad (21)$$

Equation (21) can now be interpreted as leading to the usual Luttinger sum rule for physical fermions: With  $\mu$  calculated under relation  $\langle n^d \rangle = \langle n^f \rangle$  from equation (14) for  $f$ -fermions, this equality is obtained back from equation (21). Moreover, the resonant band at the energy  $\varepsilon_c(\mathbf{k})$  close to  $\varepsilon_d + \lambda$ , is just the MF  $f$ -band, with its weight rescaled by  $b_0^2$ . The Fermi surface in the resonant band of equation (21)  $\mu = \varepsilon_c(\mathbf{k})$  is of the same shape as the Fermi surface of  $f$ -fermions in equation (14). Under the Fermi surface of the resonant band, oxygen component included, there are  $\langle n^d \rangle + 2\langle n^p \rangle$  occupied states, the local contribution of equation (21) at energy  $\varepsilon_c(\mathbf{k}) - \lambda$ , close to  $\varepsilon_d$ , included too.

Further discussion depends on the energy scales  $\lambda$ ,  $b_0 t_0$  and  $t'$  involved in equation (21) and  $b_0$  determined from the minimization of the ground state energy. When  $\lambda$  is large with respect to the bandwidth of  $\varepsilon_c(\mathbf{k})$ , controlled by  $b_0$ , the narrow resonant band is well separated from the narrow dispersionless background. On the other hand, when  $\lambda$  becomes of the order of the bandwidth, two spectral densities tend to come together. For large  $\varepsilon_p - \varepsilon_d$  and small positive or negative doping, this corresponds to charge-transfer (CT) or Hubbard-like limits, respectively, for the MFSB  $\lambda$ ,  $b_0$  values of the Emery model [30,31].

## 6 Relation to the perturbation theories

Equation (21) was obtained retaining the component of  $|G_{MF}\rangle$  in the  $Q_R > 1$  space, but choosing appropriately the slave boson representation of number and single-particle propagation operators to compensate for its effects. The correction in equation (21) is achieved by introducing a local, deep level  $\nu$  term, in line with the understanding that the straightforward MF approximation treats poorly the local correlations, better taken into account *e.g.* by the DMFT [6]. After the introduction of this term  $G^d$  of equation (21) is meant to approximate the “exact”  $G^d$  and it is interesting to compare it with the result of the adiabatic/antiadiabatic separation in the Bethe-Salpeter equation of Figure 1. When the (local)  $b_R$ -boson propagator is assumed to separate in the central peak entirely responsible for  $\langle b_R^\dagger b_R \rangle$  and the antiadiabatic component, analogous to the one of equation (16), *i.e.* with  $\lambda$  sufficiently large, the first term in Figure 1 generates, as easily seen, the first two terms in equation (16), which correspond at  $\tau = 0_+$  to equation (5). The  $\nu$ -correction in equation (16) corresponds then necessarily to the second term in Figure 1 taken at  $R = R'$ . At  $\tau = 0_+$ , it corresponds then to the contribution of the  $Q_R = 1$  excited states to equation (4). In addition, at  $R \neq R'$ , the second term corresponds to the contribution of equation (15). All this with the identification  $\langle b_R^\dagger b_R \rangle = b_0^2$ , but with  $\langle b_R^\dagger \rangle = \langle b_R \rangle = 0$ . In this representation the  $\nu$ -term corrects the error in equation (5), as it was correcting it in the MFSB equation (8), establishing the bridge between two at first sight unrelated errors, assured by the same, adiabatic/antiadiabatic separation in the background. Further study of this correspondence on the level of internal consistency of the Bethe-Salpeter equation of Figure 1 is however required.

An expression for  $G^d$  similar to equation (21), which also conserves the Luttinger sum rule, was proposed earlier [28], (also) based on the analysis of the time and space scales of the (outright) Hubbard model. A mixed picture, combining the long-time treatment of the local term and long-range expression for the non-local terms was used there. In the treatment of the local term, the propagation operator (11) was replaced by  $Tf_R^\dagger(\tau)f_R$  in equation (6) with  $|G_{MF}\rangle$  instead of  $|G\rangle$ . In the intermediate step  $b_R(\tau)$  is replaced by  $b_R$ , respecting in fact the time ordering of  $b_R^\dagger$  and  $b_R(\tau)$ . The obvious result is  $G_{RR}^d = G_{RR}^f$ . The same result follows from equation (6) assuming that the transfer of the boson spectral weight to low frequencies in Figure 1 is complete. Further on,  $G_{RR}^d = G_{RR}^f$  is artificially decomposed according to  $G_{R,R}^d = b_0^2 G_{R,R}^f + (1 - b_0^2) G_{R,R}^f$ , instead of equation (16), while at  $R \neq R'$  equation (15) was retained with general  $b_0^2$ ,  $G_{R,R'}^d = b_0^2 G_{R,R'}^f$ . On the other hand, equation (21), with  $G_{R,R}^d = b_0^2 G_{R,R}^f + (1 - b_0^2) \hat{G}_{R,R}^f$  and  $G_{R,R'}^d = b_0^2 G_{R,R'}^f$  in obvious notations, suggests that when  $b_0^2$  is taken equal to unity in the local  $G_{R,R}^d$  term, it should be taken as such in the intersite term too. In this case the earlier expression [28] and equation (21) reduce to the same  $G^d(\mathbf{k}) = G^f(\mathbf{k})$ . However, for a general

$b_0^2 < 1$ , equation (21) is making difference between  $G_{R,R}^f$  and  $\hat{G}_{R,R}^f$ , for the reasons explained in its derivation, modifying thus the earlier suggestion.

## 7 Summary

In summary, the present results are useful in several aspects. As the first, directly, the Luttinger sum rule of the MFSB theory places unambiguously the chemical potential in the resonant band, defining thus the shape of the Fermi surface [30,31], the property best seen by ARPES experiments [33]. As the second, more profoundly, it associates the sum rule problem with local contribution at large energies, suggesting that the low energy physics, associated with the formation of the resonant band, is weakly affected by those problems. As the third, suggesting that the long-range ordering of the MFSB theory can be understood to some extent as a long-time ordering of locally gauge-invariant theories, MFSB approximation can serve as a useful eye guideline for the more sophisticated approaches to the understanding of the low energy behavior of the strongly correlated systems, high- $T_c$  superconductors included. In particular, the Brinkmann-Rice metal-insulator phase transition obtained in the straight-forward MFSB theory [23,30,31], is expected therefore to correspond to the crossover in  $\langle b_R^\dagger b_R \rangle$  in more advanced approaches. In this spirit the MFSB theory can serve as a reasonable starting point for the study of the magnetic and superconducting correlations in the strongly interacting systems.

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