Spin and Charge Structure Factor of the 2-d Hubbard Model

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Abstract

The spin and charge structure factors are calculated for the Hubbard model on the square lattice near half-filling using a spin-rotation invariant six-slave boson representation. The charge structure factor shows a broad maximum at the zone corner and is found to decrease monotonically with increasing interaction strength and electron density and increasing temperature. The spin structure factor develops with increasing interaction two incommensurate peaks at the zone boundary and along the zone diagonal. Comparison with results of Quantum Monte Carlo and variational calculations is carried out and the agreement is found to be good. The limitations of an RPA-type approach are pointed out.

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I. INTRODUCTION

Soon after the discovery of superconductivity in the cuprate materials, it was suggested [1] that this phenomenon is closely related to strong correlation effects. Indeed correlations are responsible for the insulating state observed in the parent compounds. The simplest Hamiltonian accounting for such Mott insulators is the one band Hubbard model. It poses a serious challenge to the theoretician since ordinary many-body perturbation theory breaks down for strong coupling, being unable to account for Mott insulator state. A number of new techniques have been developed, either fully numerical such as Quantum Monte Carlo calculations or exact diagonalizations of small systems [2], or analytical using the Hubbard X-operator technique (for a recent work see [3]), the self-consistent 2-particle theory [4], the dynamical mean field approximation [5] or slave bosons. The slave boson method has been applied to a whole range of problems with local Coulomb interaction: the Kondo impurity model [6,7], the Kondo lattice model [7–10], the Anderson Hamiltonian [6,11], the Hubbard model [12,13] possibly with orbital degeneracy [14] and even the Bose-Hubbard model [15]. In the Kotliar and Ruckenstein (KR) slave boson technique [12] the Gutzwiller Approximation [16–19] appears as a saddle-point approximation of this field theoretical representation of the Hubbard model. In the latter a metal-insulator transition occurs at half-filling in the paramagnetic phase as discussed by Lavagna [20]. The contribution of the thermal fluctuations has been calculated [21] and turned out to be incomplete as this representation, even though exact, is not manifestly spin-rotation invariant. Spin-rotation invariant [22] and spin and charge-rotation invariant [23] formulations have been proposed, all sharing the advantage of treating all the atomic states on an equal footing, and the first one was used to calculate correlation functions [24] and spin fluctuation contributions to the specific heat [25]. Comparisons of ground state energy with Quantum Monte-Carlo simulations, including antiferromagnetic ordering [26] and spiral states [27], or with exact diagonalization data [28] have been done and yield excellent agreement, and a magnetic phase diagram has been proposed [29,30]. The magnetic susceptibility has been evaluated [31] and
shows in the strong coupling regime a maximum in its doping dependence in agreement with the observed behavior in the cuprates. Such a field theoretical description is especially useful since it allows for the calculation of dynamical quantities as well. This is the goal of the paper. We first derive expressions for the spin and charge auto-correlation functions, which we then evaluate numerically and determine the structure factors. We discuss how they depend on the doping, the interaction strength and the temperature.

II. RESPONSE FUNCTIONS

In this work we calculate the spin and the charge structure factors of the Hubbard model on the square lattice within the Spin Rotation Invariant (SRI) slave boson formulation \cite{23}. After having compared ground state energies, effective band widths and dispersions and magnetic susceptibilities with results obtained by other techniques, generally with very good agreement, structure factors provide another test for the approach, which is free of any adjustable parameter.

In the Spin Rotation Invariant slave boson representation, the Hubbard Hamiltonian is expressed in terms of slave boson operators $e_i$, $p_i$, $d_i$ for empty, singly occupied and doubly occupied sites and pseudo-fermions operators $f_{\sigma}$ as \cite{12,22,23}

$$H = \sum_{i,j} t_{i,j} \sum_{\sigma,\sigma'\sigma''} z_{i\sigma'\sigma''} f_{i\sigma'} f_{j\sigma''} z_{j\sigma'\sigma''} + U \sum_i d_i^+ d_i$$ (1)

where

$$z_i = e_i^+ L_i M_i R_i p_i + \bar{p}_i^+ L_i M_i R_i d_i$$ (2)

with

$$M_i = [1 + (e_i^+ e_i + p_{i0} p_{i0} + \bar{p}_i^+ \cdot \bar{p}_i + d_i^+ d_i)]^{1/2}$$

$$L_i = [(1 - d_i^+ d_i) \tau_0 - \bar{p}_i^+ \bar{p}_i]^{-1/2}$$

$$R_i = [(1 - e_i^+ e_i) \tau_0 - \bar{p}_i^+ \bar{p}_i]^{-1/2}$$ (3)
The under-bar denotes a $2 \times 2$ matrix in spin space, $\tau_0$ is the unit matrix and $\bar{p}_i$ is the time reverse of operator $p_i$. As usual the slave boson operators have to fulfill constraints. Here they read

\[ e_i^+ e_i + (p_{i0}^+ p_{i0} + \bar{p}_i^+ \cdot \bar{p}_i) + d_i^+ d_i = 1 \]
\[ \sum_{\mu} p_{i\mu} p_{i\mu} + 2d_i^+ d_i = \sum_{\sigma} f_{i\sigma}^+ f_{i\sigma} \]
\[ (p_{i0}^+ \bar{p}_i + \bar{p}_i^+ p_{i0} - i\bar{p}_i^+ \times \bar{p}_i) = \sum_{\sigma\sigma'} \bar{\tau}_{\sigma\sigma'} f_{i\sigma}^+ f_{i\sigma} \]  

(4)

and they are respectively enforced by the constraint fields $\alpha, \beta_0, \beta$. The scalar and vector slave boson fields $p_{i0}$ and $\bar{p}_i$ are defined as

\[ p_i = \frac{1}{2}(p_{i0} \tau_0 + \bar{p}_i \bar{\tau}) \]  

(5)

where $\bar{\tau}$ is the vector of Pauli matrices. The paramagnetic mean-field free energy results into

\[ F = -2T \int d\epsilon \rho(\epsilon) \ln[1 + \exp -E/T] + Ud^2 \]
\[ + \alpha(e^2 + d^2 + p_0^2 - 1) - \beta_0(p_0 + 2d^2) \].

(6)

After having fixed the notation we can proceed to the calculation of the dynamical susceptibilities. The linear response to an external field is given by the one-loop order calculation. The expression for the dynamical spin susceptibility has already been obtained by Li et al [24], but the calculation of charge fluctuations turned out to be more involved. In early calculations it has been assumed that the gauge symmetry group of both KR and SRI representations allows for gauging away the phases of all slave boson fields [21,20]. It later turned out that this conclusion is erroneous, and one Bose field has to be complex [32,13,23]. Choosing it to be the field describing double occupancy allows for describing the physics of the upper Hubbard band [33]. We note that the fully symmetric gauge approach has been applied to the calculation of the Landau parameters for liquid $^3$He by Li and Bénard [34].

The spin and charge auto-correlation functions $\chi_s$ and $\chi_c$ can be obtained out of:

\[ B_{\sigma\sigma'}(i - i', \tau - \tau') = \langle \hat{T}[n_{i\sigma}(\tau)n_{i'\sigma'}(\tau')] \rangle \]  

(7)
\[
\chi_s(i - i', \tau - \tau') = \sum_{\sigma \sigma'} \sigma \sigma' B_{\sigma \sigma'}(i - i', \tau - \tau')
\]
\[
\chi_c(i - i', \tau - \tau') = \sum_{\sigma \sigma'} B_{\sigma \sigma'}(i - i', \tau - \tau') \tag{8}
\]

Using the constraints and the mapping
\[
n_{i\sigma} = \frac{1}{2} \sum_{\mu=0}^{3} p_{i\mu} p_{i\mu} + d_i^+ d_i + \frac{1}{2} \sigma[p_{i0}p_{i3} + p_{i3}p_{i0} - i(p_{i1} p_{i2} - p_{i2} p_{i1})] , \tag{9}
\]
one can express the density fluctuations in terms of the slave boson fields as
\[
\sum_{\sigma} \delta n_{\sigma} = \delta(d^+ d - e^+ e) \equiv \delta N
\]
\[
\sum_{\sigma} \sigma \delta n_{\sigma} = \delta(p_{0}^+ p_{3} + p_{3}^+ p_{0}) \equiv \delta S \ . \tag{10}
\]
The correlation functions can be written in terms of the slave boson correlation functions as:
\[
\chi_s(k) = \sum_{\sigma \sigma'} \sigma \sigma' \delta n_{\sigma}(-k) \delta n_{\sigma'}(k) = \langle \delta S(-k) \delta S(k) \rangle
\]
\[
\chi_c(k) = \sum_{\sigma \sigma'} \delta n_{\sigma}(-k) \delta n_{\sigma'}(k) = \langle \delta N(-k) \delta N(k) \rangle . \tag{11}
\]
Performing the calculation to one-loop order, one can make use of the propagators given in the appendix to obtain:
\[
\chi_c(k) = 2e^2 S_{11}^{-1}(k) - 4edS_{12}^{-1}(k) + 2d^2 S_{22}^{-1}(k)
\]
\[
\chi_s(k) = 2p_0^2 S_{11}^{-1}(k) . \tag{12}
\]
Including the inverse matrix elements, we get
\[
\chi_c(k) = \frac{\left(S_{33}(k)S_{55}(k)e^2[-2p_0^2 \Gamma_1(k) + 8dp_0 \Gamma_2(k) - 8d^2 \Gamma_3(k)] - 2e^4 p_0^2 S_{55}(k) \omega^2\right)}{S_{33}(k)(\Gamma_1(k) \Gamma_3(k) - \Gamma_2^2(k)) + \omega^2 \Gamma_3(k) S_{55}(k) e^2} \tag{13}
\]
and
\[
\chi_s(k) = \frac{\chi_0(k)}{1 + A_k \chi_0(k) + A_1 \chi_1(k) + A_2(\chi_2(k) - \chi_0(k) \chi_2(k))} , \tag{14}
\]
where

\[ A_k = (2p_0^2)^{-1} \left[ \alpha - \beta_0 + \varepsilon_0 z_0 \frac{\partial^2 z_{\uparrow}}{\partial p_3^2} + \varepsilon \frac{\partial z_{\uparrow}}{\partial p_3} \right] \]

\[ A_1 = p_0^{-1} z_0 \frac{\partial z_{\uparrow}}{\partial p_3} \]

\[ A_2 = (4p_0^2)^{-1} z_0^2 \left( \frac{\partial z_{\uparrow}}{\partial p_3} \right)^2 \]

and

\[ \Gamma_1(k) = -S_{55}(k)(e^2 S_{22}(k) - 2ed S_{12}(k) + d^2 S_{11}(k)) + (eS_{25}(k) - dS_{15}(k))^2 \]

\[ \Gamma_2(k) = -S_{55}(k)(e^2 S_{24}(k) - p_0 e S_{12}(k) - ed S_{14}(k) + dp_0 S_{11}(k)) \]

\[ + (eS_{25}(k) - dS_{15}(k))(eS_{45}(k) - p_0 S_{15}(k)) \]

\[ \Gamma_3(k) = -S_{55}(k)(e^2 S_{44}(k) - 2ep_0 S_{14}(k) + p_0^2 S_{11}(k)) + (eS_{45}(k) - p_0 S_{15}(k))^2 \] .

(15)

In the following we shall evaluate numerically the spin and charge structure factors:

\[ S_x(q) = - \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} \frac{\text{Im} \chi_x(q, \omega + i0)}{1 - \exp(-\omega/T)} ; \quad x = s, c . \]

(17)

Note that while deriving the expressions (12) for the spin and charge correlation functions, we are dealing with both complex \((d)\) and real \((e, p_\mu)\) fields. For the latter, following an argument by Read and Newns [9], the contribution from the measure to the action \((\sum_{i,n} \ln (e_{i,n} \prod_{\mu} p_{i,n}^{e_{i,n}}))\) has been neglected. This aspect has been recently re-investigated in the framework of the \(1/N\) expansion of the large \(U\) Hubbard model [35]. It has been shown that including this contribution only leads to a minor change of the action, leaving its numerical value unchanged. This argument holds in the present context as well.

III. RESULTS

We first determine the spin structure factor as given by Eq. (17). In the weak coupling limit our result reduces to the RPA [36], and thus for small coupling and particle densities, the agreement with the exact solution is expected to be very good. However the RPA is getting less and less reliable as the interaction strength increases. This leads to unreasonable
results in RPA as e.g. a magnetic instability of the paramagnetic state for any particle filling above a critical coupling $[37]$. Such a deficiency is corrected in slave boson mean field theory. At zero temperature magnetic instabilities appear only beyond a certain particle filling $[30]$. For increasing temperature the region of magnetic long-range order is shrinking rapidly $[31]$. Strictly speaking, long-range order is absent at any finite temperature due to thermal excitations of spin waves (Mermin-Wagner theorem), which are not taken into account in slave boson mean-field theory.

Here we display results in the paramagnetic state, away from the instability line. Let us start by comparing (Fig. 1) our result for the spin structure factor to Quantum Monte Carlo results $[38]$. Here the structure factor is plotted as a function of wave number along straight lines $\Gamma-X-M-\Gamma$ in the Brillouin zone. For $U = 4t$, temperature $T = t/6$ ($\beta = 6; \beta = t/T$) and a doping $\delta = 0.275$, the overall agreement is good and the trends of the simulations are reproduced. Especially the peak is very broad and is centered around $(3\pi/4, \pi)$ for the QMC data. Out of our approach we get two peaks located away from $(\pi, \pi)$, which are indicating the onset of incommensurate short ranged spin order. As compared to the QMC calculations we obtain a second peak along the diagonal of the Brillouin zone which cannot be resolved in the simulations due to the small size of the system. The height of the peak which is located along the zone boundary is larger than the one of the peak which is lying on the diagonal of the Brillouin zone. We note that we are comparing the slave boson results for an infinite system to the raw QMC data on the $8 \times 8$ lattice. We believe that this comparison is meaningful since we observed that finite size effects are small (in the percent range as compared to the $6 \times 6$ lattice) for the set of parameters we are using. The agreement between the 2 approaches is mostly qualitative, and the slave boson calculation tends to overestimate the tendency towards magnetic ordering. But it also allows for gaining additional informations which are not revealed by the simulations like the presence of a second peak along the diagonal of the Brillouin zone. QMC data are not available in the complete parameter range. As an alternative there exist variational approximations at $T = 0$ to which we can compare our data. A very promising variational
ansatz is provided by a generalized Baeriswil-Gutzwiller wave-function \[39\]. In Fig. 2 we compare our result for \( U = 2t \) and \( U = 4t \) (\( \beta = 8 \), because of onset of long range order in our mean-field treatment) and \( \delta = 0.218 \) with the zero temperature results of ref. \[39\], and we reach the same conclusions as when comparing with the QMC simulations. On top of that we notice that the agreement is better for weaker interaction. Note that the position of the peaks is temperature dependent. At low temperature it is systematically located away from \((\pi, \pi)\), except at half-filling, but it moves towards \((\pi, \pi)\) for increasing temperature, as shown on Fig. 3 for \( U = 4t \). The first result of a small increase of the temperature is to suppress the value of the structure factor at its peak position, while the one at the zone corner is increasing, up to the point where it becomes the dominant one, as emphasized in the inset of Fig. 3. Increasing the temperature further results into an overall reduction of the structure factor for large momenta, and an overall increase of it for small momenta.

The fluctuation-dissipation theorem relates the \( q = 0 \) value of the spin structure factor to the magnetic susceptibility. As shown in the inset of Fig. 3, the latter is growing with increasing temperature for low \( T \), reaches a maximum at \( \beta \sim 4 \), and decreases beyond. This behavior is reminiscent of the spin gap behavior observed in the High \( T_c \) superconductors, although there it occurs at a smaller energy scale. As one can see from Fig. 3, the spin structure factor appears to approach its zero temperature limiting value at \( \beta \approx 8 \). We may therefore use the result for \( U = 4t \) at \( \beta = 8 \) instead of the \( T = 0 \) (\( \beta = \infty \)) result (which is not accessible because of onset of long range order in our mean-field treatment), to compare with the variational Monte Carlo (VMC) result at doping concentration \( \delta = 0.218 \) (Fig. 2). Whether incommensurate long range order occurs off half-filling using Otsuka’s wave-function is not known. In any case it sets in using the Gutzwiller wave-function \[40\].

We now consider the dependence of the spin structure factor on the interaction and the density. Here we fix the temperature to \( \beta = 8 \), and we calculate \( S_s(q) \) for \( U = t \) and \( U = 2t \) and display it on Fig. 4 for \( \delta = 0.1 \), on Fig. 5 for \( \delta = 0.2 \) and \( U/t = 1, 2, 3 \) and 4, and on Fig. 6 for \( \delta = 0.3 \) and \( U/t = 2, 4, 6, 7 \) and 8. In all cases we obtain that raising up the interaction generates more spin ordering, and the structures in the curves are
much more pronounced. At this temperature the position of the peak remains at the zone corner for small doping (see Fig. 4), while it is shifted away from its commensurate value for larger doping (see Fig. 5 and 6). The influence of the interaction is stronger when the system is denser, and this effect is enhanced by the vicinity of the perfect nesting point. For large doping the peaks become much broader resulting in an incommensurate very short ranged spin order. Also increasing the hole doping shifts the positions of the maxima of $S_s(q)$ further away from $(\pi, \pi)$, both along the $M - X$ line and along the $\Gamma - M$ line. One may ask to what extent the results presented above can be obtained in the framework of an RPA-type (or Fermi liquid type) scheme. For this purpose we compare the result for $\chi_s$ obtained by replacing the effective interaction $A_k(q)$ by its $q = 0$ limit and putting $A_1$ and $A_2$ equal to zero in Eq. (14,15). This allows for investigating the influence of the momentum dependence of the effective interaction on the spin order. The result is displayed on Fig. 7 for $U/t = 2, 4$ and 6. Clearly the approximation is very good for moderate couplings, but gets gradually worse for increasing interaction. Thus the dispersion of the effective interaction has a negligible influence on the structure factor for moderate interaction, but an important one for intermediate to large couplings, where it strongly shifts and suppresses the peaks of the structure factor. We thus conclude that knowing the Landau parameter $F_0^a$ is not all what is needed in order to determine the spin structure factor, especially when the fluctuations have a dominant short wavelength character.

We now turn to the charge structure factor. In Fig. 8 we compare our result for $U = 4t$ and $\delta = 0.275$ at temperature $T = t/6$ with the Quantum Monte Carlo result of Dzierzawa [38]. The charge structure factor consists of one broad peak which is centered at $(\pi, \pi)$. Fig. 8 clearly shows that the agreement between both approaches is excellent, and that the difference does not exceed a few percent. In Fig. 9 our result at zero temperature and $\delta = 0.218$ for $U = 4t$, $U = 8t$, and $U = 16t$ are compared with the variational Monte Carlo result of [39], and the dependence on $U$ is also displayed on Fig. 10. As expected, increasing the interaction strength $U$ leads to a suppression and a further broadening of the charge structure factor. In Fig. 11, the dependence on doping is shown for $U = 8t$ at zero
temperature. In weak coupling, one would expect $\chi_c$ to decrease upon doping. However the opposite behavior holds in a dense strongly correlated system, and our approach succeeds in obtaining this subtle effect. As compared to the 2-particle self-consistent theory [4], the reason of the success is however quite different. Indeed if we use the “RPA” approximation (the same procedure as above, but now in the charge fluctuation sector), we again obtain that the difference as compared to the full expression grows under an increase in the interaction strength as displayed in Fig. 12. Thus in our theory it is essential to take the dispersion of the interaction into account in order to obtain a good result, while such a dispersion is neglected in the 2-particle self-consistent theory [4]. We also performed the calculation at finite temperature. In contrast to the spin structure factor, the charge structure factor is mostly temperature independent at low $T$. This is a pure interaction effect, since in the non-interacting limit both structure factors have the same $T$-dependence. A further increase in $T$ simply leads to an overall reduction of the charge structure factor for large momenta, and an increase of it for small momenta, as shown in Fig. 13, where $S_c(q)$ is plotted for $U = 4t$ and $\delta = 0.275$ at temperatures ranging from $T = t/1.3$ down to $T = t/8$. Furthermore the temperature has no influence on the position of the peak of the charge structure factor. The fluctuation-dissipation theorem relates the charge structure factor at $q = 0$ to the charge susceptibility. As indicated in the inset of Fig. 13, the latter decreases monotonously with increasing Temperature, in agreement with Fermi liquid theory.

IV. SUMMARY

In this work we derived and evaluated the spin and charge structure factors of the Hubbard Model within the Spin Rotation Invariant six-slave boson formulation of the Hubbard model. We considered Gaussian fluctuations about the paramagnetic saddle-point, at small hole doping and for finite temperature, where the mean field solution is the paramagnetic one. The agreement with available exact numerical results for finite size systems and for variational wave functions was found to be very good. It is found that increasing either
the interaction strength or the density leads to more incommensurate spin order, and less
commensurate charge order. The slave boson mean field theory appears to provide a good
starting point for describing dynamical correlations on the level of Gaussian fluctuations.
It would be of interest to extend the calculations to the magnetically ordered phases, dis-
cussed e.g. in ref. [28]. Also the consideration of short range antiferromagnetic order [41] is
presumably important at low temperature, and should be taken into account.

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VI. APPENDIX

In second order in the bosonic variables the action is given by [23]:

\[ S = \sum_{q,\mu,\nu} \psi_\mu(-q)S_{\mu,\nu}(q)\psi_\nu(q) \]  

with \( \psi_1 = e, \psi_2 = d', \psi_3 = d'', \psi_4 = p_0, \psi_5 = \beta_0, \psi_6 = \alpha, \psi_7 = p_1, \psi_8 = \beta_1, \psi_9 = p_2, \psi_{10} = \beta_2, \psi_{11} = p_3, \psi_{12} = \beta_3 \). Here \( d' \) and \( d'' \) are the real and imaginary parts of the complex
d-field. The propagator matrix decouples into 4 blocks, one for the charge fluctuations and
3 for the spin fluctuations. Since the calculation is straightforward and most results can be
gathered from ref [24], we only quote the results. The charge part of the fluctuation matrix
is given by:

\[ S_{11}(k) = \alpha + \tilde{S}_{11}(k) \]
\[ S_{22}(k) = \alpha - 2\beta_0 + U + \tilde{S}_{22}(k) \]
\[ S_{33}(k) = \alpha - 2\beta_0 + U + \tilde{S}'_{33}(k) \]
\[ S_{23}(k) = \omega_{\mu} \]
\[ S_{44}(k) = \alpha - \beta_0 + \tilde{S}_{44}'(k) \]
\[ S_{ij}(k) = \tilde{S}_{ij}(k); i \neq j; i, j = 1, 2, 4 \]
\[ S_{15}(k) = -\frac{1}{2}\chi_1(k)\frac{\partial z}{\partial e} \]
\[ S_{16}(k) = e \]
\[ S_{25}(k) = -2d - \frac{1}{2}\chi_1(k)\frac{\partial z}{\partial \tilde{d}^0}z_0 \]
\[ S_{26}(k) = d \]
\[ S_{45}(k) = -p_0 - \frac{1}{2}\chi_1(k)\frac{\partial z}{\partial p_0}z_0 \]
\[ S_{46}(k) = p_0 \]
\[ S_{55}(k) = -\frac{1}{2}\chi_0(k) \] (19)

and the spin part by:
\[ S_{77}(k) = S_{99}(k) = S_{11,11}(k) = \alpha - \beta_0 + \tilde{S}_{77}(k) \]
\[ S_{88}(k) = S_{10,10}(k) = S_{12,12}(k) = -\frac{1}{2}\chi_0(k) \]
\[ S_{78}(k) = S_{9,10}(k) = S_{11,12}(k) = -p_0 - \frac{1}{2}\chi_1(k)\frac{\partial z^+}{\partial p_3}z_0 \] . (20)

We also defined:
\[ \tilde{S}_{\mu\nu}(k) = \varepsilon_0z_0\frac{\partial^2 z}{\partial \psi_\mu \partial \psi_\nu} + [\varepsilon_k - \frac{1}{2}z_0^2\chi_2(k)]\frac{\partial z}{\partial \psi_\mu} \frac{\partial z}{\partial \psi_\nu} \quad \mu, \nu = 1, 2, 4, 7, 9, 11 \]

\[ \tilde{S}'_{33}(k) = \varepsilon_0z_0\frac{\partial^2 z}{\partial \tilde{d}^0 \partial \tilde{d}^0} + [\varepsilon_k - \frac{1}{2}z_0^2\chi_2(k)]\frac{\partial z^+}{\partial \tilde{d}^0} \frac{\partial z}{\partial \tilde{d}^0} \] (21)

and
\[ \varepsilon_k = \sum_{p\sigma} t_{p\sigma-k} G_0(p) \] (22)

in terms of the pseudo-fermion Greens function \( G_0(p) = 1/(i\omega_n - E_k) \) and the effective dispersion:
\[ E_k = z_0^2t_k - \mu + \beta_0 \] . (23)
We also introduced the dynamical response functions of the fermionic system:

\[
\chi_n(k) = - \sum_{\sigma}(t_{\vec{p} + \vec{k}} + t_{\vec{p} + \vec{k}})^n G_{0\sigma}(p) G_{0\sigma}(p + k) = \chi_n(-k) \quad (n = 0, 1, 2)
\]

\[
\chi_2'(k) = - \sum_{\sigma}(t_{\vec{p} + \vec{k}} - t_{\vec{p}})^2 G_{0\sigma}(p) G_{0\sigma}(p + k)
\]

In Eq. (21) the derivatives are given by:

\[
\frac{\partial z}{\partial d'} = \sqrt{2} p_0 \eta (1 + \frac{2xd}{1 + \delta})
\]

\[
\frac{\partial z}{\partial d''} = i \sqrt{2} p_0 \eta
\]

\[
\frac{\partial^2 z}{\partial d'^2} = \frac{2 \sqrt{2} p_0 \eta}{1 + \delta} (2d + x + \frac{3xd^2}{1 + \delta})
\]

\[
\frac{\partial^2 z}{\partial d'd''} = i \frac{2 \sqrt{2} p_0 d \eta}{1 + \delta}
\]

\[
\frac{\partial^2 z}{\partial d'^2} = \frac{2 \sqrt{2} p_0 x \eta}{1 + \delta}
\]

\[
\frac{\partial^2 z}{\partial d'd''} = \frac{2 \sqrt{2} p_0 d \eta}{1 + \delta} (\frac{e}{1 - \delta} + \frac{d}{1 + \delta} + 2edx \eta^2)
\]

\[
\frac{\partial^2 z}{\partial d' \partial p_0} = \sqrt{2} \eta (1 + 2p_0^2 \eta^2 + \frac{2xd}{1 + \delta} + \frac{6p_0^2 xd}{(1 + \delta)^2} + 2p_0^2 \eta^2)
\]

\[
\frac{\partial^2 z}{\partial d'' \partial p_0} = i \frac{2 \sqrt{2} p_0 e \eta}{1 - \delta}
\]

\[
\frac{\partial^2 z}{\partial d'' \partial p_0} = i \sqrt{2} \eta (1 + 2p_0^2 \eta^2)
\]

With \( x = e + d \) and \( \eta^2 = 1/(1 - \delta^2) \). The other derivatives can be found in Ref. [24]. This extends the result of Bang \textit{et al} [13] to the metallic regime.
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FIGURE CAPTIONS

FIG. 1. Comparison of the Quantum Monte Carlo (circles) and Slave Boson (full line) spin structure factors for $U = 4t$, $\delta = 0.275$ and $\beta = 6$.

FIG. 2. Comparison of the Variational Monte Carlo (circles for $U = 2t$ and squares for $U = 4t$) and Slave Boson (dashed line for $U = 2t$, $\beta = 8$ and full line for $U = 4t$, $\beta = 8$) spin structure factors for $\delta = 0.218$ and $T = 0$.

FIG. 3. Temperature dependence of the spin structure factor for $U = 4t$, and $\delta = 0.275$. The temperatures are $\beta = 8$ (full line), 4 (dotted line), 2 (dashed-dotted line) and 1.3 (long dashed-short dashed line). Left inset: Magnification of the latter around the M-point. Right inset: Temperature dependence of the magnetic susceptibility for $U = 4t$ and $\delta = 0.275$.

FIG. 4. $U$-dependence of the Slave Boson spin structure factor for $U = 1t$ (circles) and $U = 2t$ (triangles), for $\delta = 0.1$ and $\beta = 8$.

FIG. 5. $U$-dependence of the Slave Boson spin structure factor for $U = 1t$ (circles), $U = 2t$ (triangles), $U = 3t$ (pluses) and $U = 4t$ (x’s), for $\delta = 0.2$ and $\beta = 8$.

FIG. 6. $U$-dependence of the Slave Boson spin structure factor for $U = 2t$ (circles), $U = 4t$ (triangles), $U = 6t$ (pluses), $U = 7t$ (x’s) and $U = 8t$ (diamonds), for $\delta = 0.3$ and $\beta = 8$.

FIG. 7. Comparison of the Slave Boson (x’s resp. diamonds resp. stars) and RPA (circles resp. triangles resp. pluses) spin structure factors for $U = 2t$ resp. $U = 4t$ resp. $U = 6t$, and $\delta = 0.3$ and $\beta = 8$.

FIG. 8. Comparison of the Quantum Monte Carlo (triangles) and Slave Boson (full line) charge structure factors for $U = 4t$, $\delta = 0.275$ and $\beta = 6$.

FIG. 9. Comparison of the Variational Monte Carlo (circles, pluses, diamonds) and Slave Boson (full, dashed, dashed-dotted line) charge structure factors for $U = 4t$, $U = 8t$
and $U = 16t$, and $\delta = 0.218$ and $T = 0$.

FIG. 10. U-dependence of the Slave Boson charge structure factor for $U = 2t$ (circles), $U = 4t$ (triangles), $U = 8t$ (pluses) and $U = 16t$ (x’s), for $\delta = 0.275$ and $T = 0$.

FIG. 11. Doping-dependence of the Slave Boson charge structure factor for $\delta = 0.1$ (circles), $\delta = 0.2$ (triangles), and $\delta = 0.3$ (pluses), and for $U = 8t$ and $T = 0$.

FIG. 12. Comparison of the Slave Boson (circles, pluses, diamonds) and RPA (squares, triangles, x’s) charge structure factors for $U = 2t$ resp. $U = 4t$, resp. $U = 8t$, and $\delta = 0.218$ and $T = 0$.

FIG. 13. Temperature dependence of the charge structure factor for $U = 4t$, and $\delta = 0.275$. The temperatures are $\beta = 8$ (circles), 6 (triangles), 4 (pluses), 2 (x’s) and 1.3 (diamonds). Inset: Temperature dependence of the charge susceptibility for $U = 4t$ and $\delta = 0.275$. 

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