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Lower and upper Hubbard bands: A slave-boson treatment

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We analyze the single-particle spectral density and the optical conductivity of the single-band Hubbard model in the insulating Mott phase within the slave-boson technique. We show that the boson fluctuations around the saddle-point solution build up the lower and upper Hubbard bands and give rise to the optical conductivity which describes transitions between these incoherent bands. We find that the Brinkman-Rice metal-insulator transition is characterized by the simultaneous vanishing of the jump in the chemical potential, the single-particle spectral density gap, and the optical gap.

In a recent paper the single-particle spectral density and the optical conductivity for the three-band infinite- U Hubbard model near and in the charge-transfer insulating phase were analyzed using the slave-boson approach.¹ It was shown that the metal-charge-transfer-insulator transition can be interpreted as a softening of an auxiliary Bose excitation. The energy of the boson mode, in the insulating phase, at zero doping, was related to the jump of the chemical potential for adding or removing a particle. Furthermore the presence of the collective excitations resulted in broad features both in the optical absorption and in the single-particle spectral density, reminiscent of the pioneering Hubbard picture in terms of lower and upper bands. It was conjectured that a similar description must hold also for the single-band finite- U Hubbard model and results for the zero momentum boson excitations were presented to support this suggestion.

In this paper we undertake to extend that analysis, by using the slave-boson technique introduced by Kotliar and Ruckenstein to deal with the finite-U Hubbard model.² Our results are the following: (1) In the Mott insulating phase, above the Brinkman-Rice metal-insulator transition point, 3 the slave bosons have, at Gaussian level, two dispersive modes. The mode at low energies is the holon mode previously found in a number of theories of

the single-band infinite- U Hubbard and $t - J$ models. The mode at high energies is associated with the finite- U charge-transfer energy and corresponds to the exciton mode of the three-band model. (2) The contributions from these Gaussian modes lead to the formation of the lower and upper Hubbard bands in the single-particle spectral density and to the high-energy broad absorption above the optical gap in the conductivity. (3) Upon doping, new quasiparticle states are introduced at the bottom and the top of the upper and lower Hubbard bands, respectively. (4) In Ref. ¹ the Brinkman-Rice transition, present in the saddle-point treatment of the Hubbard model of Kotliar and Ruckenstein,² was associated with the softening of the high-energy mode at zero momentum, whose energy equals the jump $\Delta \mu$ in the chemical potential in the Mott phase. We show that, in analogy with the three-band infinite- U Hubbard model, both the single-particle and optical gaps are equal to $\Delta \mu$ and vanish at the metal-insulator transition. (5) Finally, in the limit of vanishing hopping amplitude, our solution recovers the atomic limit, as in the original Hubbard work.

Our starting point is the four slave-boson functionalintegral representation of the Hubbard model introduced by Kotliar and Ruckenstein.² The partition function can be written in terms of the Lagrangian

$$
\mathcal{L}(\tau) = -t \sum_{i,j,\sigma} z_{i\sigma}^{\dagger} z_{j\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i,\sigma} c_{i\sigma}^{\dagger} (\partial/\partial \tau + \lambda_{i\sigma}^{(2)} - \mu) c_{i\sigma} + \sum_{i} d_{i}^{\dagger} \left[\partial/\partial \tau + \lambda_{i}^{(1)} + U - \sum_{\sigma} \lambda_{i\sigma}^{(2)} \right] d_{i} + \sum_{i} e_{i}^{\dagger} (\partial/\partial \tau + \lambda_{i}^{(1)}) e_{i} + \sum_{i,\sigma} p_{i\sigma}^{\dagger} (\partial/\partial \tau + \lambda_{i}^{(1)} - \lambda_{i\sigma}^{(2)}) p_{i\sigma} - \sum_{i} \lambda_{i}^{(1)} ,
$$
\n(1)

where the sum over i and j is restricted to nearestneighbor sites of a d-dimensional square lattice. The Bose fields d_i , $p_{i\sigma}$, and e_i represent doubly, singly occupied with a given spin, and empty sites, respectively. The atomic single-particle level is taken to be the zero of the energy. The fields $z_{i\sigma}$ are given by $z_{i\sigma} = g_{1i\sigma} (e_i^{\dagger} p_{i\sigma} + p_{i-\sigma}^{\dagger} d_i) g_{2i\sigma}$ where the factors $g_{1i\sigma}$ and $g_{2i\sigma}$ can be chosen in a quite arbitrary way as far as the functional integral is solved exactly. Kotliar and Ruckenstein showed that a particular choice must be done in order to recover the results of the Gutzwiller approach at the saddle-point level.² In what follows the actual choice of the g factors is to some extent irrelevant and for the time being we will leave them unspecified.

The time-independent Lagrange multipliers $\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$ introduced in Eq. (1) enforce at each lattice site the constraints $e_i^{\dagger}e_i + d_i^{\dagger}d_i + \sum_{\sigma} p_{i\sigma}^{\dagger} p_{i\sigma} = 1$ and $d_i^{\dagger}d_i + p_{i\sigma}^{\dagger} p_{i\sigma}$ $=c_{i\sigma}^{\dagger}c_{i\sigma}$ necessary to ensure the equivalence with the original Hubbard model.

Our idea now is to'study the model at half-filling in the Mott phase. This must be understood in the sense of considering the limit of vanishing particle or hole doping $\delta \rightarrow 0^{\pm}$. Despite the fact that the mean-field values of the parameters and the Bose excitations depend on which side the zero doping limit is actually being considered, the continuity is recovered in evaluating physical quantities.

The mean-field theory² is obtained by substituting the Bose fields with a c number, $\langle d_i \rangle = d_0$, $\langle e_i \rangle = e_0$, and $\langle p_{i\sigma} \rangle = p_{0\sigma}$. At the mean-field level the constraints are satisfied only on average with the Lagrange multipliers taken to be constant throughout the sample as $\langle \lambda_i^{(1)} \rangle = \lambda_0^{(1)}$ and $\langle \lambda_{i\sigma}^{(2)} \rangle = \lambda_{0\sigma}^{(2)}$. In Table I of Ref. 5 the analysis of the mean-field paramagnetic solution is synthetically reported. At zero doping, as U increases, the saddle-point solution recovers the Brinkman-Rice metalinsulator transition at $U = U_c$. In the Mott phase ($\delta = 0$, $U > U_c$) the Bose fields e and d are not condensed, while $p_{0\sigma} = 1/\sqrt{2}$ independent of σ . It follows that at Gaussian level the fluctuations of the e and d Bose fields are actually decoupled from those of the p fields. This fact is a consequence of the particular boson interaction term which derives from the hopping term of the original Hubbard model. In this way our task of considering charge fluctuations described by the e and d fields is enormously simplified, because the Gaussian fluctuations of these two fields can be treated by means of a 2×2 matrix, where the other boson fields only appear through their mean-field values. Furthermore, as was realized by Jolicoeur and Le Guillou, 6 in the finite-U Hubbard model it is impossible to study the fluctuations by fully reducing to the so-called "radial" gauge, which amounts to absorb the phases of the four Bose fields in the Lagrange multipliers. In what follows we will see that in the insulating Mott phase it is more convenient to work directly in the "Cartesian" gauge where all Bose fields maintain their own phase.

By integrating out the fermion degrees of freedom the Lagrangian for the e_i and d_i fluctuating fields is

$$
\mathcal{L} = \sum_{\mathbf{q}} (e_{\mathbf{q},\mathbf{v}}^{\dagger} d_{-\mathbf{q},-\mathbf{v}}) \Gamma(\mathbf{q}, i\omega_{\mathbf{v}}) \begin{bmatrix} e_{\mathbf{q},\mathbf{v}} \\ d_{-\mathbf{q},-\mathbf{v}}^{\dagger} \end{bmatrix},
$$
 (2)

where

$$
\Gamma(\mathbf{q}, i\omega_{\nu}) = \begin{bmatrix} -i\omega_{\nu} + \lambda_0^{(1)} + \Sigma(\mathbf{q}) & \Sigma(\mathbf{q}) \\ \Sigma(\mathbf{q}) & i\omega_{\nu} + \lambda_0^{(1)} + U - 2\lambda_0^{(2)} + \Sigma(\mathbf{q}) \end{bmatrix}.
$$
 (3)

The self-energy appearing in Eq. (3) is obtained by contracting the four-leg vertex originated from the hopping term

$$
\Sigma(\mathbf{q}) = -p_0^2 \overline{g}_1^2 \overline{g}_2^2 T \sum_{\mathbf{k}, n, \sigma} 2t \epsilon_{\mathbf{k} + \mathbf{q}} G(\mathbf{k}, i\omega_n) = -\frac{1}{d} p_0^2 \overline{g}_1^2 \overline{g}_2^2 \epsilon_{\mathbf{q}} \varepsilon,
$$
\n(4)

where $\epsilon_k = \sum_{\alpha=1}^d \cos(k_\alpha)$ and $\epsilon = 2 \int_{-\infty}^{\mu} \omega \rho_0(\omega) d\omega$, $\rho_0(\omega)$ being the uncorrelated density of states. The factors \bar{g}_1 and \bar{g}_2 are the saddle-point values of the corresponding functions $g_{1\sigma}$ and $g_{2\sigma}$. $G(\mathbf{k}, i\omega_n) = 1/(i\omega_n - E_{\mathbf{k}} + \mu)$ is the c-fermion single-particle Green function at the saddle-point level. $E_k = \lambda_0^{(2)} - 2\overline{g}_1^2 \overline{g}_2^2 p_0^2 (e_0 + d_0)^2 t \epsilon_k$ is the quasiparticle band, which is obtained at mean-field level and has a width vanishing at the metal-insulator transition $(E_k \rightarrow \lambda_0^{(2)}$ when $\delta \rightarrow 0$, $U > U_c$). While working in the Matsubara framework the $T=0$ limit is everywhere understood. By inserting Eq. (4) in (3) and taking the determinant we get

det
$$
\Gamma(\mathbf{q}, i\omega_{\nu}) = \omega_{\nu}^2 - i\omega_{\nu} (U - 2\lambda_0^{(2)})
$$

 $+ \lambda_0^{(1)} (\lambda_0^{(1)} + U - 2\lambda_0^{(2)})$
 $- p_0^2 \overline{\mathbf{g}}_1^2 \overline{\mathbf{g}}_2^2 \varepsilon \epsilon_{\mathbf{q}} / d (2\lambda_0^{(1)} + U - 2\lambda_0^{(2)})$. (5)

In order to solve Eq. (5), we borrow from Table I of Ref. 5 the values for $\lambda_0^{(1)}$ and $\lambda_0^{(2)}$ in the $\delta = 0^{\pm}$ limit:

$$
\lambda_0^{(1)} = \lambda_0^{(2)} = (U/2)(1 \pm \zeta) \tag{6}
$$

and $\zeta = (1-U_c/U)^{(1/2)}$ with $U_c = 4p\frac{2\pi}{3} \frac{2}{\epsilon^2} \epsilon$. It is easy to verify that $U - 2\lambda_0^{(2)} = \pm U\xi$, $\lambda_0^{(1)} + U - 2\lambda_0^{(2)} = (U/\lambda_0^{(1)})$

2)(1+ ζ), and $2\lambda_0^{(1)} + U - 2\lambda_0^{(2)} = U$.

H + 5), and $2\lambda_0$ + θ - $2\lambda_0$ - θ .
Having defined $\gamma_q^2 = 1 - \epsilon_q/d$, Eq. (5) then reads

$$
\omega_v^2 \pm i \omega_v U \zeta + (UU_c / 4) \gamma_q^2 = 0 \tag{7}
$$

By going to real frequencies $i\omega_v \rightarrow \omega$, Eq. (7) has two roots

$$
\omega_{1q} = \frac{1}{2} \{ \pm U\zeta + [(U\zeta)^2 + UU_c\gamma_q^2]^{1/2} \}, \qquad (8)
$$

$$
\omega_{2q} = \frac{1}{2} \{ \pm U\zeta - [(U\zeta)^2 + UU_c\gamma_q^2]^{1/2} \}, \qquad (9)
$$

which in the large- U limit reduce to

$$
\begin{split} \omega_{1\mathbf{q}} & = \tfrac{1}{2}U(\pm\zeta+\zeta) + \tfrac{1}{4}(U_c\,\slash\zeta)\gamma_{\mathbf{q}}^2\;,\\ \omega_{2\mathbf{q}} & = \tfrac{1}{2}U(\pm\zeta-\zeta) - \tfrac{1}{4}(U_c\,\slash\zeta)\gamma_{\mathbf{q}}^2 \end{split}
$$

depending on δ =0^{\pm}.

These collective modes show the same "phenomenology" found in the three-band infinite- U Hubbard model [compare Eq. (5) of Ref. 1]. The mode at high positive (negative) energy at $\delta = 0^+$ ($\delta = 0^-$) is the equivalent of the exciton mode in the three-band infinite- U Hubbard model. Its energy at $q=0$ was previously derived in Ref. ¹ and shown to be equal to the jump in the chemical potential, at zero doping, for adding or removing a particle. This is clearly seen by noticing that $\Delta \mu = \mu(\delta = 0^+) - \mu(\delta = 0^-) = \lambda_0^{(2)}(\delta = 0^+) - \lambda_0^{(2)}(\delta = 0^-)$ $= U \xi$.

The mode at low energy is the holon mode of the single-band infinite- U Hubbard model. In fact, the single-band infinite- U limit is recovered from the above equation by sending $U \rightarrow \infty$; at $\delta = 0^-$ the exciton mode is pushed to $-\infty$ and we are left with the holon mode only with energy $\omega_{\mathbf{q}} = (U_c / 4) \gamma_{\mathbf{q}}^2$.

We want now to evaluate, at the Gaussian level, the one-particle spectral density $A(\omega)$ of the original fermions which are expressed in terms of the c_{σ} fermions and e, d, and p_{σ} and Bose fields as $\tilde{c}_{\sigma} = z_{\sigma} c_{\sigma}$. $A(\omega)$ is given by $A(\omega) = -(1/\pi)\text{Im}g_{ii}(\omega)$ sgn ω with

$$
\mathcal{G}_{ij}(\tau) = -p_0^2 \overline{g}_1^2 \overline{g}_2^2 \langle c_i(\tau) c_j^{\dagger}(0) \rangle \langle b_i^{\dagger}(\tau) b_j(0) \rangle , \qquad (10)
$$

where we introduced in Eq. (10) the boson combination $b_i^{\dagger} = e_i^{\dagger} + d_i$. Notice that in the Mott phase the mean-field contribution to $A(\omega)$ is identically zero and only the fluctuating contributions from the e and the d fields appear in Eq. (10) since e and d have vanishing condensate in the insulating limit. The other boson fields are set equal to their mean-field values. From the fluctuation matrix we get

$$
D(q,i\omega_{\nu}) \equiv \langle b(q,i\omega_{\nu})b^{\dagger}(q,i\omega_{\nu}) \rangle = \sum_{\alpha=1,2} Z_{q}^{\alpha} \frac{1}{i\omega_{\nu} - \omega_{\alpha,q}}
$$
(11)

with

$$
Z_q^{\alpha} = (-1)^{\alpha} U / [(U \zeta)^2 + U U_c \gamma_q^2]^{1/2} .
$$

The fermion single-particle spectral density is then given by

$$
A(\omega) = (\overline{g}_1^2 \overline{g}_2^2 p_0^2 / 2N_s) \sum_{\mathbf{q}, \alpha} |Z_{\mathbf{q}}^{\alpha}| \delta(\omega - \lambda_0^{(2)} + \omega_{\alpha \mathbf{q}}) , \qquad (12)
$$

 N_s being the number of lattice sites. We recall that $\lambda_0^{(2)}$ is the energy of the renormalized atomic level and coincides with the chemical potential at $\delta = 0^{\pm}$. Notice that in obtaining Eq. (12) we have taken the bare atomic energy level as the reference zero. By inserting in Eq. (12) the expressions of the collective modes found in Eqs. (8) and (9) we reconstruct the lower and upper Hubbard bands whose energy positions are at the bare atomic level $\omega \sim 0$ and U. Specifically the gap between the two bands is given by $U\zeta = \Delta\mu$ and their width ΔW is of the order of the bare band width, $\Delta W \sim \alpha U_c$, with α ranging from $1/\sqrt{2}$ at $U = U_c$ to $\frac{1}{2}$ for $U \gg U_c$. As soon as the system is doped, mean-field quasiparticle states start to appear at $\lambda_0^{(2)}(\delta=0^{\pm})$, i.e., at the top (bottom) of the lower (upper) Hubbard band for $\delta < 0$ ($\delta > 0$).

At this point a possible criticism to our treatment may arise from the absence of magnetism in the scenario we are illustrating. In the present discussion we focused mainly on the role of charge fIuctuations which are relevant in order to understand the high-energy features of the electron and optical spectra. However, our expectation is that the inclusion of magnetic correlations, which will appear to higher orders in the loop expansion, should be mostly important as far as the low-energy behavior is concerned, but will not substantially modify, at high energies, the picture we have obtained. Actually, in this framework it is possible to recover the atomic limif the numerous it is possible to recover the atomic limit $t \rightarrow 0$, i.e., zero kinetic energy. This is done by letting $U_c \rightarrow 0$ and $|Z_q^{\alpha}| \rightarrow 1$, so that $\lambda_0^{(2)} = U$, $\omega_{1q} = U$, $\omega_{2q} = 0$ at $\delta = 0^+$ and $\lambda_0^{(2)} = 0$, $\omega_{1q} = 0$, $\omega_{2q} = -U$ at $\delta = 0$

The atomic spectral density reads

$$
A^{\text{atomic}}(\omega) = (\overline{g}_1^2 \overline{g}_2^2 p_0^2 / 2) [\delta(\omega) + \delta(\omega - U)] . \tag{13}
$$

Let us now comment on the specific form of the $g_{1\sigma}$ and $g_{2\sigma}$ factors. As far as the model is exactly solved, the $g_{1\sigma}$ and $g_{2\sigma}$ could be chosen in a quite general way. Kotliar and Ruckenstein² showed that in order to recover the uncorrelated limit $(U=0)$ a particular form must be chosen, namely, $g_{1\sigma} = f_{KR}(\vec{d}^\dagger d, p^\dagger_{\sigma} p_{\sigma})$
and $g_{2\sigma} = f_{KR}(e^\dagger e, p_{-\sigma}^\dagger p_{-\sigma})$ with $f_{KR}(x, y) = (1-x - y)^{-1/2}$. On the other hand, this choice gives the wrong spectral weight in the atomic limit, as is apparent from Eq. (13). This is not entirely surprising. The point is that, at the present level of approximation, the sum rule for the integrated spectral density is not expected to be satisfied. More generally we can derive what the sum rule would be, when the single-particle spectral density is evaluated bv neglecting vertex corrections in $(c_{i\sigma}(\tau)z_{i\sigma}(\tau)c_{j\sigma}^{\dagger}(0)z_{j\sigma}^{\dagger}(0))$ and just convoluting the Fermi and the Bose propagators. For the integrated spectral density we obtain

$$
\int_{-\infty}^{\infty} d\omega \, A(\omega) = \langle z_{\sigma}^{\dagger} z_{\sigma} \rangle + (1 - \langle c_{\sigma}^{\dagger} c_{\sigma} \rangle) \langle [z_{\sigma}, z_{\sigma}^{\dagger}] \rangle \qquad (14)
$$

which acquires different values in the metallic and insulating phase, and in general would differ from unity. In order to get the correct spectral weight, at the present order of approximation, one would be tempted to adjust the g factors depending on which saddle-point solution is actually being taken. In the Mott limit, to recover unity in Eq. (14), the average product $\bar{g}_1^2 g_2^2$ needs to be a function of U/ε which approaches 2 in the atomic limit. The possible functional forms for the g's leading to the above mean values have to be different from the Kotliar-Ruckenstein choice for which $\bar{g}^2_1 \bar{g}^2_2 \equiv 4$ in the Mott phase (and therefore the mean-field analysis of the Brinkman-Rice point would differ from the results of the Gutzwiller approach). We think, however, that to settle the problem of a proper choice of the g factors requires further analysis.

Let us now consider the optical conductivity. The current operator in the \hat{x} direction is $J_{i,x}$
= $it \sum_{\sigma} [\tilde{c}_{i\sigma}^{\dagger} \tilde{c}_{i+x\sigma} - \tilde{c}_{i+x\sigma}^{\dagger} \tilde{c}_{i\sigma}]$ or in momentum space $J_{q,x} = -(2t/\sqrt{N_s})\sum_{k\sigma} \sin(k_x)\tilde{\sigma}_k^{\dagger} - q/2\tilde{\sigma}_k^{\dagger} + q/2\sigma^{\dagger}$

The optical conductivity is obtained by $\text{Re}\sigma(\mathbf{q},\omega)$ $=-\text{Im}[\Pi^R_{I}(\mathbf{q},\omega)/\omega]$ with

$$
\Pi_J^{xx}(\mathbf{q}, i\omega_\nu) = -\langle T_r J_{\mathbf{q},x}(\tau) J_{\mathbf{q},x}^\dagger(0) \rangle .
$$

By expressing the original fermion as usual, i.e., $\tilde{c}_{k\sigma} = p_0 \overline{g}_1 \overline{g}_2/\sqrt{N_s \sum_p c_{k+p\sigma} b_p^{\dagger}}$ we get

$$
\Pi_{J}^{xx}(\mathbf{q}, i\omega_{v}) = 2[(2t)^{2}/N_{s}]T \sum_{n,k} \sin^{2}(k_{x})
$$

\$\times g(\mathbf{k} - \mathbf{q}/2, i\omega_{n})\$
\$\times g(\mathbf{k} + \mathbf{q}/2, i\omega_{n} + i\omega_{v})\$ (15)

By performing the analytic continuation $i\omega_v \rightarrow \omega + i0^+$ we obtain

$$
\text{Im}\Pi_{J}^{Rxx}(\mathbf{q},\omega) = 2\frac{(2t)^2}{N_s} \int_{-\infty}^{\infty} \frac{dz}{\pi} \sum_{\mathbf{k}} \sin^2(k_x) \times [f(z+\omega)-f(z)] \times \text{Im}\mathcal{G}^R(\mathbf{k}-\mathbf{q}/2,z) \times \text{Im}\mathcal{G}^R(\mathbf{k}+\mathbf{q}/2,z+\omega) \tag{16}
$$

with

Im
$$
\mathcal{G}^R(\mathbf{k}, z) = -\frac{p_0^2 \overline{g}_1^2 \overline{g}_2^2}{N_s} \sum_{\mathbf{p}} \text{Im} D^R(\mathbf{p}, E_{\mathbf{k}+\mathbf{p}} - z)
$$

$$
\times [b(E_{\mathbf{k}+\mathbf{p}} - z) + f(E_{\mathbf{k}+\mathbf{p}})].
$$
 (17)

In the above equations, $f(x)$ and $b(x)$ are the Fermi and the Bose functions, respectively, and it is understood that the chemical potential is subtracted from E_{k+p} . To make further progress in Eq. (16) we consider the case $\omega > 0$ and $T = 0$. For the q=0 limit of the optical conductivity (at $\delta = 0^{\pm}$) we obtain

$$
\sigma(\omega) = 2(2p_0^2 \overline{g}_1^2 \overline{g}_2^2 t)^2 \pi \frac{1}{N_s^2}
$$

$$
\times \sum_{\mathbf{p}_1, \mathbf{p}_2} \beta_{\mathbf{p}_1 \mathbf{p}_2}^2 \frac{|Z_{\mathbf{p}_1}^1| |Z_{\mathbf{p}_2}^2|}{\omega_{1\mathbf{p}_1} - \omega_{2\mathbf{p}_2}} \delta(\omega - \omega_{1\mathbf{p}_1} + \omega_{2\mathbf{p}_2}). \qquad (18)
$$

 $\beta_{\text{P}_1\text{P}_2}^2 = (1/N_s)\sum_k f(E_{k+\text{P}_1})[1-f(E_{k+\text{P}_2})]\sin^2(k_x)$ where
the limit $T\rightarrow 0$ is understood before taking the limit $\delta \rightarrow 0$ (i.e., $E_{k+p_{1,2}} \rightarrow 0$). From Eq. (18) we see that, in the Mott phase, the optical absorption starts at $\omega = U \zeta$, the same energy which controls the gap in the one-particle spectral density, and extends up to one-particle spectral density, and extends up to
max $\{\omega_{1p_1} - \omega_{2p_2}\} = [(U\zeta)^2 + 2UU_c]^{1/2}$. Upon doping, the

presence of quasiparticle states gives rise to a Drude absorption already at mean-field level.

We are now in a position to draw a general picture for the Hubbard model from our slave-boson treatment up to the first nontrivial corrections beyond mean field. We have shown that the slave-boson fluctuations, at Gaussian level, build up the lower and upper Hubbard bands and give rise to the optical conductivity which describes transitions between these incoherent bands. As doping is turned on, quasiparticles start to appear and a redistribution of spectral weight is expected.⁸ It follows that near the metal-insulator transition the spectral density and the optical conductivity have two distinct contributions: (i) a coherent one which derives form quasiparticles and controls the low-energy behavior and (ii) an incoherent one, which mainly contributes to the high-energy features of the spectra. The incoherent contribution is the result of the complicated motion of a quasiparticle surrounded by the cloud of charge excitations it leaves behind and becomes the leading one in the insulating phase. This picture agrees with the available numerical results on finite clusters⁹ and has strong analogies with the exact solution which can be obtained in infinite dimension. 10,11 In this last case however the Brinkman-Rice transition appears to be first order¹¹ with a finite jump of the chemical potential at the transition.¹² Whether this discrepancy must be ascribed to the $d = \infty$ limit or to the approximations used in this paper is an interesting open problem.

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- ¹C. Castellani, G. Kotliar, R. Raimondi, M. Grilli, Z. Wang, and M. Rozenberg, Phys. Rev. Lett. 69, 2009 (1992).
- ²G. Kotliar and A. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986).
- 3W. F. Brinkman and T. M. Rice, Phys. Rev. B2, 4302 (1970).
- ⁴J. Hubbard, Proc. R. Soc. London Ser. A 276, 238 (1963).
- 5M. Lavagna, Phys. Rev. 8 41, 142 (1990).
- ⁶Th. Jolicoeur and J. C. Le Guillou, Phys. Rev. B 44, 2403 (1991).
- ⁷In this case it would be more appropriate to write $z_{\sigma} = e^{\tau}g_{\tau}g_{\sigma}g_{\sigma} + p^{\tau}g_{\tau}g_{\tau}g_{\sigma}d$ [see E. Arrigoni, G. C. Strinati, and C. Castellani, Phys. Rev. B 41, 4838 (1990)] in order to avoid spurious singularities in z_{σ} when applied to physical states. This is, however, immaterial to the present context.
- ⁸A detailed analysis of the evolution of the various spectral weights with the doping will be the subject of a future publication.
- ⁹E. Dagotto, A. Moreo, F. Ortolani, D. Poilblanc, and J. Riera, Phys. Rev. B 45, 10741 (1992).
- ¹⁰W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
- $¹¹M$. J. Rozenberg, X. Y. Zhang, and G. Kotliar, Phys. Rev.</sup> Lett. 69, 1236 (1992); A. Georges and W. Krauth, ibid. 69, 1240 (1992), and references therein.
- ¹²Further, we recall that in our Gaussian approximation the broadening of the incoherent lower and upper Hubbard bands are related to the dispersion of the collective modes while the same broadening has a different source at $d = \infty$ where momentum dependence is absent.