## Collective Excitations, Photoemission Spectra, and Optical Gaps in Strongly Correlated Fermi Systems

C. Castellani, <sup>(1)</sup> G. Kotliar, <sup>(2)</sup> R. Raimondi, <sup>(1)</sup> M. Grilli, <sup>(1)</sup> Z. Wang, <sup>(2)</sup> and M. Rozenberg<sup>(2)</sup>

stenam, " G. Kotnar, " K. Kannondi, " M. Grini, " Z. Wang, " and M. Kozenber<br>Dipartimento di Fisica, Università "La Sapienza," 2, Piazzale Aldo Moro, 00185 Roma, Italy  $^{(2)}$ Serin Physics Laboratory, Rutgers University, P.O. Box 849, Piscataway, New Jersey 08854

(Received 4 March 1992)

We analyze the single-particle and collective excitations near the metal to charge-transfer insulator transition, using the slave-boson technique. We show that the Mott transition can be interpreted as a softening of an auxiliary Bose excitation. In the insulating phase the energy of the boson at zero momentum is related to the jurnp in the chemical potential at zero doping. The dispersion of the collective modes gives rise to the structure of the incoherent Hubbard bands. A similar picture holds for the single-band Hubbard model.

PACS numbers: 79.60.-i, 71.28.+d, 71.30.+h, 74.70.Vy

The one-particle Green's function in Mott and chargetransfer insulators has been a subject of renewed interest following the discovery of the superconducting transition-metal oxides. In broad terms, the main features of the insulating compound single-particle spectra are understood in terms of the Hubbard picture supported by small-cluster and impurity model calculations. While it is clear that doping modifies the spectral functions there is no universally accepted scenario. In the rigid Mott-Hubbard picture, the doping electron or hole occupies preexistent states at the top or the bottom of the lower and upper Hubbard bands, respectively [1]. In the marginal-Fermi-liquid scenario new states are generated upon doping inside the charge-transfer gap [2]. The experimental situation is still unclear [3].

In this Letter we reexamine this problem using the slave-boson method and the large- $N$  expansion. Our contribution to this problem is as follows: (1) We first observe that at small doping, near the insulating regime at half filling, the slave bosons have two well-defined dispersive modes, a mode analogous to the holon [4,5] in the one-band system and an exciton mode which brings in the finite- $U$  (or charge-transfer energy) character of the problem. In the insulating limit these collective modes are not direct physical excitations of the system but appear as intermediate entities in several observables. They are the hidden variables which provide a simple interpretation for the incoherent features of the single-particle and the optical spectra of the Mott insulator. (2) We show that the Mott transition acquires a simple physical picture as the softening of the exciton mode. This insight is significant because there is no obvious order parameter for the Mott transition, and therefore the standard Landau-Ginzburg analysis is of no avail for identifying a soft mode directly associated with this phase transition. We show that, on the insulating side the energy of the charge-transfer exciton mode is identical to the jurnp in the chemical potential  $(\Delta \mu)$  for adding or removing a particle. A finite  $\Delta \mu$  corresponds to a gap in the singleparticle excitation spectrum and is a criterion for insulating behavior. On phenomenological grounds, the copper

oxides are characterized by having a charge-transfer gap to hybridization ratio which is smaller than that of all known insulating transition-metal oxides. In this sense they are close to the metal to charge-transfer insulator transition and the existence of a soft mode is relevant as a potential source of deviations from canonical Fermiliquid behavior. (3) In both Mott and charge-transfer systems the doping introduces states at the top and the bottom of the lower and upper Hubbard bands for electron and hole doping, respectively. However, these states are new quasiparticle resonance states which are not simply related to preexisting states in the insulator. The Mott-Hubbard picture holds as a result of the identity between the jump in the chemical potential and the  $q=0$ limit of the exciton mode dispersion. The lower and upper Hubbard bands and the optical absorption spectra are simply related to the dispersion of the sound and the exciton mode.

Most of our analysis is based on the solution of the infinite-U extended Hubbard model, solved to next to leading order in 1/N. We believe, however, that our conclusions are quite general and support this conjecture with an analysis of the one-band finite-U Hubbard model in the framework of the four-boson technique [6].

The starting point is the Lagrangian of the extended three-band Hubbard model with SU(2) spin generalized to  $SU(N)$  flavors for the CuO<sub>2</sub> planes [7]:

$$
\mathcal{L} = \sum_{i,\sigma} d_{i\sigma}^{\dagger} (\partial/\partial \tau + \varepsilon_d^0) d_{i\sigma} + \sum_{i,a,\sigma} p_{i\alpha\sigma}^{\dagger} (\partial/\partial \tau + \varepsilon_p^0) p_{i\alpha\sigma} \n+ \sum_i b_i^{\dagger} \partial/\partial \tau \ b_i - \frac{t_{pd}}{\sqrt{N}} \sum_{i,\eta,\sigma} \text{sgn}(\eta) (p_{i\eta\sigma}^{\dagger} d_{i\sigma} b_i^{\dagger} + \text{H.c.}) \n+ i \sum_i \lambda_i \left( \sum_{\sigma} d_{i\sigma}^{\dagger} d_{i\sigma} + b_i^{\dagger} b_i - N/2 \right),
$$
\n(1)

where  $\alpha = x, y$  and  $\eta = \pm x, \pm y$ , and  $\lambda_i$  is a Lagrange multiplier enforcing the infinite- $U_d$  constraint on the copper site. The  $b_i$  is a slave boson whose expectation value measures the hybridization between the copper  $3d_{x^2-y^2}$  orbitals  $(d_{\sigma}^{\dagger})$  and the oxygen  $2p_x$  and  $2p_y$  orbitals  $(p_{x\sigma}, p_{y\sigma})$ , and the hole representation is used. This is a minimal charge-transfer model which at several points

of the discussion will be supplemented by

$$
H_{\rm c} = \frac{V_{\perp}}{N} \sum_{i,\eta,\sigma,\sigma'} d_{i\sigma}^{\dagger} d_{i\sigma} p_{i\eta\sigma'}^{\dagger} p_{i\eta\sigma'} + \frac{V_{2}}{N} \sum_{i,\eta,\sigma,\sigma'} d_{i\sigma}^{\dagger} d_{i\sigma'} p_{i\eta\sigma'}^{\dagger} p_{i\eta\sigma},
$$
 (2)

with  $V_1$  and  $V_2$  representing the *direct* and *exchange* part of the nearest-neighbor Coulomb repulsion whose importance for the high- $T_c$  oxides has been emphasized by Varma, Schmitt-Rink, and Abrahams [8]. The phase diagram of the model defined by  $(\mathcal{L}+H_{v})$  has been studied recently [9].

The metal to insulator transition at half filling was first discussed by Kotliar, Lee, and Read [71 form the point of view of the fermionic quasiparticles. In the large-N limit, mean-field theory applies,  $\lambda_0 = i \langle \lambda_i \rangle$  and  $r_0 = \langle |b_i| \rangle / \sqrt{N}$ , and the model describes three renormalized quasiparticle bands  $\Phi_{k\sigma,l}=(c_{k\sigma,1}, c_{k\sigma,2}, c_{k\sigma,3})$  of the hybridized copperoxygen orbitals  $\Psi_{k\sigma, l} = (d_{k\sigma}, i p_{k\sigma, x}, i p_{k\sigma, y})$ . When  $V_{1, 2} = 0$ , the dispersions of the bonding and the antibonding bands are  $E_{1,2}(k) = (\varepsilon_p + \varepsilon_d \mp R_k)/2$  with  $R_k^2 = (\varepsilon_p - \varepsilon_d)$ +16r $_0^2 t_{pd}^2 \gamma_k^2$  and  $\gamma_k^2 = \sin^2(k_x/2) + \sin^2(k_y/2)$ , whereas that of the nonbonding band  $E_3 = \varepsilon_p$ . The renormalized atomic level difference is  $\Delta \equiv \varepsilon_p - \varepsilon_d = \varepsilon_p^0 - \varepsilon_d^0 - \lambda_0$ . The parameters  $r_0$  and  $\lambda_0$  are determined by the meanfield equations which minimize the free energy,  $\lambda_0$  $N_s^{-1} \sum_k (4t_{pd}^2 \gamma_k^2 / R_k) (f_{1k} - f_{2k})$  and  $r_0^2 = \frac{1}{2} - N_s^{-1}$  $x \sum_{k} (u_k^2 f_{1k} + v_k^2 f_{2k})$ , where  $N_s$  is the number of unit cells,  $f_{ik} = f(E_i(k) - \mu)$  are the Fermi distribution functions, and  $u_k^2(v_k^2) = (1 \pm \Delta/R_k)/2$ . The mean-field equations can be solved analytically to conclude that a second-order Brinkman-Rice transition takes place at a critical value of the charge-transfer gap  $(\varepsilon_p^0 - \varepsilon_d^0)_c$  $=4t_{pd}(\overrightarrow{\gamma_k})^{1/2}$  where  $\lambda_0^2 = \Delta_c = 2t_{pd}(\overrightarrow{\gamma_k})^{1/2}$  and  $\overrightarrow{\gamma_k} = N_s$  $\sum_{k} \gamma_{k}^{2} f_{1k} = 1/2 + 2/\pi^{2}$ . This transition is similar to the Brinkman-Rice transition if we identify the bare chargetransfer gap  $E = \varepsilon_p^0 - \varepsilon_d^0$  with the Hubbard U. Close to the critical point  $r_0^2$  vanishes according to  $r_0^2$ <br>=  $[(\gamma_k^2)^{3/2} / \gamma_k^4] (E_c - E) / t_{pd}$  at half filling. Here  $\gamma_k^4$  $=N_s^{-1}\sum_k \gamma_k^4 f_{1k} = 5/8+4/\pi^2$ . It is important to emphasize that, on the insulating side  $(E > E<sub>c</sub>)$ , the chemical potential jumps discontinuously as one goes from hole to electron doping:  $\Delta \mu = \lambda_0(\delta = 0^+) - \lambda_0(\delta = 0^-)$  characteristic of a Mott insulating state. This quantity is given by

$$
\Delta \mu = (E^2 - 16t_{pd}^2 \overline{\gamma_k^2})^{1/2} = |\lambda_0 - \Delta|
$$
 (3)

and vanishes at the metal to insulator transition as  $E$  approaches  $E_c = 4t_{pd}(\overrightarrow{y_k})^{1/2}$  from above according to  $\Delta \mu \propto (E - E_c)^{1/2}$ . The compressibility vanishes as  $dn/d\mu$  $\propto E - E_c$ .

We mention in passing that in the presence of the copper-oxygen repulsion term  $H<sub>v</sub>$  the minimum value of  $t_{pd}$  to sustain a metallic state is increased by  $V_1$  and decreased by  $V_2$  which enhances the  $p-d$  hybridization by a

factor  $\kappa = 1 + \lambda_0 V_2 / 4t_{pd}^2$ . For  $V_1 < V_c = 1.75t_{pd} + 0.73V_2$ , the Brinkman-Rice transition remains second order and  $\Delta \mu = |\lambda_0 - \Delta/\kappa|$  vanishes at the transition where  $\kappa \lambda_0^c = \Delta_c$ . For  $V_1 > V_c$ , the Brinkman-Rice point becomes the origin of a first-order transition line ending at another secondorder transition point at finite doping, around which the model exhibits phase separation [9].

We now discuss this transition from the point of view of the Bose degrees of freedom. This picture, which is dual to the fermionic picture, illuminates a different aspect of the Mott phenomenon. To this end, we focus on the half-full limit  $\delta \rightarrow 0^{\pm}$ . The action for the Bose degrees of freedom is obtained by integrating out the  $p$  and d fermion excitations from  $\mathcal{L}$ . It has a very simple form in Cartesian gauge. Denote  $(\tilde{b}, \tilde{b}^{\dagger}) \equiv (b, b^{\dagger})/\sqrt{N}$ ; then  $\mathcal{L}_b = N \sum_{\mathbf{q}, \omega_n} \tilde{b}^\dagger(\mathbf{q}, i\omega_n) [-i\omega_n + \lambda_0 - \Pi_{pd}(\mathbf{q}, i\omega_n)] \tilde{b}(\mathbf{q}, i\omega_n),$ where  $\Pi_{pd}$  is the usual interband polarization bubble,

$$
\Pi_{pd}(\mathbf{q}, i\omega_n) = 4t_{pd}^2 \overrightarrow{\gamma_{k+q}} / (i\omega_n + \Delta) ,
$$
  

$$
\overrightarrow{\gamma_{k+q}} = N_s^{-1} \sum_k \gamma_k^2 + qf_{1k} .
$$

We obtain the Bose field propagator

$$
N\langle \tilde{b}(\mathbf{q}, i\omega)\tilde{b}^\dagger(\mathbf{q}, i\omega)\rangle = \frac{Z_\mathbf{q}^s}{i\omega_n - \omega_\mathbf{q}^s} + \frac{Z_\mathbf{q}^e}{i\omega_n - \omega_\mathbf{q}^e},\qquad(4)
$$

with  $Z_q^{\alpha} = -(\omega_q^{\alpha} + \Delta)/(\omega_q^{\alpha} - \omega_q^{\beta})$ ,  $\alpha \neq \beta = s, e$ . The poles in the propagator (4) define two collective modes  $\omega^s$  and  $\omega^e$  corresponding to the holon and to the charge-transfer exciton, respectively. The general dispersion of the modes is given by

$$
\omega_{\mathbf{q}}^{1,2} = \frac{1}{2} (\lambda_0 - \Delta) \pm \frac{1}{2} [(\lambda_0 - \Delta)^2 + 4\lambda_0 \Delta \Omega(\mathbf{q})]^{1/2},
$$

which simplifies in the large-charge-transfer-gap limit into

$$
\omega_{\mathbf{q}}^{s} = -\frac{\lambda_{0}\Delta}{\lambda_{0}-\Delta}\,\Omega\left(\mathbf{q}\right)\,,\quad\omega_{\mathbf{q}}^{e} = \lambda_{0}-\Delta + \frac{\lambda_{0}\Delta}{\lambda_{0}-\Delta}\,\Omega\left(\mathbf{q}\right)\,,\qquad(5)
$$

and  $\Omega(q) = 1 - \overline{\gamma_{k+q}^2/\gamma_{k}^2} = (2/\pi^2) \gamma_q^2/\gamma_k^2 \propto q^2$  for small q. Therefore, in the hole-doped case  $(\delta \rightarrow 0^+)$ ,  $\omega_q^s < 0$  and  $\omega_q^s > 0$ , whereas this situation is reversed for electron doping  $(\delta \rightarrow 0^-)$  where  $\omega_q^s > 0$  and  $\omega_q^s < 0$ . Note that<br>for  $\delta > 0$ ,  $\lambda_0 \approx \varepsilon_p^0 - \varepsilon_d^0 - t_{pd}^2/(\varepsilon_p^0 - \varepsilon_d^0)$  is large and<br> $\Delta = \varepsilon_p - \varepsilon_d$  is small. The opposite is true when  $\delta < 0$ . We will see in the following that the one-particle spectra are reconstructed by convolving the Bose spectral function with the spectral function of the fermions. The fermionic spectral function changes discontinuously as we go from positive to negative doping. The reversal of roles (and the discontinuous change) of the two modes as we go from  $\delta \leq 0$  to  $\delta \geq 0$  is necessary to insure the fact that the incoherent part of the spectral weight changes continuous-  $\lambda y$ , and in particular has the same limiting value form  $\delta = 0^+$  and  $\delta = 0^-$ . The modes disperse over a characteristic energy scale  $t \equiv t_{pd}^2/(\varepsilon_p^0 - \varepsilon_d^0)$ . Expressions (3) and (5) establish that the energy of the charge-transfer exciton is identical to the jurnp in the chemical potential as one goes from hole to electron doping:  $\Delta \mu = \omega_q^e = 0$ . This statement holds for  $V_{1,2} \neq 0$  where  $\Delta \mu = \omega_{\mathbf{q}}^e = \left[ \lambda_0 - \Delta/\kappa \right]$ and will be verified in the context of single-band Hubbard model with finite U.

At moderate hole concentration, the system forms a neutral Fermi liquid and the holon mode smoothly crosses over to the usual zero sound mode in the long-wavelength limit [5], which would show up in  $\omega_0^s$  had we kept the next to leading order in  $r_0^2$  contributions. In addition, in the presence of a finite intra-atomic repulsion  $V_{1,2}$ , excitonic effects emerge and the energy of the charge-transfer mode is reduced upon doping  $\omega_{\mathbf{q}}^e=0 \approx [(\lambda_0-\Delta/\kappa)^2]$  $-8r_0^2\lambda_0V_1]^{1/2}$ .

At finite doping, the modes  $\omega_{\mathbf{q}}^{s,\epsilon}$  appear as poles (which turn into resonances by including the damping effects) in the density-density and stress-stress correlation functions, identifying themselves with the collective modes of the strongly correlated metal. However, near half filling, for  $E > E_c$ , these collective modes have a vanishing ( $\approx r_0^2$ ) spectral weight, as direct excitations in the response functions.

At this point the modes appear as poles in the Bose propagators which are auxiliary quantities. Physical quantities are obtained as convolutions of these entities with fermionic or other bosonic excitations. To relate these modes to observables we compute the optical absorption in the insulating limit. The current operator is given by  $(e = \hbar = 1)$ ,

$$
J_{i,a} = i(t_{pd}/2) [d_{i\sigma}^{\dagger}b_i(p_{i+a/2,\sigma} + p_{i-a/2,\sigma}) - \text{c.c.}]
$$

The optical conductivity is determined by the imaginary part of the current-current correlator

$$
\Pi_J(\mathbf{q}, \tau) = -\langle T_\tau J_x^\dagger(\mathbf{q}, \tau) J_x(\mathbf{q}, 0) \rangle ,
$$
  
Re $\sigma(\mathbf{q}, \omega) = -\operatorname{Im}[\Pi_J(\mathbf{q}, \omega)/\omega],$ 

which can be evaluated using our Bose field propagators. For  $\delta \rightarrow 0^+$ , the only nonvanishing contribution comes from the 1/N corrections, which involve a convolution of boson propagators with an interband fermion bubble. We found

$$
\text{Re}\sigma(\mathbf{q},\omega) = \frac{\pi t_{pd}^2}{2NN_s} \sum_{\mathbf{p}} (1 - \overline{\gamma_{\mathbf{k}+\mathbf{q}-\mathbf{p}}^2}) \left[ \frac{1}{\omega - \Delta - \omega_{\mathbf{p}}^2} \delta(\omega - \Delta - \omega_{\mathbf{p}}^e) + (\omega \to -\omega) \right]. \tag{6}
$$

Clearly, in the insulating limit for  $\delta \rightarrow 0^+$  the exciton mode gives rise to the continuum in the optical spectrum whereas the sound (holon) mode is completely screened out at half filling. The opposite happens for  $\delta \rightarrow 0^-$  and the roles of the holon and the exciton modes are interchanged, but one reconstructs the same incoherent spectrum. The onset of absorption at this order  $(1/N)$  begins at  $\Delta \mu + \Delta = \lambda_0(\delta = 0^+)$  and this can be understood as an optical transition between an atomic sharp level and a d level which is broadened (i.e., our Feynman diagram describes a transition between the incoherent part of the d Green function and the bare  $p$  level). In the next order  $O(1/N^2)$ , we find the optical gap equals  $\Delta \mu = |\lambda_0 - \Delta|$ [101. At finite positive (negative) doping, the screening of the sound (exciton) is no longer complete, because all modes  $(\pm \omega_{\mathbf{q}}^s, \pm \omega_{\mathbf{q}}^e)$  start to be present in the boson propagators. Moreover intraband processes have to be taken into account. Eventually absorption develops inside the insulating gap.

Even though  $\omega_a^s$  is not involved in the current-current correlator in the zero-hole-doping limit  $(\delta=0^+)$ , it is essential for the understanding of the single-particle spectral function which appears in the photoemission and inverse photoemission spectrum. The spectral density on the copper site is  $A_d(\omega) = -2/\pi N \operatorname{sgn}\omega \operatorname{Im} G_d(\omega)$ , where  $G_d(i\omega_n) = FT[-\langle d_i(\tau) b_i^{\dagger}(\tau) b_i(0) d_i^{\dagger}(0)\rangle]$  is the Green function for the physical d fermions. In the limit  $\delta \rightarrow 0$ the quasiparticle contribution of order  $1/N<sup>0</sup>$  vanishes and  $A_d(\omega)$  is given by the first 1/N correction considered by Sá de Melo and Doniach [11] and Pattnaik and Newns [12]. Following their analysis, we obtained

$$
A_d(\omega) = \frac{1}{NN_s} \sum_{\mathbf{q}, a} \delta(\omega - \varepsilon_d + \omega_{\mathbf{q}}^a) |Z_{\mathbf{q}}^a| \,. \tag{7}
$$

The momentum summation in (7) spreads out the  $\delta$  functions giving rise to two broad continua synonymous with the upper and lower Hubbard bands. Their positions are determined by the arguments of the  $\delta$  functions which for  $\delta \rightarrow 0^+$ ,  $\Delta \approx 4t_{pd}^2 \gamma_k^2/(e_p^0 - e_q^0) \ll \lambda_0$ , are given by  $\varepsilon_d - \omega_q^0$  $= \epsilon_d + \Delta \Omega$  (q) and  $\epsilon_d - \omega_q^2 = \epsilon_d^2 + \Delta[1 - \Omega(q)]$ . For  $\delta \to 0^-$ ,  $\lambda_0 \approx 4t_{pd}^2 \gamma_k^2/(\epsilon_p^0 - \epsilon_d^0) \ll \Delta$ , we obtain  $\epsilon_d - \omega_q^2$  $\Rightarrow$  0,  $\kappa_0 \approx 4I_p d^2 k / k_p$   $\epsilon_d \approx 2 \times \Delta$ , we obtain  $\epsilon_d$   $\omega_q$ <br> $\approx \epsilon_d - \lambda_0 \Omega(q)$  and  $\epsilon_d - \omega_q^e \approx \epsilon_p^0 - \lambda_0 [1 - \Omega(q)]$ . It is clear now that both modes are essential to construct the spectral function. The spectral density is schematically depicted in Fig. 1 which shows that in the  $p-d$  chargetransfer system quasiparticle states are introduced at the top of the lower  $(Cu^{++})$  and at the bottom of the upper  $(0<sup>-</sup>)$  ionic bands for electron and hole doping, respectively, resembling the Mott-Hubbard picture from the energetic point of view. The quasiparticle states which are induced by doping, however, are strong coupling limits of the Kondo resonances [13] describing states which have no analog in the insulating state. The spectral weight associated with the quasiparticle states increases with doping. Therefore the effect of doping is not a simple redistribution of spectral weight among states which existed in the insulator but causes a drastic modification of the nature of low-energy excitations, contrary to the rigid Mott-Hubbard picture. They form the narrow quasiparticle band  $E_1(k)$  of width  $\sim 8r_0^2t_{\text{pd}}^2/\Delta$  around the renormalized level  $\varepsilon_d$  with a Luttinger Fermi surface and give



FIG. l. A schematic picture of the single-particle spectral density in the charge-transfer model given by Eq. (7) in the insulating limit (solid lines) and upon hole doping (dashed line). The bare and renormalized energy scales are indicated and  $\Delta \mu = \omega_{\mathbf{q}}^e = |\lambda_0 - \Delta|$ . The width of the continuum is determined by the dispersion for the modes at the zone boundary  $Q = (\pi, \pi).$ 

rise to the dispersive features observed in angle-resolved photoemission. Thus the closing of the charge-transfer gap is equivalent to the softening of the exciton mode at zero q. The picture outlined in this paper is not restricted to charge-transfer systems or to the large- $N$  expansion which was used to derive the results.

To confirm this conjecture we analyze the one-band Hubbard model with finite  $U$  following the functional integral approach introduced by Kotliar and Ruckenstein [6] based on four auxiliary bosons representing the empty site  $e^{\dagger}$ , the double occupied site (doublon)  $d^{\dagger}$ , and the single occupied site  $p_{\sigma}$ ,  $\sigma = \uparrow$ ,  $\downarrow$ , and three Lagrange multipliers  $\lambda_i$  and  $\Lambda_{i\sigma}$ .

The mean-field analysis [6,14] in the paramagnetic case at half filling shows a metal to insulator transition at  $U=U_c \equiv 8|\epsilon(\delta=0)|$  where  $\epsilon$  is the unrenormalized kinetic energy. On the insulating side  $(U > U_c)$  the mean-field values of the Bose fields are given by the self-consistency equations in the small doping limit [6,14,15]. Similar to the charge-transfer model, the jump in the chemical potential from hole to electron doping is given by  $\Delta \mu$  $=\Lambda_0(\delta=0^+) - \Lambda_0(\delta=0^-) = U\zeta$ , where  $\zeta \equiv [(U-U_c)/\zeta]$  $U]^{1/2}$ .

To study the Gaussian fluctuations and the collective modes it is essential to notice the absence of a full radial gauge, an observation due to Jolicoeur and Le Guillou [15], i.e., it is not possible to transform all the phases of the four Bose fields to the Lagrange multipliers. At least one boson, taken to be  $e_i$  in the following, maintains its own phase. In the following we shall partially follow the notation of Ref. [14] extended to correctly include both the e and  $e^{\dagger}$  fields. At the Gaussian level, the charge fluctuations decouple from the spin fluctuations and are described by a 6×6 matrix  $D(q, \omega)$  of the propagators for 201?

the fields  $a_i(\mathbf{q}, \omega) = (R_q, A_q, d_q, p_q^s, \lambda_q, \Lambda_q^s)$  with  $q = (\mathbf{q}, \omega)$ ,  $R_q = e_q + e_{-q}^{\dagger}, A_q = e_q - e_{-q}^{\dagger}, p_q^s = \frac{1}{2} (p_{q\uparrow} + p_{q\downarrow}),$  and  $\Lambda_q^2$  $=\frac{1}{2}(\Lambda_{q_1}+\Lambda_{q_1})$ . To determine the energy of the exciton mode in the insulating limit  $(U > U_c)$ , we focus on the limit  $q \rightarrow 0$  of the inverse of the Bose propagator  $D^{-1}$ . The evaluation of the determinant of  $D^{-1}(\mathbf{q}=0, \omega)$  is straightforward and gives

$$
\det D^{-1} = 2d_0^2 \{ -\omega^2 + [ (e_0^2 - d_0^2)/d_0^2 ]^2 [(U_c/4) + \lambda_0]^2 \}.
$$

The collective mode arises from the poles in the Bose field propagators, which is determined by det $D^{-1}(0, \omega_g) = 0$ , so that by using the mean-field values  $e_0$ ,  $d_0$ , and  $\lambda_0$  as given in Ref. [14], one obtains  $\omega_g = \Delta \mu = [U(U - U_c)]^{1/2}$ in agreement with the analysis of the charge-transfer model.

To conclude, we have shown that the slave-boson technique provides a simple picture of the finite- $U$  and finitecharge-transfer-energy aspects of the strong correlation problem. The physics of the Mott and the metal to charge-transfer insulator transition as well as the distribution of the single-particle spectral density can be understood in terms of collective bosonic excitations which evolve into the physical collective modes in a strongly correlated metal upon doping.

The group in Rome acknowledges the support of the European Economic Community under Contract No.  $SC1 * 0222-C(EDB)$ . The work at Rutgers was supported by the NSF under Grants No. DMR-89-15895 and No. DMR-89-96285.

- [1] H. Eskes, M. Meinders, and G. A. Sawatzky, Phys. Rev. Lett. 67, 1035 (1991).
- [2] A. Ruckenstein and C. M. Varma, Physica (Amsterdam) 185-189C, 134 (1991).
- [3] For a recent review see Physica (Amsterdam) 185-189C, (1991).
- [4] P. W. Anderson, Science 235, 1196 (1987).
- [5] Z. Wang, Y. Bang, and G. Kotliar, Phys. Rev. Lett. 67, 2733 (1991).
- [6] G. Kotliar and A. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986).
- [7] G. Kotliar, P. A. Lee, and N. Read, Physica (Amsterdam) 153-155C, 538 (1988).
- [8] C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. 62, 681 (1987).
- [9] M. Grilli, R. Raimondi, C. Castellani, C. Di Castro, and G. Kotliar, Phys. Rev. Lett. 67, 259 (1991).
- [10] At order  $1/N^2$  transitions are allowed involving the  $(1/N)$ -dressed fermion propagators, which have a spectral weight gap  $\Delta \mu$ ; see below in the text.
- [11] C. A. R. Sá de Melo and S. Doniach, Phys. Rev. B 41, 6633 (1990).
- [12] P. C. Pattnaik and D. M. Newns, Phys. Rev. B 41, 880 (1990),
- [13] M. Grilli, G. Kotliar, and A. Millis, Phys. Rev. B 42, 329 (1990).
- [14] M. Lavagna, Phys. Rev. B 41, 142 (1990).
- t15) Th. Jolicoeur and J. C. Le Guillou, Phys. Rev. B 44, 2404 (1991).