Chapter 1

DENSITY RESPONSE OF CUPRATES AND RENORMALIZATION OF BREATHING PHONONS

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Abstract
We analyse the dynamical density fluctuation spectra for cuprates starting from the $t-J$ model in a slave-boson $1/N$ representation. The results obtained are consistent with diagonalization studies and show novel low-energy structure on the energy scale $J + \delta t$ due to the correlated motion of holes in a RVB spin liquid. The low-energy response implies an anomalous renormalization of several phonon modes. Here we discuss the renormalization of the highest breathing phonons in La$_{2-x}$Sr$_x$CuO$_4$. ¹

1. INTRODUCTION

High-temperature superconductors are doped Mott-Hubbard insulators, therefore the low-energy density response is proportional to the doping, due to transitions in the lower Hubbard band. In one dimension the Hubbard physics is characterized by charge and spin separation, which implies that the density response is spinless fermion like, i.e., showing vanishing excitation energy at $4k_F$. Exact diagonalization studies[1, 2] for the $t$-$J$ model have revealed that the dynamical density response $N(q, \omega)$ for the 2D model relevant for the cuprates is very different from the 1D case. On the other hand these calculations show several features also unexpected from the point of view of weakly correlated fermion systems: (i) a strong suppression of low energy $2k_F$ scattering in the density response, (ii) a broad incoherent peak whose shape is rather insensitive to hole concentration and exchange interaction $J$, (iii) a very different form of $N(q, \omega)$ compared to the spin response function $S(q, \omega)$, which share common

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features in usual fermionic systems. Finite temperature diagonalization studies [3] show only weak temperature dependence for $T < 0.3t$ even at low energy. While considerable analytical work has been done to explain the spin response of the $t$-$J$ model only few authors analysed $N(q, \omega)$. Wang et al.[4] studied collective excitations in the density channel and found sharp peaks at large momenta corresponding to free bosons. Similar results were obtained by Gehlhoff and Zeyher[5] using the X-operator formalism. Lee et al[6] considered a model of bosons in a fluctuating gauge field and found a broad incoherent density fluctuation spectrum at finite temperature, due to the coupling of bosons to a quasistatic disordered gauge field.

Starting from a slave-boson representation we show that the essential features observed in the numerical studies can be obtained in the framework of the Fermi-liquid phase of the $t$-$J$ model at zero temperature[7]. Our main findings are: (i) at low momenta the main effect of strong correlations is to transfer spectral weight from particle-hole excitations into a pronounced collective mode. Because of the strong damping of this mode (linear in $q$) due to the coupling to the spinon particle-hole continuum, this collective excitation is qualitatively different from a sound mode. (ii) At large momenta we find a strict similarity of $N(q, \omega)$ with the spectral function of a single hole moving in a uniform RVB spinon background. In this regime $N(q, \omega)$ consists of a broad peak at high energy whose origin is the fast, incoherent motion of bare holes. (iii) The polaronic nature of dressed holes leads to the formation of a second peak at lower energy, which is more pronounced in $(\pi, 0)$ direction in agreement with diagonalization studies[1, 2].

The anomalous renormalization of certain phonon modes as observed in inelastic neutron scattering provides a sensitive test of the peculiarities of the low-energy density response. In this contribution we shall analyse the strong, doping-dependent renormalization of the highest breathing phonon modes which is a generic feature in the high-$T_c$ compounds.

2. SLAVE BOSON THEORY OF DENSITY RESPONSE

Following Kotliar and Liu[8] and Wang et al[4] we start from the $N$-component generalization of the slave-boson $t$-$J$ Hamiltonian, $H_{t,J} = H_t + H_J$, which is obtained by replacing the constrained electron creation operators $\tilde{c}_{i,\sigma}^+ = c_{i,\sigma}^+(1 - n_{i,-\sigma}) \rightarrow f_{i,\sigma}^+ b_i$:

$$H_t = -\frac{2t}{N} \sum_{<i,j>_{\sigma}} (f_{i\sigma}^+ h_j^+ h_i f_{j\sigma} + h.c.),$$

$$H_J = \frac{J}{N} \sum_{<i,j>_{\sigma\sigma'}} f_{i\sigma}^+ f_{i\sigma'} f_{j\sigma'}^+ f_{j\sigma} (1 - h_i^+ h_i)(1 - h_j^+ h_j),$$

(1.1)
where $f_{i\sigma}^+$ is a fermionic (spinon) operator, $\sigma = 1, \cdots, N$ is the fermionic flavor index, and $h_i$ denotes the bosonic holes. These operators obey standard commutation rules, yet the number of these auxiliary particles must obey the constraint $\sum \sigma f_{i\sigma}^+ f_{i\sigma} + h_i^+ h_i = N/2$. The original $t$-$J$ model is recovered for $N = 2$.

The slave boson parametrization provides a straightforward description of the strong suppression of density fluctuations of constrained electrons through the representation of the density response in terms of a dilute gas of bosons. A common treatment of model (1) is the density-phase representation (“radial” gauge[9]) of the bosonic operator $h_i = r_i \exp(i\theta_i)$ with the subsequent $1/N$-expansion around the Fermi-liquid saddle point. While this gauge is particularly useful to study the low energy and momentum properties, it is not very convenient for the study of the density response in the full $\omega$ and $q$ space. Formally the latter follows in the radial gauge from the fluctuations of $r_i^2$.

If one considers for example convolution type bubble diagrams, one realizes that their contribution to the static structure factor is correctly of order $1/N$,
but is not proportional to the density of holes $\delta$ as it should be. According to Arrigoni et al.[10] such unphysical results originate from a large negative pole contribution in the $\langle r_{-q} r_{q} \rangle$ Green's function of the real field $r$, which is hard to control by a perturbative treatment of phase fluctuations. We follow therefore Popov[11] using the density-phase treatment only for small momenta $q < q_0$, while keeping the original particle-hole representation of the density operator, $b^+ b$, at large momenta. More precisely $h_i = r_i \exp(i\theta_i) + b_i$, where $b_i = \sum_{|q| > q_0} h_q \exp(iqR_i)$. The cutoff $q_0$ is introduced dividing “slow” (collective) variables represented by $r$ and $\theta$ from “fast” (single-particle) degrees of freedom. As explained by Popov[11] this “mixed” gauge is particularly useful for finite temperature studies to control infrared divergences. We start formally with “mixed” gauge and keep only terms of order $\delta$ and $1/N$ in the bosonic self energies. In this approximation our zero temperature calculations become quite straightforward: The cutoff $q_0 < \delta$ actually does not enter in the results and we arrive finally at the Bogoliubov theory for a dilute gas of bosons moving in a fluctuating spinon background.

\begin{center}
\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Density fluctuation spectra $N(q, \omega)$ for $J/t = 0.4$ and $\delta = 0.15$ along $(\pi, 0)$ (top) and $(\pi, \pi)$ directions (bottom). Energy in units of $t$.}
\end{figure}
\end{center}
The Lagrangian corresponding to the model (1) is then given by (the summation over \( \sigma \) is implied)

\[
L = \sum_i \left( (f^+_i \frac{\partial}{\partial \tau} - \mu_f)f_{i\sigma} + (b^+_i \frac{\partial}{\partial \tau} - \mu_b)b_i \right) + H_t + H_J
\]

\[
+ \frac{i}{\sqrt{N}} \sum_i \lambda_i \left( f^+_i f_{i\sigma} + (r_i + b^+_i)(r_i + b_i) - \frac{N}{2} \right),
\]

\[
H_t = -\frac{2t}{N} \sum_{<ij>} f^+_i f_{j\sigma} (b^+_j b_i + r_i r_j + r_j b_i + b^+_j r_i) + h.c.
\]

Here the \( \lambda \) field is introduced to enforce the constraint, and \( \mu_f, \mu_b \) are fixed by the particle number equations \( \langle n_f \rangle = \frac{N}{2}(1 - \delta) \) and \( \langle r_i^2 + b_i^+ b_i \rangle = \frac{N}{2} \delta \), respectively. The uniform mean field solution \( r_i = r_0 \sqrt{N/2} \) leads in the large \( N \) limit to the renormalized narrow fermionic spectrum \( \xi_k = -\tilde{t}\gamma_k - \mu_f \), with \( \tilde{t} = J\chi + t\delta, \gamma_k = \frac{1}{2}(\cos k_x + \cos k_y) \), \( \chi = \sum_\sigma \langle f^+_i f_j \rangle / N \), and \( z = 4 \) the number of nearest neighbors. In the \( N = \infty \) limit \( \chi_\infty \approx 2/\pi^2 \) is given by that of free fermions, while for the original \( t-J \) model its value should be larger[12] due to Gutzwiller projection. In the following \( \chi = \frac{3}{2}\chi_\infty \) will be used. Distinct from the finite-temperature gauge-field theory of Nagaosa and Lee[13] the bond-order phase fluctuations acquire a characteristic energy scale in this approach[4], and the fermionic ("spinon") excitations can be identified with Fermi-liquid quasiparticles. The mean field spectrum of bosons is \( \omega_q = 2z\chi t(1 - \gamma_q) \). Thus the effective mass of holes \( m^*_h \propto 1/t \) is much smaller than that of the spinons.

Due to the diluteness of the bosonic subsystem, \( \delta \ll 1 \), the density correlation function \( \chi_{q,\omega} = \langle \delta n^h b^\dagger n^h \rangle_{q,\omega} \) is mainly given by the condensate induced part which is represented by the Green’s function \( \langle (b^+_q + b^-_q)(b^\dagger_q + b^\dagger_q) \rangle_{\omega} \) for \( q > q_0 \), and \( 2\langle r_q r^\dagger_q \rangle_{\omega} \) for \( q < q_0 \), respectively:

\[
\chi_{q,\omega} = \frac{N}{2} r_0^2 \left( \langle (b^+_q + b^-_q)(b^\dagger_q + b^\dagger_q) \rangle_{q > q_0} + 2\langle r_q r^\dagger_q \rangle_{q < q_0} \right).
\]

The \( 1/N \) self-energy corrections to these functions are calculated in a conventional way[9, 8] expanding \( r_i = (r_0 \sqrt{N} + (\delta r)_i)/\sqrt{2} \) and considering Gaussian fluctuations around the mean field solution. Neglecting all terms of order \( \delta/N \) and \( q_0^2/N \), only one relevant \( 1/N \) contribution remains which corresponds to the dressing of the slave-boson Green’s function by spinon particle-hole excitations. Within this approximation and at zero temperature no divergences occur at low momenta, thus one can take the limit \( q_0 \to 0 \). The final result for the dynamic structure factor (normalized by the hole density) is:

\[
N_{q,\omega} = \frac{2}{\pi} Im \left( (\omega_q a + S_{q,\omega}^{(1/N)} - \mu_b) / D_{q,\omega} \right),
\]
\[
D_{q,\omega} = (\omega_q + S_{q,\omega}^{(1/N)} - \mu_b)(\omega_q + S_{q,\omega}^{(1)} + S_{q,\omega}^{(1/N)} - \mu_b) - (\omega - A_{q,\omega}^{(1/N)})^2. \tag{1.7}
\]

The origin of the contribution

\[
S_{q,\omega}^{(1)} = z t r_0^2 \frac{(1 + \Pi_2)^2}{\Pi_1} - \Pi_{q,\omega}, \tag{1.8}
\]

\[
\Pi_m = z t \sum_k \frac{n(\xi_k) - n(\xi_{k+q})}{\xi_{k+q} - \xi_k - \omega - i0^+} (\gamma_k + \gamma_{k+q})^{m-1}, \tag{1.9}
\]

is the indirect interaction of bosons via the spinon band due to the hopping term (which gives \(\Pi_3\) in (4)) and due to the coupling to spinons via the constraint field \(\lambda\). The latter channel provides a repulsion between bosons, making \(S^{(1)}(\omega = 0)\) positive and therefore ensuring the stability of the uniform mean-field solution. The \(1/N\) self energies \(S^{(1/N)}\) and \(A^{(1/N)}\) are essentially a single boson property. They are given by the symmetric and antisymmetric combinations (with respect to \(\omega + i0^+ \rightarrow -\omega - i0^+\)) of the self energy

\[
\Sigma_{q,\omega}^{(1/N)} = \frac{1}{N} \sum_{|k|<k_F<|k'|} (z t \gamma_{k'-q})^2 G_{q+k-k'}^0(\omega + \xi_k - \xi_{k'}). \tag{1.10}
\]

Here \(G_{q}^0(\omega) = (\omega - \omega_q - \Sigma_{q,\omega}^{(1/N)} + \mu_b)^{-1}\) is the Green’s function for a single slave boson moving in a uniform RVB background. Although in the context of \(1/N\) theory the \(G_{q}^0\) function in (5) should be considered as a free propagator, we shall use here the selfconsistent polaron picture for a single hole[14]. This is crucial when comparing the theory for \(N = 2\) with diagonalization studies. Finally, the constants \(a\) and \(\mu_b\) in (3) are given by \((1 - t r_0^2 / \tilde{t})\) and \(S^{(1/N)}(\omega = q = 0)\), respectively. The parameter \(r_0^2\) in Eq.(1.8), which formally corresponds to the condensate fraction in our theory, is determined selfconsistently from \(r_0^2 = \frac{1}{2} \sum_{q \neq 0} \tilde{n}_q\). The momentum distribution \(\tilde{n}_q = \langle b^+_q b_q \rangle\) is calculated from the corresponding bosonic Green’s function for finite hole-density.

In the small \(\omega, q\) limit \(N(q, \omega)\) (3) is mainly controlled by the interaction of bosons represented by the \(S^{(1)}\) term (\(\propto r_0^2\)), while the internal polaron structure of the boson determined by \(S^{(1/N)}\) is less important. \(N(q, \omega)\) consists of a weak spinon particle-hole continuum with cutoff \(\propto v_F q\), and a very pronounced linear collective mode which nearly exhausts the sum rule. The velocity of this mode is always somewhat smaller than the spinon Fermi velocity, \(v_s \lesssim v_F \approx z \tilde{t}\), which implies a strong damping \(\propto \omega\) (or \(q\)) of this mode (Fig.1.2).

The density response \(N(q, \omega)\) at large momenta, \(q > \delta\), which we can compare with diagonalization results, is dominated by the properties of a single boson selfenergy \(S^{(1/N)}\). The calculated density response of the \(t-J\) model has three characteristic features on different energy scales: (i) The main spectral weight of the excitations at large momenta is located in an energy region of
order of several $t$. This high energy peak is very broad and incoherent as a result of the strong coupling of bosons to low-energy spin excitations. The position of this peak and its shape are rather insensitive to the ratio $J/t \lesssim 1$ in agreement with conclusions of [1, 2]. This is simply due to the fact that the high-energy properties of the $t$-$J$ model are controlled by $t$. (ii) The theory predicts also a second peak at lower energy (Fig. 1.2) which is more pronounced in the direction $(\pi, 0)$, while its weight is strongly suppressed for $q$ near $(\pi, \pi)$. The origin of this excitation is due to the formation of a polaron-like band of dressed bosons. The relative weight of this contribution increases with $J$ as a result of the increasing spinon bandwidth. (iii) In addition there is the spinon particle-hole continuum which is generated by $S^{(1)}$ with relatively small weight ($\propto \delta^2$). At $(\pi, 0)$ the high energy cutoff of the spinon continuum is at $z(\chi J + \delta t)$ (Fig. 1.2), while the polaron peak is at about $(\chi J + \delta t)$.

We note that the polaron peak in $N(q, \omega)$ is in the same energy range as the high energy phonons in cuprates.

3. **RENORMALIZATION OF BREATHING PHONONS**

Inelastic neutron scattering experiments on high-$T_c$ superconductors have shown that in particular the highest energy longitudinal optic phonons near $(\pi, 0)$ soften and broaden strongly as holes are doped into the insulating parent compound. Whereas the corresponding breathing mode at $(\pi, \pi)$ shows much smaller softening and no anomalous broadening. This effect seems to be generic for cuprates and detailed neutron scattering studies have been reported for La$_{2-x}$Sr$_x$CuO$_4$ [16, 17, 18] and YBa$_2$Cu$_3$O$_{6+x}$ [18].

![Figure 1.3](image-url) Atomic displacements of oxygen ions (a) for the $q = (\pi, \pi)$ breathing phonon and (b) for the $(\pi, 0)$ half-breathing mode.

The renormalization of these phonons can be calculated in the framework of the $t$-$J$ model, since these modes modulate the energy of a hole in a Zhang-Rice singlet state, and therefore couple directly to the density of doped holes. Expanding the Zhang-Rice energy $E_{ZR} = 8 \frac{\epsilon^2}{2\Delta}$ with respect to the oxygen displacements $u^i_x, v^i_y$ (see Fig.1.3) of the four O-neighbors of the Cu-hole.
yields the linear electron-phonon coupling

\[ H_{e-ph} = g \sum \left( u^i_x - u^i_{-x} + v^i_y - v^i_{-y} \right) \hbar \hat{h}_i. \]  

(1.11)

We assume that the resonance integral obeys the Harrison relation \( t_{pd} \propto r_0^{-7/2} \), where \( r_0 \) is the Cu-O distance, and obtain \( g = 7E_{ZR}/4r_0 \), i.e., \( g \approx 4\text{eV/Å} \). The lattice part of the Hamiltonian is determined by the force constant \( K \approx 25\text{eV/Å}^2 \) for the longitudinal O-motion. Due to the structure of \( H_{e-ph} \) the breathing modes couple directly to \( \chi_{q,\omega} \).

We have studied the renormalization of the phonon Green’s functions along \((\pi, 0)\) and \((\pi, \pi)\) directions

\[ D^{ph}_{q,\omega} = \frac{\omega_{q,0}}{\omega^2 - \omega_{q,0}^2 (1 - \alpha_q \chi_{q,\omega})}. \]  

(1.12)

where \( \omega_{q,0} \) is the bare phonon frequency, i.e. measured in the undoped parent compound, and \( \alpha_q = \frac{4g^2}{K}(\sin^2 q_x/2 + \sin^2 q_y/2) \). Based on the parameters of the pd-model we estimate for the dimensionless coupling constant \( \xi = g^2/ztK \sim 0.3 - 0.5 \).

Figure 1.4 shows the strong renormalization of the \((\pi, 0)\) half-breathing mode for La\(_{1.85}\)Sr\(_{0.15}\)CuO\(_4\) with a twice as large shift as for the \((\pi, \pi)\) breathing phonon. The large damping of the \((\pi, 0)\) phonon results from the hybridization with the large polaron peak in \( N(q, \omega) \) at this momentum\([19]\) and is consistent with the experimental data\([17]\). The phonon energies of the undoped parent compound \( \omega_{q,0} = 80(90) \text{meV} \) for \((\pi, 0)\) and \((\pi, \pi)\), respectively, are taken from Ref.\([16]\). The strong doping dependence of this effect is shown in Fig.1.5.
Figure 1.5 Doping dependence of low-energy density response at $(\pi,0)$ (solid lines). As a consequence of the scaling of the polaron structure $\propto (\chi J + \delta t)$ there is a strong change in the renormalization and damping of the $(\pi,0)$ half-breathing phonon, which is at $\omega_0 = 0.2t$ in the undoped system.

Figure 1.6 Fano structure in fully renormalized $N(q_\perp,\omega)$ (solid line) due to the coupling to the $(\pi,0)$ phonon. The bare $N(q_\perp,\omega)$ and the phonon spectral function are indicated by dashed and dotted lines, respectively (parameters as in previous figure).

Finally we have studied the changes of the density response $\chi_{q_\perp,\omega}$ due to the additional coupling to the breathing phonon modes. This effect is displayed in Fig.1.6, which shows a rather strong Fano structure in $N(q_\perp,\omega)$ for $q_\perp = (\pi,0)$.
4. SUMMARY

We have outlined a 1/N slave-boson theory for the density response of the $t$-$J$ model, which explains the data obtained by exact diagonalization. We demonstrated that the predicted low energy polaron structure in the density response, which is particularly pronounced along $(\pi, 0)$, explains the anomalous doping induced line width and shift of the longitudinal planar $(\pi, 0)$ phonon. The energy of the polaron peak is determined by the spinon energy scale, therefore we predict a nontrivial doping dependence for the phonon renormalization. In that respect further neutron scattering studies of the doping dependence of phonons would provide a sensitive test for the low energy density response as well as for the spin structure in the different doping regimes.

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