Density response of the t-J model and renormalization of breathing and half-breathing phonon modes: A slave-fermion calculation.

P. Horsch\textsuperscript{a} \textsuperscript{*}, G. Khaliullin \textsuperscript{a} \textsuperscript{†} and V. Oudovenko\textsuperscript{a} \textsuperscript{b} \\
\textsuperscript{a}Max-Planck-Institut für Festkörperforschung, Heisenbergstr.1, D-70569 Stuttgart, Germany \\
\textsuperscript{b}Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08855-0849, USA.

The density fluctuation spectrum $N(k, \omega)$ is calculated for the $t$-$J$ model in the low-doping regime using a slave-fermion method for the constrained fermions. The obtained results for $N(k, \omega)$ are in good agreement with diagonalization results. The density response is characterized by incoherent, momentum dependent spectral functions reaching up to energies $\sim 8t$ and a low-energy structure at energy $\sim J$ due to transitions in the quasiparticle band. $N(k, \omega)$ is shown to lead to a strong renormalization of planar bond-streching and breathing phonon modes with a large phonon linewidth at intermediate momenta caused by the low-energy response. Our results are consistent with recent neutron scattering data, showing the peculiar behavior of these modes.

1. INTRODUCTION

The density response of doped Mott-Hubbard insulators like the high-$T_c$ superconductors is expected to differ strongly from that of weakly correlated metals. Due to the Mott-Hubbard gap the low-energy density response in the doped systems is proportional to the number of holes and not proportional to the electron concentration. Experimentally the peculiarities of the density response in high-temperature superconductors show up (i) in the anomalous mid-infrared absorption in the frequency dependent conductivity, (ii) in the renormalization and strong increase of linewidth of certain phonon modes upon doping, and (iii) the charge instability leading to the stripe phase. While static stripes in cuprates are found only in the LTT-phase it is expected that dynamic stripe like correlations exist also in the other cuprate materials.

Exact diagonalization studies\textsuperscript{4} of the dynamical density response $N(k, \omega)$ at large momentum transfer have revealed several features unexpected from the point of view of weakly corre-

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\textsuperscript{†}Permanent address: Kazan Physicotechnical Institute, 420029 Kazan, Russia.
the incoherent structure at high energy and the appearance of a low energy peak associated with the coherent polaron motion. The characteristic energy scale of the low-energy polaron peak is \( \tilde{J} \approx \chi J + \delta t \), where \( \chi \) is the uniform RVB-order parameter relevant for the overdoped regime studied in that work. In addition on the same energy scale \( J \) there is a smooth Fermi-liquid like particle-hole continuum, which reflects the Fermi surface, with total weight \( \sim \delta^2 \). Further studies \cite{32,33} analysed the incoherent part of \( N(k,\omega) \) yet did not obtain the low-energy structure.

The aim of the present work is to investigate \( N(q,\omega) \) in the low-doping regime. We confine our study to the AF long-range ordered phase which implies a different Fermi surface and collective spin wave excitations. There are two key questions: (i) what theory is needed to produce spectra at high energy similar to the large doping notes the number of nearest neighbours. This Hamiltonian has the structure of a polaron problem where spinless fermions (holes) are coupled to collective spin excitations\cite{32}.

The density fluctuation spectrum

\[
|n_k(n_{-k})\rangle = -i \int_0^{\infty} e^{i\omega t} \langle [n_k(t), n_k(0)] \rangle dt.
\]

where \( \gamma_k = 0.5(\cos k_x + \cos k_y) \) while \( z = 4 \) denotes the number of nearest neighbours. This Hamiltonian has the structure of a polaron problem where spinless fermions (holes) are coupled to collective spin excitations\cite{32}.

The density fluctuation spectrum

\[
N(k,\omega) = -\frac{1}{\pi} \text{Im}\chi(k,\omega),
\]

where \( \chi(k,\omega) = \langle \langle n_k | n_{-k} \rangle \rangle_\omega \) and \( n_k = \sum_{i,\sigma} \tilde{c}_{i,\sigma} \hat{c}_{i,\sigma} e^{i\mathbf{k} \mathbf{R}_i} \), is defined via the density correlation function

\[
\langle \langle n_k | n_{-k} \rangle \rangle_\omega = -i \int_0^{\infty} e^{i\omega t} \langle [n_k(t), n_k(0)] \rangle dt.
\]

Calculation of \( \chi(k,\omega) \) by expansion in a small parameter usually fails due to the singular character of this quantity for small \( \omega \). This problem can be resolved by rewriting \( \chi(k,\omega) \) in terms of the static susceptibility \( \chi_0(k) \) and a selfenergy \( M(k,\omega) \)\cite{32}:

\[
\chi(k,\omega) = \chi_0(k) \frac{M(k,\omega)}{\omega + M(k,\omega)}.
\]

The evaluation of the memory function \( M(k,\omega) \) by expanding in a small parameter (here the coupling constant \( t \)) gives correct results for \( \chi(k,\omega) \) valid for all frequencies. From this expression it is obvious that an evaluation of \( M \) to low order in the coupling constant \( t \) implies for the charge susceptibility \( \chi \) a partial resummation up to infinite order. We shall find that this form is crucial for the proper description of the charge excitations at high energy, which are of collective nature and induced by the denominator \( \omega + M \) which can become small. In second order approximation in \( t \) we can write:

\[
\omega \chi(k,\omega) \approx \chi_0(k) M(k,\omega),
\]
which moves to higher energy as variation of \( N \)ation regime by the \( N \) slave-fermion calculation are displayed in Fig. 2. The density fluctuation spectra obtained by the \( N \) function is determined from the integral relation

\[
\int \chi(k, \omega) d\omega = \frac{\omega_0}{\omega^2 - \omega_0^2 (1 + 4\xi \sin^2 \frac{\omega}{2} \chi(\omega))};
\]  

(9)

and the fact that the static charge structure factor \( N(k) \) is well approximated in the strong correlation regime by the \( N(k) \) for spinless fermions[1].

The density fluctuation spectra obtained by the slave-fermion calculation are displayed in Fig. 2. \( N(k, \omega) \) is characterized by a broad continuum which moves to higher energy as \( k \) increases. At \((\pi, \pi)\) the spectrum peaks at \( \omega \sim 6t \), i.e., the variation of \( N(k, \omega) \) with \( k \) and the energy scale are fully consistent with the diagonalization results for small systems[1]. Low energy structures on scale \( J \), due to quasiparticle scattering between hole pockets, appear at small and intermediate momentum transfers and vanish at the zone boundary. The pronounced low-energy structure at large momentum transfer in \((\pi, 0)\) direction found in the spin liquid regime[2] is absent.

3. BOND-STRETCHING PHONONS

The high energy planar breathing and bond-stretching oxygen modes in \((\pi, \pi)\) and \((\pi, 0)\) direction, respectively, show the strongest doping dependence from all phonon modes[12] which appears to be a generic feature of cuprates. Inelastic neutron scattering studies of the LO mode in \((\pi, 0)\) direction in \( La_{2-x}Sr_xCuO_4 \) \((x = 0.15)[12,13]\) reveal a \( \sim 10\% \) renormalization near \((\pi, 0)\) as compared to the undoped system, while there is no significant renormalization at the \( \Gamma \)-point. Surprisingly the linewidth assumes a maximum at intermediate \( k \)[13].

The coupling of these phonon modes to density fluctuations is described by

\[
H_{ev-ph} = g \sum_i f_i^+ f_i (-u_{i_x} - u_{i_x} + u_{i_y} - u_{i_y}),
\]

(10)

where \( u_{i_x}, u_{i_y} \) are the displacements of the four oxygen neighbors of the hole, \( g \) is the electron-phonon coupling constant. This coupling originates from the change of the Zhang-Rice singlet energy by breathing and bond-stretching modes.

The phonon Green’s function has the following form for \( k = (k, 0) \)

\[
D(k, \omega) = \frac{\omega_0}{\omega^2 - \omega_0^2 (1 + 4\xi \sin^2 \frac{\omega}{2} \chi(\omega))};
\]  

(11)

here we assume a \( k \)-independent bare phonon frequency \( \omega_0 = 0.3 \) and a normalized coupling constant \( \xi = g^2/Kt = 0.25[14] \). For momenta \( k = (k, k) \) the constant 4\( \xi \) in Eq.(11) should be replaced by 8\( \xi \). The phonon spectral function \( B(k, \omega) = -\frac{1}{\pi} ImD(k, \omega) \) is displayed in Fig. 3. Figure 3 shows a large increase of the renormalization of \( \omega_k \) with increasing \( k \), which is similar for the two directions, with rather abrupt changes in \( \omega_k \) at intermediate \( k \). The damping appears to
Figure 3. Phonon spectral function at $\delta = 0.1$ for different momenta along $(k,0)$ and $(k,k)$ directions, where $k = \pi/8$ for the top panel and increases in steps of $\pi/8$ in downward direction. Here $\omega_0 = 0.3$; arrows indicate $\omega_k$ along $(k,k)$.

be largest not at the zone-boundary but at intermediate $k$. We note that earlier calculations for larger doping, $\delta = 0.15 - 0.25$, show a significantly larger energy change at $(\pi,0)$ than at $(\pi,\pi)$, which was due to the pronounced low energy polaron related structure in $N(k,\omega)$ near $(\pi,0)$ in the spin disordered state. The low-energy structure of $N(k,\omega)$ in the AF ordered system considered here is markedly different, and suggests nontrivial changes for the phonon renormalization as function of doping.

Hence we conclude by stressing that phonon modes, and in particular those discussed here, provide a sensitive probe for the anomalous low-energy charge response of doped Mott insulators. Furthermore it is expected that measurements at different doping concentrations will reveal significant changes of phonon energies and damping due to the changes in the spin response and in the topology of the Fermi surface, which in turn strongly affect the charge response at low energy.

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