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MAGNETIC EXCITATIONS IN THE t - J MODEL: APPLICATION TO NEUTRON AND NMR EXPERIMENTS IN HIGH T_C MATERIALS.

D.R. Grempel and M. Lavagna[§]

Centre d'Etudes Nucléaires de Grenoble, DRFMC-MDN, 85X, F-38041 Grenoble Cedex, France

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We study the dynamic magnetic susceptibility of the two-dimensional t - J model using a mean-field bond slave boson approach coupled to self-consistent spin-fluctuation theory. The spectrum of the magnetic fluctuation exhibits interesting temperature dependence that is a consequence of lattice effects. We apply our results to the interpretation of recent neutron and NMR measurements on $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ systems. Our predictions for the temperature dependence of the nuclear spin relaxation rate are in good agreement with experiment.

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One of the more interesting experimental manifestations of unconventional behavior in the normal state properties of the high T_C superconductors is the temperature dependence of the spectrum of nearly antiferromagnetic fluctuations in the cuprate superconductors^{1,2,3,4}. NMR investigations show that, in $\text{La}_{2-x}\text{Sr}_x\text{Cu}_2\text{O}_4$ ¹ and $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ ², the nuclear spin lattice relaxation time on the Cu site multiplied by the temperature, T_1T , depends upon T , first decreasing and then increasing, with a minimum at a temperature T_m larger than T_C . This behavior is in contradiction with Korringa's law that states that, in normal metals, T_1T is constant. These experimental results suggest that, near the antiferromagnetic Bragg point, the low energy end of the spin fluctuation spectrum depends intrinsically upon the temperature and is strongly suppressed below T_m . This has been confirmed by direct determination of the imaginary part of the dynamic susceptibility by neutron scattering⁴ in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. Whereas in normal metals the low-frequency magnetic spectral density is linear in ω and T independent, the magnetic excitation spectrum of the systems discussed here has a gap at low temperatures in the vicinity of the antiferromagnetic point. For temperatures of the order of the gap, the response is linear in frequency, with a T dependent coefficient.

A phenomenological model⁵ for the dynamic magnetic susceptibility has been proposed in order to explain the NMR data. In this model, T_1T depends on temperature because the antiferromagnetic correlation length, ξ , does. Although some of the NMR results may be explained in this way, the proposed form of the correlation length disagrees with the neutron linewidths that are temperature independent.

In this paper we interpret the neutron and NMR experiments in terms of a nested-Fermi liquid approach^{6,7} that we derive from the microscopic t - J description of the

CuO_2 layers of the cuprates⁸. Our model accounts for the observed temperature and frequency dependence of the spin fluctuation spectrum and predicts a T -independent correlation length of the right order of magnitude.

The magnetic properties of the t - J model have been discussed at the level of the RPA by Tanamoto Kuboki and Fukuyama (hereafter, TKF) in a paper⁹ published while this work was under completion. There exist important differences between the results of TKF and ours. In particular, we found it essential to include the fluctuation corrections to the RPA susceptibility in the calculation.

The Hamiltonian of the t - J model is :

$$H = -t \sum_{\langle i,j \rangle} \left\{ f_{i\sigma}^\dagger f_{j\sigma} + \text{h.c.} \right\} + J \left(S_i S_j - \frac{1}{4} n_i n_j \right) \quad (1)$$

The electron operators $f_{i\sigma}$ act on a Hilbert space with configurations containing doubly occupied sites excluded. Therefore, they obey commutation rules that are neither those of fermions nor those of bosons. By the transformation $f_{i\sigma}^\dagger \rightarrow c_{i\sigma}^\dagger e_i$, the constrained electron operator is expressed in terms of two new operators, $c_{i\sigma}$ and e_i , representing "spinons" and "holons", that obey standard Fermi and Bose statistics, respectively. Doubly occupied sites are excluded by the condition that the total number of particles, bosons plus fermions, be one on every site.

The starting point to describe the normal state properties of the cuprates is the fluxless state of Nagaosa and Lee¹⁰. In this mean-field like description in which holons are not condensed, fermions and bosons are decoupled and described by the effective Hamiltonian :

$$H_0 = - \sum_{ij} t_{ij} B c_i^\dagger c_j - \sum_{ij,\sigma} t_{ij} F^\sigma c_{i\sigma}^\dagger c_{j\sigma} + \lambda \sum_i \left(c_i^\dagger c_i + \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} - 1 \right) - \mu \left(\sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - N(1 - \delta) \right) \quad (2)$$

where d is the number of holes relative to a half-filled band, and λ is a Lagrange multiplier that enforces the condition of no double occupancy on the average. The parameters

$B = \sum_\sigma \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$ and $F^\sigma = \langle c_i^\dagger c_j \rangle + \frac{J}{2t} \langle c_{i-\sigma}^\dagger c_{j-\sigma} \rangle$ are self-consistently determined renormalisation factors for the boson and fermion hopping amplitudes between neighboring sites i , and j ¹¹. As shown in Fig.1, the bandwidth, W_F , and chemical potential, μ_F , of the fermions vary strongly with hole concentration. An important point is that the energy scale, W_F , is vastly reduced with respect to its bare value, $8t$. For δ in the range 0.08-0.14 the reduction factor is, roughly, one order of magnitude. There is also temperature dependence in the bandwidth but, in the temperature range of interest in this paper, it is weak and may as well be neglected. The results shown in Fig. 1 are in disagreement with the ones reported by TFK, whose energy scale F is, roughly, a factor of two higher than ours. This difference, due to a problem of double counting, has since been corrected by TFK¹².

To this order, the dynamic spin susceptibility of the system is that of free fermions with the renormalised band structure $E_{\mathbf{k}} = -2\tilde{t}(\cos k_x + \cos k_y)$, $\tilde{t} = tF$. As already pointed out^{6,7,9,13}, at the zone corner, $\mathbf{Q}_0 = (\pi, \pi)$,

$$\chi''_0(\mathbf{Q}_0, \omega) = \frac{\pi}{2} \left[n_F\left(\frac{\omega}{2}\right) - n_F\left(\frac{\omega}{2}\right) \right] \rho\left(\frac{\omega}{2}\right)$$

where $\rho(E)$ is the two dimensional density of states, and n_F is the Fermi function. At $T=0$, the excitation spectrum at $\mathbf{Q}_0$ exhibits a gap of size $E_G = 2|\mu|$ ^{6,7,9,13}. The origin of this gap lies in the nesting property of the band structure, i.e., the fact that $\mathbf{Q}_0$ maps pairs of constant energy surfaces of opposite energy, $E_{\mathbf{k}} = E$ and $E_{\mathbf{k}+\mathbf{Q}_0} = -E$, into one another. Since the smallest energy difference for a single particle

Figure 1: Effective bandwidth (full lines, left scale) and chemical potential (dashed lines, right scale) for the fermions as a function of the temperature and hole density. $t/J = 4$.

transition occurs when the initial state is on the Fermi surface, the spectrum starts at $\omega = 2\mu$.

For $\mathbf{q} \neq 0$, along the diagonals of the Brillouin zone, $\chi''_0(\mathbf{Q}_0 + \mathbf{q}, \omega)$ can be evaluated exactly at $T=0$, a fact that, to our knowledge, has not been noticed before. We find:

$$\chi''_0(\mathbf{Q}_0 + \mathbf{q}_\pm, \omega) = \frac{1}{8\pi \tilde{t} \cos \frac{q_\pm}{4}} \begin{cases} [2K(k) - F(\phi_+, k) - F(\phi_-, k)], & \omega > 2|\mu| \\ [F(\phi_-, k) - F(\phi_+, k)], & \omega < 2|\mu| \end{cases} \quad (3)$$

where $q_\pm = q_x \pm q_y$, $k^2 = 1 - [\omega(8\tilde{t} \cos(q_\pm/4))]^2$, and $K(k)$, and $F(\phi, k)$ denote the complete and incomplete elliptic integrals of the first kind, respectively. The argument is $\phi_\pm = \cos^{-1}[(|\mu| \pm \omega/2) / (4\tilde{t} k \sin(q_\pm/4))]$.

The q -dependent gap, $\omega_G = 2[|\mu| - 4\tilde{t} \sin(q_\pm/4)]$ vanishes at $|q_\pm^*| = |q^*| = 4 \sin^{-1}(|\mu|/4\tilde{t})$. These points are such that $\mathbf{Q}_0 + \mathbf{q}_\pm$ span the Fermi surface. Moreover, it is at these points that the static susceptibility has its maxima¹⁴. Fig. 2 shows $\chi''_0(\mathbf{Q}_0 + \mathbf{q}, \omega)$ at $T=0$ for several values of $\mathbf{q}$ along the (1,1) direction, for a fixed value of the doping, $\delta=0.12$. Along this direction, the dynamic susceptibility at $\omega=\omega_G$ is essentially independent of q for $q \neq 0$ and equal to half the value at $q=0$. A simple geometrical construction shows that the reason for this is that, when $q \neq 0$ the contribution to $\chi''(\omega_G)$ of half of the states on the Fermi surface is the same as before.

At finite temperature, analytic results may be obtained for $q \ll \pi$, $\omega \ll W_F$.

If the frequency lies in the gap, the composition law $\chi''_0(\mathbf{Q}_0 + \mathbf{q}, \omega) = \chi''_0(\mathbf{Q}_0 + \mathbf{q}_+, \omega) + \chi''_0(\mathbf{Q}_0 + \mathbf{q}_-, \omega)$ holds, with $\mathbf{q} = \mathbf{q}_+ + \mathbf{q}_-$, and:

Figure 2: Imaginary part of the zero temperature non-interacting susceptibility as a function of frequency for wavevectors in the vicinity of the antiferromagnetic Bragg point. The inset shows the region in the q - ω plane where $\chi''_0 \neq 0$.

$$\chi''_0(\mathbf{Q} + \mathbf{q}_\pm, \omega) = \frac{1}{2\pi W_F} \times \quad (4)$$

$$\int_{-\pi}^{\pi} \frac{du}{\sqrt{\sin^2 u - (\omega/W_F)^2}} \frac{\sinh \beta(\omega/2 + i q_\pm \sin u)}{\cosh \beta \mu + \cosh \beta(\omega/2 + i q_\pm \sin u)}$$

In the limit $T \rightarrow 0$ this equation reduces to the small q and ω form of the exact result (3), as it should. It disagrees with the expression given by Maleev⁷, which fails to reproduce the correct low temperature limit.

At finite T there is spectral weight in the gap region. For small q and ω , and low temperature, $T \ll |\mu|$, χ'' is exponentially small, $\chi'' \sim \omega \ln(W_F/\omega) / T \exp(-|\mu|/T)$. In the opposite regime, $T \gg |\mu|$, we find $\chi'' \sim \omega \ln(W_F/\omega) / T$ for $\omega \ll T$, $\chi'' \sim \text{constant}$ for $\omega \gg T$. This T and ω -dependence is reminiscent of the one in the marginal Fermi-liquid model¹⁵ except for of a logarithmic correction coming from the frequency dependence of the 2-D density of states, a lattice effect. However, while the marginal Fermi liquid hypothesis postulates that this behavior should persist throughout the Brillouin zone, here, it arises in the vicinity of the zone corner.

Residual interactions, neglected in the mean-field approach, introduce corrections to the non-interacting susceptibility discussed so far. The most important ones come from the exchange term in the Hamiltonian. In the lowest order, the exchange corrected susceptibility is given by the random phase approximation:

$$\chi_{\text{RPA}}(\mathbf{Q}_0 + \mathbf{q}, \omega) = \frac{\chi_0(\mathbf{Q}_0 + \mathbf{q}, \omega)}{1 - J(\cos q_x + \cos q_y) \chi_0(\mathbf{Q}_0 + \mathbf{q}, \omega)} \quad (5)$$

This expression only makes sense if the system is far from the magnetic instability signaled by a zero in the denominator of (5) at $\omega = 0$. Using the experimental value of the exchange constant, $J \sim 1500$ K, and the commonly accepted ratio $t/J = 4$ to determine the renormalised bandwidth and chemical potential, and known expressions for the static susceptibility¹⁴, we found that the RPA ground-state instability takes place at an unrealistically high value of the hole concentration, $\delta_c > 0.15$. Due to their error in the energy scale, TKF⁹ find a much lower instability threshold which leads them to applying the RPA expression in a region of concentrations where it is no longer valid.

In order to stabilise the paramagnetic phase and improve the estimate of δ_c , it is necessary to include the effects of the quantum fluctuations that are left out in the RPA calculation. We have done this by using a self-consistent spin-fluctuation renormalisation scheme in which the lowest order fluctuation corrections are self-consistently incorporated into the static part of the susceptibility^{16,17}. These corrections reduce the susceptibility with respect to its non-interacting value pushing the system away from the RPA instability. In practice, all this amounts to is the substitution

$\chi_0(\mathbf{q}^* + \mathbf{Q}_0, 0) \rightarrow \chi_0(\mathbf{q}^* + \mathbf{Q}_0, 0) - \Lambda$ in Eq.(5), where Λ , the

fluctuation correction to the peak value of the static susceptibility, is given by:

$$\Lambda = 3 \Gamma_4 J \int_0^\infty \frac{d\omega}{\pi} \coth \beta \frac{\omega}{2} \times \quad (6)$$

$$\frac{1}{N} \sum_{\mathbf{q}} \text{Im} \left\{ \frac{1}{1 - 2J \gamma(\mathbf{q}) [\chi_0(\mathbf{Q}_0 + \mathbf{q}, \omega) - \Lambda]} \right\}$$

and Γ_4 is the effective mode-mode coupling coefficient. This vertex may, in principle, be calculated perturbatively. However, since Γ_4 is itself renormalised by the fluctuations that we are trying to determine, a reliable calculation of this quantity is not feasible. It turns out, however, that, if δ is not too high, the density dependence of the vertex may be determined analytically up to an amplitude that is left out as a single adjustable phenomenological parameter. Indeed, one may show by careful analysis of the diagrammatic perturbation expansion for Γ_4 that, to leading order in the density, this quantity has the following scaling form:

$$\Gamma_4 = \frac{1}{W^3} \left(\frac{2W}{\mu} \right)^2 \tilde{\Gamma} \left(\frac{\mu}{W} \right) \quad (7)$$

where $\tilde{\Gamma}$ is a dimensionless reduced vertex. Since, for low to moderate δ , the ratio μ/W is very small (cf. Fig.1), it seems reasonable to approximate the density dependence of Γ_4 by the one of the prefactor, replacing the full reduced vertex by its $\delta \rightarrow 0$ value, $\tilde{\Gamma}(0)$. This parameter may be fixed by the requirement that the magnetic instability takes place at the experimentally known critical hole concentration.

The first step in the calculation of the renormalised susceptibility is the determination of the T and δ -dependence of Λ by numerical solution of (6). We have chosen $\tilde{\Gamma}(0) = 1.6$ which leads to $\delta_c = 0.02$, the experimental value. There are two distinct contributions to Λ that come from zero-point and thermal fluctuations, respectively. It turns out that the contribution from the latter is of order $(T/T_0)^2$, where T_0 is a very large temperature scale¹⁶. Thus, for all practical purposes, Λ is dominated by the zero-point fluctuations and is essentially temperature independent. The same argument holds for the correlation length which is closely related to Λ . For δ in the range 8 to 14%, ξ varies between 4.5 and 1.35 lattice spacings, values that are comparable to the experimental ones⁴.

The imaginary part of the renormalised dynamic susceptibility at the antiferromagnetic point is shown in Fig. 3. There is a gap in the spectrum at zero temperature that is gradually filled with states as T increases. At high temperatures, χ'' is roughly linear in ω at low frequency, in agreement with the experimental observations. The size of gap is of the right order of magnitude. Detailed comparison with neutron experiments would require the discussion of resolution effects. Indeed, for the hole densities in the range

Figure 3 : Imaginary part of the renormalised dynamical susceptibility at the antiferromagnetic point as a function of frequency for several temperatures.

considered in this paper, q^* is small (only a few hundredths in reciprocal lattice units) and comparable to the experimental resolution. Consideration of Fig. 2, however, makes it clear that, albeit washed out, the gap structure should survive finite resolution effects.

The slope of $\chi''(\mathbf{Q}_0, \omega)$ at the origin is closely related to the nuclear spin relaxation rate on the Cu site. This quantity is exponentially small at low temperatures, reflecting the opening of the gap, goes through a maximum for $T \approx E_G$ and decreases as $1/T$ at high temperatures. The latter behaviour, first discussed¹⁵ in connection with the marginal Fermi liquid hypothesis arises here as a consequence of the nested structure of the Fermi surface. In order to confront quantitatively the present theory with experiment, we have calculated $T_1 T$ on the Cu site as a function of temperature, for several values of δ . The results are shown in Fig. 4 together with NMR data for $\text{YBa}_2\text{Cu}_3\text{O}_{6.51}$ ¹⁸. There is good agreement between the experimental results and the theoretical curve for $\delta = 0.12$.

To conclude, we have shown that the t - J model in the mean-field approach provides an adequate basis for the un-

Figure 4: $T_1 T$ as a function of temperature and density. Data points are experimental results for the Cu nuclear spin relaxation rate in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, $x = 0.5$.

derstanding of the experimental properties of spin-fluctuations in the cuprate superconductors provided spin fluctuation effects are properly taken into account. We find that the magnetic correlation length is temperature independent, in agreement with experiment, but in contradiction with other theories. The predicted low frequency properties of the magnetic fluctuation spectrum agree with neutron scattering results and compare very well with NMR measurements of $T_1 T$.

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