Effect of antiferromagnetic instability on two-dimensional electrons in the antiadiabatic limit

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Abstract

Electrons at the van Hove point of a two-dimensional band model are studied in the weak-coupling limit as the condensation of the AF mode is approached from the paramagnetic phase. The interaction with fluctuations is treated in the one–loop approximation. It is found that for underdamped fluctuations the quasiparticle peak at the Fermi level is preserved down to the transition point, *i.e.* the van Hove singularity is not suppressed by the pseudogap, in contrast to what was found previously in the adiabatic approximation. However, the strength of the peak vanishes quadratically with the frequency of the AF mode when the latter is small.

1 Introduction

The influence of antiferromagnetic (AF) correlations on the electronic properties of high T_c materials has been the object of intense study [1, 2, 3, 4, 5]. The AF correlations may be studied either in the limit of strong Coulomb repulsion on the Cu sites ('large U_d' limit), or in the weak-coupling limit ('small U_d'). In the first case, the system orders itself antiferromagnetically after a Mott charge-transfer gap has opened first [6], while in the other AF order is described by an SDW instability [5, 7]. In this work we adopt the latter language, as in [5]. We note that similar results are obtained [8] in the slave-boson treatment [9] of the strongly correlated case.

It has recently been observed that the optical phonon mode in the CuO_2 lattice, associated with the lifting of the degeneracy of the O_2 and O_3 oxygen sites, is in strong competition with the superconducting transition. This is most obvious when it condenses [10], but an anomaly is observed in the corresponding Raman mode as well [11]. The large susceptibility of the intracell O–O charge transfer to the oxygen energy splitting has been associated in previous work [12, 13, 14] with the Fermi energy being on the logarithmic van Hove (vH) singularity of the square lattice. Of course, this can also affect the superconducting transition itself.

In order to test the validity of this point of view, it is important to calculate the effects of an impending AF transition on the electrons at the vH singularity, what has not been singled out for attention before. As the AF mode softens, a pseudogap appears in the density of states at the Fermi energy, as a precursor of the AF gap. The question is, will it suppress the vH singularity?

Note that the usual argument in favor of a pseudogap does not apply. It is based on the adiabatic approximation, in effect claiming that fast electrons see little difference between an almost static AF mode and a truly static one.

However, electrons at the vH point are not fast; their velocity is zero, and it is known from a previous one-dimensional electron-phonon calculation that the pseudogap appears only for electron velocities larger than the phonon velocity at the instability [15].

We shall show in this work that an analogous situation exists in two dimensions. For quasi-static electrons at the vH singularity, there is no damping and no energy shift, *i.e.* the singularity is not suppressed by the softening of the AF mode, assuming that the latter is characterized by a finite frequency. The strength of the singularity does, of course, decrease as the transition is approached.

2 Model and Approach

The essential physical assumption of the present work is that the AF fluctuations in the paramagnetic phase have a gap which goes to zero only at their condensation temperature. This gap has been observed in neutron scattering [3, 4] and is modeled by the parameter $\tilde{\omega}$ in the dispersion introduced below. We do not expect our result to depend critically on other aspects of the phenomenology.

As for the electrons, the only assumptions we use are that the vH point is a saddle-point of the dispersion, and that hopping is isotropic in the plane, characterized by some scale t.

The objection can be made that the procedure we use is not self-consistent: it is assumed that there is a gap in the spin excitations, while the electron spectrum used has no gap. However, we investigate precisely that one-loop diagram which one expects to be dominant (see, *e.g.*, Ref. [5]) in the opening of a gap in the electron spectrum. Indeed, we obtain a gap at nearly the whole Fermi surface, but we show that it is absent in the immediate vicinity of the v.H. points. The absence of a gap in this region is due to the electrons being slow there, and is the main result of our work.

Another type of consistency objection would be to ask why we have not included both charge and spin instabilities. A careful treatment of all such effects by the weak-coupling parquet approach is found in Ref. [7]. These authors find that the behavior of the model in most of parameter space is RPA-like, *i.e.* there exist stable regimes of the parquet equations in which one of these two instabilities is dominant.

Furthermore, the reader should note that our 'gap' in the spin excitations is at the nesting wave vector $\mathbf{q} = \mathbf{Q} \equiv (\pi, \pi)$, and not at $\mathbf{q} = 0$, which is what first comes to mind when one mentions a gap. It might be interesting to see what is the effect of v.H. singularities on the real part of the spin structure factor at $\mathbf{q} = 0$, $\chi'(\mathbf{q} = 0)$, especially since the latter is experimentally accessible via the Knight shift, whose behavior, to the best of our knowledge, has so far not been satisfactorily explained. Again, the work of Ref. [7] treats v.H. effects properly, but $\chi'(\mathbf{q} = 0)$ has not been looked at.

Working at finite temperature and above the instability, we assume that the AF fluctuations have the dispersion

$$\omega_D(\mathbf{Q} + \mathbf{q}) = \sqrt{\tilde{\omega}^2 + c^2\mathbf{q}^2}\ , \tag{1}$$

where c is their velocity away from $\mathbf{Q} = (\pi, \pi)$. Since the AF mode is anomalously populated as the transition ($\tilde{\omega} \to 0$) is approached, the Fermi occupation numbers can be neglected with respect to the Bose ones, which are approximated classically. The one-loop expression for the electron self-energy without vertex corrections [16] then becomes

$$\begin{aligned} \Sigma(\omega) &\equiv \Sigma^R(\mathbf{p}, \omega) \\ &\propto \int d^2q \int d\omega' \frac{1}{\omega - \epsilon_{\mathbf{p}-\mathbf{Q}+\mathbf{q}} + i\delta} \frac{kT}{\hbar\omega'} \chi''(\omega')\ . \end{aligned} \tag{2}$$

where we use the following phenomenological expression for χ'':

$$\chi''(\omega) = \frac{2\Gamma\omega_0^2\omega}{(\omega^2 - \omega_D^2)^2 + 4\Gamma^2\omega^2} \tag{3}$$

Putting the external electron momentum $\mathbf{p}$ precisely at the vH point $\mathbf{K} = (0, \pi)$, we expand the electron dispersion to quadratic terms (the velocity is zero!) and obtain

$$\Sigma(\omega) = F \int_{\underline{\tilde{\omega}}}^{\underline{\omega_0}} \frac{du}{u + i\underline{\Gamma}} \left[\frac{1}{\sqrt{P_+(\underline{\omega}; u)}} + \frac{1}{\sqrt{P_-(\underline{\omega}; u)}} \right] , \tag{4}$$

where P_+ and P_- are fourth-order polynomials (complex for $\Gamma > 0$), coming respectively from the absorption and emission diagrams. A dimensionless reduction has appeared, to be denoted by an underline,

$$\underline{\omega} \equiv \frac{\omega t}{2c^2} . \tag{5}$$

The integration over a disk around the vH point is restricted by a frequency cutoff for the fluctuations, $\underline{\omega_0}$. The factor F contains the physical constants:

$$F \propto kTg^2 \frac{\omega_0^2 t}{c^4} , \tag{6}$$

where $\underline{\omega_0}$ is a characteristic frequency of the bare fluctuations, and g^2 (of dimension energy) is model-dependent. The appearance of a 'universal' scale (5) is, of course, a consequence of the simplicity of our assumptions.

3 Results and Discussion

The basic result is that for zero damping, $\mathrm{Im}\Sigma(\omega) = 0$ for $|\omega| < \tilde{\omega}$ and $\mathrm{Re}\Sigma(0) = 0$. Thus the quasiparticle peak is preserved as long as the fluctuation 'bandhead' $\tilde{\omega} > 0$. In the underdamped regime with damping Γ, the quasiparticle peak gets smeared out (see Fig. 1), while its integrated strength remains more or less the same as in the case of zero damping (see Fig. 2).

Figure 1 shows the dimensionless spectral density,

$$\tilde{A}(\underline{\omega}) \equiv \frac{2c^2}{t} A(\omega) = \frac{1}{\pi} \frac{-\mathrm{Im}\underline{\Sigma}}{(\underline{\omega} - \mathrm{Re}\underline{\Sigma})^2 + (\mathrm{Im}\underline{\Sigma})^2} \ , \tag{7}$$

over three orders of magnitude of $\underline{F}$. It is obvious how the strength of the side lobes increases with $\underline{F}$, while the gap between them widens.

The strength of the quasiparticle peak is mostly sensitive to $\underline{\tilde{\omega}}$. We show it in Fig. 2 both with and without damping. In the latter case, the strength is calculated through Eq. (9) below, while for a finite Γ we fit the calculated curves to a sum of Lorentzians, and read off the strength of the central peak (which *is* Lorentzian) from the best fit by a Levenberg–Marquardt [17] procedure. As may be seen, the strength depends very little on the damping, at least in the underdamped regime.

The sensitivity to $\tilde{\omega}$ is mainly contained in the fact that, when $\underline{\tilde{\omega}}$ is not too large,

$$\left.\frac{\partial \mathrm{Re}\Sigma}{\partial \omega}\right|_{\omega=0} \approx -\frac{\underline{F}}{2\underline{\tilde{\omega}}^2} \ . \tag{8}$$

This gives an excellent approximation for the spectral weight of the quasiparticle peak,

$$P \equiv \left.\frac{1}{1 - \frac{\partial \mathrm{Re}\Sigma}{\partial \omega}}\right|_{\omega=0} \ , \tag{9}$$

as shown in Fig. 2. As the AF mode condenses, the strength P vanishes quadratically with $\underline{\tilde{\omega}}$, thus opening a true gap in the electron spectrum.

This behavior is different from the usual pseudogap situation, where the density of states at $\underline{\omega} = 0$ comes from the tails of damped quasiparticle peaks centered elsewhere, *i.e.* it is due to $\mathrm{Im}\Sigma(0) \neq 0$, while here we have a quasiparticle at the Fermi level all the way down to the transition, albeit the probability of finding an electron there (Fig. 2) gets lower as condensation is approached.

Finally let us discuss the physical values of the parameters. It is important to establish that we may use Eq. (3) in the underdamped regime, *i.e.* for $\Gamma < \tilde{\omega}$. In Fig. 3, we fit Eq. (3) to the experimental data of [3]. The quantitative aspects of the fit are not very relevant here; qualitatively, we find that the damping is about 50% of the 'bandhead' $\tilde{\omega}$. We identify the large frequency ω_0 with c/ξ, the cutoff in Eq. (4). The experimental data contain an arbitrary vertical scale factor, so we cannot obtain ω_0 from the fit. Taking ω_0 at 200–300 meV, with $\xi \sim 2$, enables us to estimate the reduction (5) at $\sim 1eV^{-1}$.

As to the physical prefactor F, we need to estimate the coupling g^2, of dimension energy. In the worst case, it is $\sim U^2/\omega_0$ (static external perturbation), giving $\underline{F} \sim 10^{-3}$. More physically, one would put $\sim t^2/U$ (Hubbard model in the $t - J$ limit) or $\sim t^2/\Delta$ (Emery model in the large-U limit, with Δ the copper-oxygen splitting), which gives $\underline{F} \sim 10^{-5}$ or 10^{-4}. This analysis would imply that in Fig. 2 it is the regime of small $\underline{F}$ which is physical. Although, as we have already noted, the appearance of a universal scale in our calculation should not be taken too seriously, it is encouraging that the effective coupling constant seems to be reduced for vH electrons.

Incidentally, due to the fact that at $T = 5K$ the measured χ'' is strictly zero below 10 meV, the experimental situation at that temperature is better described by the zero-damping situation than by the damped curve (3) with which we fit the data in Fig. 3.

If one moves slightly off the vH singularity, writing $\mathbf{p} = \mathbf{K} + \mathbf{k}$ for the electron momentum, worst-case estimates in the case of zero damping indicate that the quasiparticle regime persists, but in a narrowed region: instead of $|\underline{\omega}| < \underline{\tilde{\omega}}$, one now has $|\underline{\omega}| < \underline{\tilde{\omega}} - \underline{\omega_k}^2/2$, where $\underline{\omega_k} \equiv tk/2c$. This is a quadratic correction in the reduced frequencies and thus always negligible for small enough $\mathbf{k}$. Thus the antiadiabatic effect found here should contribute with finite measure in the momentum integral when one calculates the density of states.

Finally, since the factor kT in F (whose reduction by (5) is basically what makes $\underline{F}$ small) is due to our taking the high-temperature limit of the structure factor, we note that the coupling in the low-temperature limit becomes exponentially small.

We conclude that the previous interpretation of certain anomalies in the behavior of optical phonons as being due to the logarithmically singular density of states is not imperiled by an impending AF transition.

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Figure Captions

Figure 1. The dimensionless spectral density for $\underline{\tilde{\omega}} = 0.03$, $\underline{\Gamma} = 0.015$, $\underline{\omega_0} = 0.4$, and three values of the reduced coupling constant. Full line : $\underline{F} = 0.0001$. Dotted line : $\underline{F} = 0.001$. Dashed line : $\underline{F} = 0.01$.

Figure 2. Strength of the quasiparticle peak in Fig. 1. Squares: $\underline{F} = 0.0001$. Triangles: $\underline{F} = 0.001$. Diamonds: $\underline{F} = 0.01$. Empty symbols: no damping. Filled symbols: damping is 50% of $\tilde{\omega}$. Full lines: Eq. (9) with the analytical approximation (8).

Figure 3. Fits of Eq. (3) at $\mathbf{q} = 0$ to the experimental data of Ref. [3]. The parameters are, with increasing temperature, $\Gamma = 5.8, 7.6, 14.4, 14.5$, $\tilde{\omega} = 24, 25, 30, 28$, $\omega_0 = 200, 220, 320, 270$, all in meV. Note that ω_0 cannot be estimated from the fits because the experimental data are arbitrarily scaled.