Quasiparticle spectrum in a nearly antiferromagnetic Fermi liquid: shadow and flat bands

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Abstract

We consider a two-dimensional Fermi liquid in the vicinity of a spin-density-wave transition to a phase with commensurate antiferromagnetic long-range order. We assume that near the transition, the Fermi surface is large and crosses the magnetic Brillouin zone boundary. We show that under these conditions, the self-energy corrections to the dynamical spin susceptibility, \( \chi(q, \omega) \), and to the quasiparticle spectral function function, \( A(k, \omega) \), are divergent near the transition. We identify and sum the series of most singular diagrams, and obtain a solution for \( \chi(q, \omega) \) and an approximate solution for \( A(k, \omega) \). We show that (i) \( A(k) \) at a given, small \( \omega \) has an extra peak at \( k = k_F + \pi \) (‘shadow band’), and (ii) the dispersion near the crossing points is much flatter than for free electrons. The relevance of these results to recent photoemission experiments in \( YBCO \) and \( Bi2212 \) systems is discussed.
The problem of fermions interacting with low-energy magnetic fluctuations has attracted a considerable interest over the past few years particularly in connection with high-$T_c$ superconductivity [1–9]. In this paper, we consider a two-dimensional system of interacting fermions near the antiferromagnetic instability with $Q = (\pi, \pi)$. We assume that the Fermi-liquid theory is valid on the disordered side of the transition (i.e., near the Fermi surface, $G(k, \omega_m) = Z/(i\omega_m - \bar{\epsilon}_k)$, where $\bar{\epsilon}_k = \epsilon_k - \mu$, and $Z$ is a positive constant), and that the Fermi surface is large and crosses the Brillouin zone boundary - under these conditions, the transition has a mean-field dynamical exponent $z = 2$ [1–3,6]. We will show in this paper that due to strong interaction between fermions and paramagnons, the actual form of $G(k, \omega)$ and of the dynamical spin susceptibility at intermediate energies is qualitatively different from the prediction of a Fermi-liquid theory. At the critical point, this new behavior stretches up to $\omega = 0$.

The point of departure for our analysis is the spin-density wave (SDW) theory of an antiferromagnetic transition in a Fermi liquid [10]. In this theory, the instability towards antiferromagnetism occurs when the total magnetic susceptibility $\chi(q, \omega) = \chi^0(q, \omega)/(1 - U_{eff}(q)\chi^0(q, \omega))$ diverges at $q = Q, \omega = 0$. Here $\chi^0(q, \omega)$ is a Pauli susceptibility of an ideal gas (a particle-hole bubble), and $U_{eff}(q)$ is an effective interaction. The precise form of $U_{eff}(q)$ is irrelevant for our low-energy analysis, we only assume that $U_{eff}(Q) > 0$, and $U_{eff}(Q)Z \leq t$. A model computation of $\chi$ in Ref. [6] yields $\chi(q, \omega_m) = C/(\omega_m^2 + 2\gamma|\omega_m| + E^2_{\tilde{q}})$, where $C$ is a constant of the order of the hopping integral, $E^2_{\tilde{q}} = v_s^2\tilde{q}^2 + \Delta^2$, $\tilde{q} = Q - q$. This form of the susceptibility was also suggested on phenomenological grounds [11,12]. It is essential for our consideration that the $\omega_m^2$ and $E^2_{\tilde{q}}$ terms in $\chi$ come from the integration over the fermionic momentum in the particle-hole bubble over the regions far from the Fermi surface. At such scales, the perturbation theory is non-singular, and we expect that the full $\text{Re } \chi^{-1}(q, \omega)$ will not differ qualitatively from the RPA result. At the same time, due to energy constraint, the damping term at $q \approx Q$ comes from the momentum integration over near vicinity of the crossing points between the Fermi surface and the magnetic Brillouin zone boundary. At such scales, fermionic and bosonic energies are both small, and we will
show that the perturbation corrections are singular.

Let us first obtain the explicit expression for $\gamma$ in the PRA formalism. Near each of the crossing points, the fermionic energies $\bar{\epsilon}_k$ and $\bar{\epsilon}_{k+Q}$ can be expanded quite generally as

$$\bar{\epsilon}_k = v \bar{k} \cos \phi, \quad \bar{\epsilon}_{k+Q} = v \bar{k} \cos(\phi + \phi_0),$$

where $\bar{k} = k - k_0$ is the deviation from the crossing point, $v = (v_x^2 + v_y^2)^{1/2}$, and for $v_x > v_y > 0$, $\phi_0$ is given by $\phi_0 = \pi/2 + 2 \tan^{-1} v_y/v_x$. A direct calculation of the particle-hole bubble then yields

$$\gamma = U^2(Q) Z^2 C / (\pi v^2 |\sin \phi_0|).$$

Notice that $\gamma$ diverges when $\phi_0 = \pi$ (the $2k_F = Q$ case [13]).

We now go beyond the RPA approximation. Consider first whether the $2\gamma|\omega_m|$ term in the magnetic susceptibility survives the effects of self-energy and vertex corrections at the transition point. The lowest-order corrections to the fermionic bubble are shown in Fig. 3b. We explicitly computed the corrections to $\gamma$ from all three diagrams and found that the two diagrams with the self-energy corrections are free from singularities. However, the diagram with the vertex correction is logarithmically singular for $Q = (\pi, \pi)$, and changes $\gamma$ to $\tilde{\gamma} = \gamma (1 - 2\beta \log(\omega_0/\omega))$ where $\omega_0$ is the cutoff frequency, and

$$\beta = \frac{U_{eff}^2 Z^2 C}{4\pi^3 v^2} \text{Re} \int_0^\pi d\phi \frac{\log[\sin(\phi/2)]}{\cos \phi + \cos \phi_0} \tag{1}$$

Substituting the result for $\gamma$, we find that $\beta$ in fact depends only on $\phi_0$. When $\phi_0$ varies between $\pi/2$ and $\pi$, $\beta$ continuously varies between $-1/16$ and $-1/8$. For $Q \neq (\pi, \pi)$, the logarithmical term is also cut by $(\pi, \pi) - Q$ [3].

We further considered second order corrections to the polarization bubble, and found that (i) the dominant contribution comes from the ladder-type diagram in Fig. 3a, which contributes $O(\beta^2 \log^2 \omega)$, while all other second-order diagrams give either finite, or $O(\beta^2 \log \omega)$ contributions, and (ii) the logarithmical terms are cut by the largest of the external frequencies. In this situation, the logarithms sum up to a power law, and solving the renormalization group (RG) equation for the full vertex, graphically shown in Fig 3b, we obtain $\Gamma \sim \omega^{\beta}$. Substituting this result into the full bubble (which in our case of the RG-like perturbation theory contains two full vertices), we find that at small frequencies, $\chi^{-1}(q, \omega_m) \propto \tilde{\gamma} |\omega_m|^{1+2\beta} + E_q^2$, where $\tilde{\gamma} \sim \gamma/\omega_0^{2\beta}$. An extra logarithmic factor in the frequency term is also possible due
to subleading, double logarithmical corrections to the full vertex which we didn’t compute. We see that the functional form of the full dynamical susceptibility at the transition point is different from the RPA and phenomenological predictions, though the numerical value of $\beta$ turns out to be small \cite{14}. Away from the transition, the logarithmical singularities are cut by $\Delta$, and there is a crossover, at $|\omega_m| \sim \Delta^2/\gamma$, from an anomalous $|\omega_m|^{1+2\beta}$ dependence of $\chi$ at higher frequencies to a Fermi-liquid-type frequency dependence $|\omega_m|\Delta^{4\beta}$ at the lowest frequencies.

Having obtained the result for the spin susceptibility, we now turn to the discussion of the form of the full fermionic Green function. Consider first the lowest-order self-energy correction to the fermionic propagator (Fig. 1a). We have $G^{-1} = (i\omega_m - \bar{\epsilon}_k - \Sigma(k, \omega_m))/Z$, where $\Sigma(k, \omega_m) = ZU^2(Q) \int \chi(q, \Omega_m)G(k + q, \Omega_m + \omega_m)$, where $\chi(q, \Omega_m)$ is the RPA susceptibility. The evaluation of the self-energy is tedious but straightforward. We obtained

$$
\Sigma(k, \omega_m) = -i\omega_m \left( \frac{2\gamma}{|\omega_m|} \right)^{1/2} \frac{v |\sin \phi_0|}{4v_s} \times \Phi \left( \frac{\Delta^2}{2\gamma|\omega_m|}, \frac{v^2 \bar{\epsilon}_{k+Q}^2}{2v_s^2 \gamma|\omega_m|} \right) - \frac{L |\sin \phi_0|}{4\pi} (\bar{\epsilon}_{k+Q} - i\omega_m) \tag{2}
$$

where $L = \log[\omega_0/\max(\omega, \Delta, \bar{\epsilon})]$. The function $\Phi(x, y)$ has a simple form in the two limits: at the crossing point, $\bar{\epsilon}_{k+Q} = 0$, we have $\Phi(x, 0) = (x^{1/2} + (x+1)^{1/2})^{-1}$, and at the transition point, $\Delta = 0$, we found that it is well approximated by $\Phi(0, y) = \pi^{-1}(1 + y)^{-1/2} \cot^{-1}((y - 1)a/(y + 1)^{3/2})$, where $a \sim (2\gamma/|\omega_m|)^{1/2} \gg 1$.

The key observation from eq. (2) is that the self-energy correction to the quasiparticle Green function at $\bar{k} = 0$ has a power-law singularity: $\Sigma(k_0, \omega_m) \propto i\omega_m/|\omega_m|^{1/2}$, which for $\omega \ll \gamma$ clearly overshadows the zero-order, $i\omega_m$ term in $G_0^{-1}$. At the same time, the self-energy correction at zero frequency is only logarithmically divergent \cite{15}. The singular behavior of $\Sigma(\omega)$ was first obtained analytically by Millis \cite{3}, and then used in the ‘spin gap’ calculations in \cite{5}. Numerically, the analogous frequency dependence was obtained by Monthoux and Pines \cite{2}. The logarithmical divergence of the self-energy at zero frequency has not been studied before, to the best of our knowledge. Notice also that (2) does not lead to the shift in the location of the crossing point.
We now discuss the form of the full $G(k, \omega_m)$. The diagram for the full self-energy is shown in Fig 2c. It contains two full vertices, full spin propagator, and full fermionic Green function. We found above that the lowest-order corrections to vertices and spin propagator contain logarithms while the correction to the fermionic propagator contains both square-root and logarithmical singularities. Because of three different sources for logarithms, the explicit summation of the perturbation series is hardly possible. Below we obtain an approximate solution for $G(k, \omega_m)$: we neglect all logarithmical terms but keep power-law divergencies. This approximation is not fully self-consistent, as the series of logarithms may eventually give rise to extra powers of frequency and momentum, similar to what we found above for the spin propagator. However, the lowest-order logarithmical corrections contain small numerical factors ($\beta \ll 1$ for susceptibility and vertex function, and $|\sin \phi_0|/4\pi$ for the Green function, see eq. (2)), so the logarithmical terms are likely to be irrelevant for all practical purposes.

We now proceed with the calculations. Assume that the fully renormalized fermionic propagator has a form $G(k, \omega_m) = S(k, \omega_m) / (i\omega_m |\tilde{\omega}_0/\omega_m|^{1/2} - \bar{\epsilon}_k)$. Substituting this Green function into the self-energy term, we obtain after simple manipulations that at the transition point, $\Sigma(0, \omega_m) \propto S (i\omega_m |\tilde{\omega}_0/\omega_m|^{1/2}$ independent on $\alpha$. At the same time, at zero frequency, we find, neglecting logarithms, $\Sigma(k, 0) \propto S \bar{\epsilon}_k + \pi$. Self-consistency on $G(k, 0)$ then implies that $S = O(1)$. Substituting $S$ into a self-consistency condition on $G(k_0, \omega_m)$, we obtain $\alpha = 2$.

The extension of the above arguments to $\Delta \neq 0$ is straightforward, and we finally obtain

$$G(k, \omega_m) = \frac{Z}{i\omega_m |\tilde{\omega}_0/\omega_m|^{1/2} \Phi \left( \frac{\Delta^2}{2\gamma|\omega_m|}, \frac{v^2 \bar{\epsilon}_k + \pi}{2\gamma^2/|\omega_m|} \right) - \bar{\epsilon}_k}, \quad (3)$$

where $\tilde{\omega}_0 \sim \gamma v^2/v_s^2 \sim \omega_0 \sim t$, and the function $\tilde{\Phi}$ has the same asymptotic behavior as $\Phi$ introduced earlier (in particular, $\tilde{\Phi}(0, 0) = 1$), but may differ from $\Phi$ at intermediate values of arguments. Eq. (3) is the key result of this paper.

We now discuss two applications of this result relevant to experiments. First, we show that eq. (3) yields flat quasiparticle dispersion near each of the crossing points. In the
photoemission experiments, the quasiparticle energy is associated with the position of the maximum in the spectral function $A(k,\omega)$ at a given $k$. In a Fermi-liquid, $A(k,\omega)$ has a peak at $\omega = \bar{\epsilon}_k \propto v|k-k_0|$, where $k_0$ is one of the crossing points. The full spectral function near $k_0$, which one obtains from (3) after a transformation to real frequencies, however, has a maximum at $\omega = B_k \bar{\epsilon}_k^2/\omega_0 \propto (k-k_0)^2$ at $\Delta = 0$, and at $\omega \propto \Delta(k-k_0) + O((k-k_0)^2)$ in the disordered phase. The factor $B_k$ depends on the ratio $\bar{\epsilon}_k +\pi/\bar{\epsilon}_k$, but we have checked numerically that this dependence is actually very weak. We see that for $\Delta \ll v \sim \omega_0$, which we assume to hold near the magnetic transition, the effective quasiparticle dispersion near $k_0$ is nearly quadratic rather than linear, which obviously means that it is much flatter than the dispersion of free fermions.

Another application relevant to experiments is the appearance of a ‘shadow band’ near the transition. Suppose that we are some distance away from $k_0$, such that self-energy corrections are non-singular. In this situation, $A(\omega)$ at a given $k \approx k_F$ is dominated by a conventional quasiparticle peak, i.e., $A(\omega) \propto Z\gamma\omega^2/(\gamma^2\omega^4 + (\omega - \bar{\epsilon}_k)^2)$. Right at the Fermi surface we have $A(0) > 0$, while at $k \neq k_F$, $A(\omega)$ behaves as $\omega^2$ at the lowest frequencies, and has a sharp peak at $\omega = \bar{\epsilon}_k$. As we move away from the Fermi surface, the peak shifts to higher frequencies, and the low-frequency part of $A(\omega)$ flatters. This behavior breaks down however when $k$ reaches the value $k = k_F + Q$. At this point, $\bar{\epsilon}_{k+Q} = 0$, and the self-energy term has the same singularity at small $\omega$ as in eq. (2), i.e., at $\Delta = 0$ we have $\Sigma(\omega_m) \propto i\omega_m/|\omega_m|^{1/2}$ \[3,5\]. Doing the standard manipulations, we obtain at small frequencies, $A(\omega > 0) \sim \omega^{1/2}/\omega_0^{3/2}$ rather than $A(\omega) \sim \omega^2/\omega_0^3$ which holds when both $\bar{\epsilon}_k$ and $\bar{\epsilon}_{k+Q}$ are finite. If $\Delta > 0$, the quadratic dependence exists also at $k = k_F + Q$, but at these $k$, $A(\omega) \propto \omega^2/\Delta^3$, i.e., for $\Delta \ll \omega_0$, the slope is still substantially larger than for other momenta. The increase in the slope of $A(\omega)$ at $k = k_F + Q$ can be detected if one fixes $\omega$ at some small value, and plots $A$ as a function of $k$. Clearly, $A(k)$ should have two maxima: one where $\bar{\epsilon}_k = \omega$, and the other (smaller and broader) where $\bar{\epsilon}_{k+Q} = 0$. The second peak is usually referred to as a ‘shadow band’ \[4\]. Notice however the important difference between conventional and ‘shadow’ peaks: at $\bar{\epsilon}_k = 0$, $A(\omega)$ tends to a finite value at $\omega = 0$, while

\[6\]
at $\tilde{\epsilon}_{k+Q} = 0$, we have $A(0) \equiv 0$. This argument shows that in the absence of long-range magnetic order, the ‘shadow Fermi surface’, strictly speaking, does not exist (cf. Ref [16]). In practice, however, the measurements always involve averaging over some finite frequency range due to resolution, in which case the second peak in $A(k)$ should indeed be present in the data.

We now discuss possible experimental realizations of these effects. First, recent photoemission measurements of $A(k)$ at small $\omega$ in pure and lead-doped $Bi2212$ [20] have shown that the intensity has a second, ‘shadow’ peak located at $k = k_F + Q$, where $\tilde{\epsilon}_{k+Q} = 0$. This is totally consistent with our findings. Second, the flat quasiparticle dispersion near $(0, \pi)$ has been observed in nearly optimally doped $YBCO$ [17] and in $Bi2212$ [18,19]. In both systems (particularly in $Bi2212$) the Fermi surface crosses the magnetic Brillouin zone boundary near $(0, \pi)$ and symmetry related points [18,20,21]. Assume that $\tilde{\epsilon}_{(0,\pi)} \ll \omega_0$, i.e, eq. (3) is valid near $(0, \pi)$. Then the effective quasiparticle dispersion is $E_k = E_{(0,\pi)} + \delta \Delta \epsilon_k$, where $\Delta \epsilon_k = \epsilon_k - \epsilon_{(0,\pi)}$, $\delta \sim (\epsilon_{(0,\pi)}^2 + \lambda \Delta^2)^{1/2}/\omega_0$, $\lambda = O(1)$, and $E_{(0,\pi)} - \mu \propto \epsilon_{(0,\pi)}^2/\omega_0 \ll \epsilon_{(0,\pi)}$. We see that if $\epsilon_{0,\pi}$ and $\Delta$ are both substantially smaller than $\omega_0 \sim t$, then $\delta \ll 1$, and the actual quasiparticle dispersion near $(0, \pi)$ has an extra small factor compared to the mean-field dispersion. Note, however, that in $YBCO$, the measured Fermi surface was fitted to the $t - t'$ model with $t' = -0.45t$ [22]. In this model, the dispersion of free fermions is already flat: $\Delta \epsilon_k = -0.1t \ (\pi - y)^2$ for $x = 0$, and $\Delta \epsilon_k = 1.9t \ x^2$ for $y = \pi$. We see that the dispersion along $(0, y)$ (but not along $(x, \pi)$) is flat already at the mean-field level, and it is actually difficult to judge to which extent the measured flat band is due to the effects of the interaction, and to which extent it is a property of a dispersion of free fermions near the Fermi surface. In $Bi2212$, the value of $t'$ is unknown, but the measured location of the crossing point $k_0$ is closer to $(0, \pi)$ than in $YBCO$ [18,20], so we expect our theory to be more relevant. There is a clear indication from the recent data [18] that the dispersion around $(0, \pi)$ is flat along both $(0, y)$ and $(x, y_0)$ directions, where $y_0$ is close to $\pi$. This phenomenon is consistent with the scenario of the fluctuation-induced softening.

To summarize, we found that the interaction between fermions and low-energy spin fluc-
tuations strongly affects the frequency-dependent part of the the fermionic quasiparticle Green function. To lesser extent, the renormalization also affects the imaginary part of the staggered spin susceptibility, and the momentum-dependent part of the fermionic propagator. The full spectral function $A(\omega)$ at a given $k$ located near the point where the Fermi surface crosses the magnetic Brillouin zone boundary, has a peak at $\omega \sim (\epsilon_k - \mu)^2$ (up to logarithms), i.e., fluctuation corrections flatten the quasiparticle dispersion. The spectral function $A(k)$ measured as a function of momentum at a given (small) frequency has two peaks: a conventional quasiparticle peak, and a ‘shadow’ peak located where $\epsilon_{k+Q} = \mu$.

The results above are related to other works on shadow and flat bands. The ‘shadow bands’ in a nearly antiferromagnetic Fermi liquid were first obtained by Kampf and Schrieffer [4]. Our approach is similar to theirs except that we considered here a conventional ‘small $U$’ SDW transition, when the SDW gap is zero at the transition point and gradually increases in the ordered phase, while Kampf and Schrieffer considered semiphenomenologically the ‘large $U$’ limit near half-filling, when there exists a pseudogap in the electronic spectrum in the paramagnetic phase. Dagotto et al [23] argued recently that the shadow and flat bands both have antiferromagnetic origin. Our conclusions are consistent with theirs. They however related the measured flat dispersion near $(0, \pi)$ to the flatness of the spectrum of a single hole in a half-filled $t-J$ model, which, they argue, persists at finite doping. We have shown here that there exists an additional, model independent mechanism which flattens the quasiparticle dispersion near the magnetic transition.

Note added. After this paper was completed, I received a preprint from B.L. Altshuler, L.B. Ioffe and A.J. Millis [13] on the analysis of the SDW transition at $Q = 2k_F$. They consider a case $Q \neq (\pi, \pi)$, but also discuss scaling behavior at intermediate momenta when the difference between $Q$ and $(\pi, \pi)$ can be neglected. In this regime, they identify the series of logarithmical corrections, and their results are very similar to the ones presented here.

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FIGURES

FIG. 1. (a). Lowest-order self-energy correction due to interaction with magnetic fluctuations. The solid and wavy lines are fermion and paramagnon propagators, respectively; (b). the lowest-order corrections to the polarization bubble

FIG. 2. (a). Diagram for the dominant second-order correction to the polarization bubble; (b). diagrammatic expressions for the fully renormalized polarization bubble and for the full vertex, thick wavy line is the fully renormalized paramagnon propagator; (c). diagram for the full self-energy. Thick solid line is the full Green function
Fig. 1
