Theory for Dynamical Short Range Order and Fermi Surface Volume in Strongly Correlated Systems

J. Schmalian, M. Langer, S. Grabowski, and K.H. Bennemann
Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany
(March 26, 1996)

Using the fluctuation exchange approximation of the one band Hubbard model, we discuss the origin of the changing Fermi surface volume in underdoped cuprate systems due to the transfer of occupied states from the Fermi surface to its shadow, resulting from the strong dynamical antiferromagnetic short range correlations. The momentum and temperature dependence of the quasi particle scattering rate shows unusual deviations from the conventional Fermi liquid like behavior.

Their consequences for the changing Fermi surface volume are discussed. Here, we investigate in detail which scattering processes might be responsible for a violation of the Luttinger theorem. Finally, we discuss the formation of hole pockets near half filling.

It is clear that the evolution of the Fermi surface (FS) upon doping and the occurrence of a very flat band crossing the Fermi level is of great importance for an understanding of the anomalous properties of high-Tc materials. Near half filling, the cuprates are antiferromagnetically ordered. Therefore, we expect due to the low carrier concentration small Fermi surface pockets. Strong indications for this behavior were experimentally observed in YBa$_2$Cu$_3$O$_6.3$ and in Sr$_2$CuO$_2$Cl$_2$. In contrast, for optimally and overdoped cuprates, large Fermi surfaces are well established. One could simply expect a transition from a small to a large FS at the antiferromagnetic-paramagnetic phase transition, occurring for $x \approx 0.025$ in La$_2$-$x$Sr$_x$CuO$_4$. Interestingly, no abrupt changes of the transport properties or the details of the electronic structure were found at this transition. Furthermore, pronounced short ranged antiferromagnetic correlations were observed in the paramagnetic state, even for optimally doped materials. An alternative scenario for the transition from a large to a small FS is the gradual evolution of shadows of the FS in the paramagnetic state, first observed by Aebi et al. In a recent letter, we gave a theoretical explanation for these states with correct excitation energy and consistent with the observed relatively short antiferromagnetic correlation length. Here, the shadow states reflect a dynamically broken symmetry on a short range which demonstrates the dynamical character of these new structures in the excitation spectrum of the cuprates. This is related to an unusual behavior of the electronic self energy leading for low doping concentrations to a small change of the Fermi surface volume compared to the uncorrelated case for equal particle density.

It is the aim of this paper to discuss in detail the anomalous momentum and temperature dependence of the quasi particle scattering rate and how it causes the change of the Fermi surface volume of underdoped systems due to the occurrence of shadow states outside the Fermi surface. Although quantitatively small, the change of the Fermi surface volume, found in our FLEX calculations, are directly related to these new structures in the spectral density. It will be shown that the anomalous frequency, momentum and temperature dependence of the electronic self energy, reflecting the dynamical character of the antiferromagnetic correlations, are responsible for this qualitatively new behavior. Furthermore, we argue that the dynamical formation of short range correlations which modifies the translation symmetry of the underlying lattice on a certain time scale is a general phenomenon related to the non Fermi liquid behavior of a strongly correlated system. Therefore, the original derivation of the Luttinger theorem is extended to an arbitrary frequency and momentum dependence of the quasi particle scattering rate, not restricted to the usual Fermi liquid behavior $\text{Im}\Sigma_k(\omega) \propto \omega^2$. This enables us to investigate in detail which scattering processes are responsible for a violation of the Luttinger theorem. This might be of importance for an understanding of the evolution of the Fermi surface of the high-Tc materials upon doping. Finally, we discuss that the changing FS-volume and the formation of hole pockets near half filling are both closely related with the formation of shadow states.

The shadow states derived within the self consistent and conserving fluctuation exchange approximation (FLEX) by Langer et al. result from a dynamical coupling of states with momentum $k$ at the FS with states at its shadow at $k + \mathbf{Q}$, where $\mathbf{Q} = (\pi, \pi)$. Due to the absence of long range antiferromagnetic order, this coupling has to be generated via decay of particles with momentum $k$ into a state with $k + \mathbf{Q}$ and vice versa. This is related to an unconventional behavior of the quasi particle scattering rate, i.e. of the imaginary part of the self energy $\Sigma_k(\omega)$. By calculating $\Sigma_k(\omega)$ within the FLEX approximation of the one band Hubbard model, we
found this anomalous momentum and frequency dependence.

In Fig. 1 we show our results for the momentum dependence of \( \text{Im} \Sigma_k(\omega = 0) \) for two different doping concentrations \( x = 1 - n \). Here, \( n \) is the particle density per lattice site. The calculation was performed using an unperturbed dispersion \( \varepsilon_k = -2t(\cos(k_x) + \cos(k_y)) \) with nearest neighbor hopping element \( t = 0.25 \text{eV} \), and a value of the on site Coulomb interaction \( U = 4t \). While for larger doping \( (x = 0.16) \) a double well structure with large quasi particle scattering rate at the Fermi energy and at its shadow occurs, we find for \( x = 0.12 \) the dominant scattering phenomena are at the FS-shadow, leading to the formation of shadow states in the spectral density.

In Fig. 2 we show the temperature dependence of \( \Gamma_k \equiv -\text{Im} \Sigma_k(\omega = 0) \) for \( k \) at the Fermi surface (solid squares) and at its shadow (open triangles), which dramatically differs from the conventional \( \Gamma_k \propto T^2 \) dependence occurring in overdoped systems. The scattering rate at the FS-shadow increases with decreasing temperature since the corresponding short range correlations, which build up the \( k \)-dependencies of \( \Gamma_k \), are getting stronger for \( T \to 0 \).

In view of this anomalous behavior of the electronic self energy, it is of interest to explore its consequences on the shape and volume of the Fermi surface. Therefore, we consider the FS-volume, characterized by

\[
n_{\text{Latt}}(T) = \frac{2}{N} \sum_{k} \theta (\mu - \varepsilon_k - \text{Re} \Sigma_k(\omega = 0)),
\]

and compare it with the particle concentration

\[
n(T) = -\frac{2}{N} \sum_{k} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} f(\omega) \text{Im} G_k(\omega + i0^+).
\]

Here, \( G_k(z) = (z + \mu - \varepsilon_k - \Sigma_k(z))^{-1} \) is the Green’s function with chemical potential \( \mu \), and self energy \( \Sigma_k(z) \), respectively. \( f(\omega) = (e^{\omega/T} + 1)^{-1} \) is the Fermi function, and \( N \) is the number of lattice sites.

We show in Fig. 3 our results for the doping dependence of the difference \( n - n_{\text{Latt}} \) (solid line) demonstrating that in underdoped systems the volume of the Fermi surface differs from its value \( n \) for \( U = 0 \). This is of importance since

\[
n(T) = n_{\text{Latt}}(T)
\]

is for \( T = 0 \) the Luttinger theorem \([24,25]\) (LT), implying an independence of the FS-volume on the interaction strength for given particle density. We argue on physical grounds that this shrinking of the Fermi surface \([23]\) results from a transfer of occupied states from the main FS to its shadow \([7]\) and gives strong indications for a violation of the LT, and is not due to the finite temperature of the calculation. The following analysis of our numerical results strongly supports this point of view although such a transfer of states does not necessarily lead to a violation of the LT, since \( n_k < 1 \) inside and \( n_k > 0 \) outside the FS is well known for interacting fermions.

For an explanation of the deviation of \( n_{\text{Latt}}(T) \) from \( n(T) \), it is helpful to reconsider the derivation of the Luttinger theorem. The Luttinger theorem applies if: (i) perturbation theory is applicable, (ii) the theory is conserving \([22]\), (iii) the temperature is zero, and (iv) the imaginary part of the self energy vanishes at the Fermi energy, e.g. like \( \text{Im} \Sigma_k(\omega) \propto \omega^2 \). Note that for an arbitrary FS-shape (iv) does not follow from the first three prerequisites. In the following we investigate in particular the importance of (iii) and (iv) on a possible violation of the LT. We start from the following identity for the particle density valid for arbitrary temperatures:

\[
n(T) = \frac{2T}{N} \sum_{k,m} G_k(i\omega_m) e^{i\omega_m 0^+} = \tilde{n}(T) + I(T),
\]

with

\[
\tilde{n}(T) = \frac{2T}{N} \sum_{k,m} \frac{\partial}{\partial(i\omega_m)} \ln \left( G_k(i\omega_m)^{-1} \right) e^{i\omega_m 0^+}
\]

and

\[
I(T) = \frac{2T}{N} \sum_{k,m} G_k(i\omega_m) \frac{\partial \Sigma_k(i\omega_m)}{\partial(i\omega_m)} e^{i\omega_m 0^+},
\]

which follows immediately if one takes Dyson equation into account. Here, \( \omega_m = (2m+1)\pi T \) is a fermionic Matsubara frequency. As shown by Luttinger and Ward \([24]\) \( I(T) \) vanishes for zero temperature order by order in perturbation theory if the theory is conserving, i.e. if there exists a diagrammatically well defined functional \( \Phi[G] \) which generates the self energy via functional derivation \([22]\). Since our numerical data are obtained for finite temperature, we obtain a finite value \( I(T) \approx 10^{-3} \), which nevertheless can be neglected compared to \( n - n_{\text{Latt}} \approx 10^{-2} \).

Considering now \( \tilde{n}(T) \) in Eq. 3, analytical continuation and partial integration yield

\[
\tilde{n}(T) = -\frac{2}{N^2 T} \sum_{k} \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \text{Im} \left[ \ln (G_k(\omega + i0^+)^{-1}) \right] f(\omega) \approx 1 - f(\omega).
\]

In order to show that our conclusion concerning the violation of the LT is also not influenced by some Fermi function smearing due to finite temperatures, we compare \( \tilde{n}(T) \) with \( \tilde{n}_o \) which is calculated from Eq. 3 using the zero temperature limit of \( f(\omega)(1 - f(\omega)) \approx \delta(\omega) \). Note that \( \tilde{n}_o \neq \tilde{n}(T = 0) \) due to the additional temperature dependence of the self energy \( \Sigma_k(0) \). In the inset of Fig. 3 we show our data for the temperature dependence of \( \tilde{n}(T) - \tilde{n}_o \approx 10^{-3} \) is much smaller than \( n - n_{\text{Latt}} \), leading to \( n \approx n_o \) with very good accuracy. Thus,
\[ n \approx n_{\text{Latt}} + \frac{2}{\pi N} \sum_k \text{arctan} \left( \frac{\Gamma_k}{\varepsilon_k + \Re \Sigma_k(0) - \mu} \right). \tag{8} \]

Eq. 8 is exact in the limit \( T \rightarrow 0 \) and can then be considered as a generalization of Luttinger’s original derivation without the assumption \( \Im \Sigma_k(\omega = 0) = 0 \), while keeping the prerequisites (i)–(iii) discussed above. Now, the volume of the FS is in general no more independent of the interaction strength. A violation of the LT occurs if the excitations at the Fermi surface cannot be described as ideal quasi particles with \( \Im \Sigma_k(\omega = 0) = 0 \). Note that one can separate in Eq. 8 one conventional contribution \( n_{\text{Latt}} \), independent of the scattering rate, from a new contribution which strongly depends on the details of \( \Gamma_k \). Consequently, the \( k \)-dependence of \( \Gamma_k \) gives a lot of interesting insights into the the origin of the difference \( n \approx n_{\text{Latt}} \). If \( \Gamma_k \neq 0 \) symmetrically for the states inside and outside the FS, the corresponding contributions from the second term in Eq. 8 cancel each other and \( n = n_{\text{Latt}} \) is fulfilled. A small value for \( n - n_{\text{Latt}} \) is also expected for systems with momentum independent self energy and large Fermi surface, independent on the details of the scattering mechanism. If however \( \Gamma_k \neq 0 \) predominantly for \( k \)-states outside (inside) the FS, it follows from Eq. 8 that \( n - n_{\text{Latt}} > 0 \) (\( < 0 \)), i.e. the FS volume shrinks (gets larger) compared with the uncorrelated system. Therefore, a strong \( k \)-dependence of \( \Gamma_k \) different for states inside and outside the FS is a general phenomenon leading to a change of the FS-volume. Consequently, the dynamical excitations which lead to \( \Gamma_k \neq 0 \) should be related to some short range order which modifies the translational symmetry and thus results in a corresponding strong momentum dependence.

Using our self consistently determined results for the electronic self energy for the lowest temperature \( T = 63 \text{K} \), the change of the FS-volume can indeed be described with Eq. 8 which is fulfilled with the expected accuracy \( \approx 10^{-3} \) for all doping concentrations, as shown in Fig. 3 (dashed line). Following the above argumentation, the FS shrinks, since \( \Gamma_k \) is largest on the shadow of the Fermi surface outside the main FS (see Fig. 3 and Fig. 4). Therefore, the change of the FS-volume is a consequence of the transfer of occupied states to the shadow of the FS due to a dynamical coupling of FS-states with states on the shadow of the FS, which confirms our original physical argumentation of Ref. 7. Such a coupling of single particle states is directly related to a violation of the Fermi liquid theory, since its basic idea is the one to one correspondence of the quasi particles of the interacting system with that of an ideal Fermi gas which is no more guaranteed if it is impossible to distinguish reasonably between the states \( k \) and \( k + Q \). Consequently, the phase space arguments of Landau’s Fermi liquid theory are no more applicable. For larger doping, the \( T \)-dependence of \( \Gamma_k \) indicates strongly \( \Gamma_k = 0 \) for \( T \rightarrow 0 \). The shadow states disappear and we find \( n = n_{\text{Latt}} \), i.e. LT is fulfilled.

Now we investigate how our numerical finite temperature results for \( \Gamma_k \) might continue in the limit \( T \rightarrow 0 \) which was performed to obtain Eq. 8. This is of importance since the temperature dependence of \( \Gamma_k \), shown in Fig. 2, strongly suggests that \( \lim_{T \rightarrow 0} \Gamma_k \neq 0 \), at least for the \( k \)-values on the shadow of the FS. Considering the FLEX equations in the zero temperature limit, the contribution \( V_q^{(s)}(\omega) \) of the effective interaction \( \Sigma_q^{(s)}(\omega) \) which results from the longitudinal and transversal spin fluctuations behaves for low frequencies like

\[ V_q^{(s)}(\omega) = \frac{3}{2} \frac{U^2 \chi_q(\omega)}{1 - U \chi_q(\omega)} \approx \frac{3}{2} \frac{c_q}{\omega_q^* - i\omega}, \tag{9} \]

with characteristic spin excitation energy \( \omega_q^* = c_q(1 - U\Re \chi_q(0))/U \) and \( c_q = (\partial \Im \chi_q(\omega)/\partial \omega)_{|\omega=0}^{-1} > 0 \). Here we assumed a conventional low frequency behavior for the particle hole bubble \( \chi_q(\omega) \approx U^{-1} - (\omega_q^* - i\omega)/c_q \). It is important to note that \( \omega_q^* \) should not be confused with the characteristic excitation energy in the dynamical spin susceptibility. The difference between the effective interaction of the FLEX and the spin susceptibility, where in such an extreme limit vertex corrections have to be considered, was recently demonstrated in Ref. [22].

We expect that even if \( \omega_q^* = 0 \) the coupling of the various spin modes due to short range correlations leads to a finite excitation energy in the spin susceptibility, in agreement with the experiment for doped cuprates. The evaluation of the FLEX diagrams yields \( \Gamma_q \neq 0 \) only if \( \omega_q^* = 0 \) for a momentum \( q \approx Q \). Then it follows

\[ \Gamma_k = \frac{3}{2} \sum_q \left( q_{k-q}(0) c_q \right). \tag{10} \]

As expected from Fig. 4b, \( \Gamma_k \) is maximal on the shadow of the FS, since the spectral density at the Fermi level \( g_k(0) \) is largest for \( k \) on the Fermi surface and because the summation is performed only for \( q \approx Q \) (indicated by the prime in Eq. 10). Our finite \( T \) calculation shows that \( \omega_q^* \) gets extremely small for \( q \approx Q \) (we find \( \omega Q^* \approx 1 - 5 \text{meV} \) which is our numerical resolution) and decreases for decreasing \( T \). This refers to a quasi instantaneous coupling of states at the FS and its shadow such that a large amount of scattering processes occurs already for very small excitation energies or temperature. Nevertheless, we cannot say whether \( \omega_q^* \rightarrow 0 \) occurs strictly for \( T \rightarrow 0 \). If \( \omega_q^* \) remains finite the scattering rate would vanish for very small temperatures and our argumentation concerning the LT refers to \( T > \omega_q^* \). Note, \( \omega_q^* = 0 \) is not necessarily related to a long range ordered state. The short range order leads to a mode mode coupling resulting in a finite but nonsingular scattering rate. Therefore, it is possible and physically reasonable that our numerical results for finite \( T \) are representative for the behavior at zero temperature. In any case, our conclusion concerning
the violation of the LT is valid with good approximation for finite but very small temperatures $T > \omega_k^*$. Finally, it is of interest to contrast our quantitatively small FS-changes with the formation of hole pockets, which occur if one considers the motion of holes within an antiferromagnetic background, relevant near half filling. As indicated in Fig. 4, the formation of shadow states leads to a considerable additional occupation outside the main Fermi surface. Due to particle conservation this results from a decrease of $n_k$ inside the FS and also from the slight shrinking of its volume discussed in this paper. Consequently, the only unoccupied region of the Brillouin zone is near the diagonal from $(0, \pi)$ to $(\pi, 0)$. Since strong coupling calculations near half filling yield a pronounced effective intrasublattice hopping [1], additional deformations of the Fermi surface shape are expected to occur for even smaller doping. This is schematically indicated in Fig. 4. Now, the corresponding unoccupied region of the Brillouin zone is the hole pocket around the $(\pi/2, \pi/2)$ point. A similar shape of the FS, and correspondingly of its shadow, occurs also if one takes from the beginning an additional next nearest neighbor hopping in $\varepsilon_k$ into account, which is believed to be of importance for $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ [27]. Thus, we conclude that the changing FS-volume discussed in this paper and the hole pocket formation are of common origin: the transfer of states from the main to the shadow Fermi surface.

In conclusion, we discussed the consequences of an anomalous momentum and temperature dependency of the quasi particle scattering rate for the volume of the Fermi surface. Therefore, we extended the calculation of Luttinger and Ward [2] to the case of a finite quasi particle scattering rate $\Gamma_k$. A non Fermi liquid behavior results in a violation of the LT if the $k$-states with $\Gamma_k \neq 0$ are asymmetrically distributed with respect to the Fermi surface. Furthermore, we showed that our numerical results obtained from the solution of the FLEX equation give evidence that the difference $n - n_{\text{Lett.}}$, obtained for small but finite temperatures reflects indeed a violation of the LT in underdoped cuprates and are not caused by the finite $T$ of the calculation. This conclusion requires that $\Gamma_k$ shown in Fig. 2 remains finite also for $T \to 0$. Based on the zero temperature behavior of the FLEX, we argued that this is at least consistent with a state of strong dynamical short range order such that our numerical results might be representative also for $T = 0$. In any case, the anomalous behavior of the scattering rate occurs for temperatures larger than an extremely small energy scale $\omega_k^*$ and shows that dynamical short range correlations change dramatically the single particle properties of the cuprates for physically relevant finite temperatures. The origin of this interesting behavior of $\Gamma_k$ is the occurrence of a many particle mode leading to a coupling of FS-states with states on the shadow of the FS. Furthermore, we discussed that the relatively small changes of the FS-volume and the formation of hole pockets are of common origin.

Finally, we believe that the result of Eq. 8 might also be stimulating for the characterization of the details of the Fermi surface in correlated systems, where the non Fermi liquid character is due to a totally different origin than that discussed in this paper. One example could be the formation of a striped phase in $\text{La}_2-x\text{Sr}_x\text{NiO}_4$ [28] where a modification of the translation invariance perpendicular to the stripes occurs which seems to result from the strong dynamical character of the corresponding excitations [29]. Other examples might be dynamical charge modulations, i.e. dynamical CDW-states or the formation bipolarons above its condensation temperature. In all these cases we expect, similar to the case where shadow states exist, a breakdown of the Fermi liquid theory and a violation of the Luttinger theorem.

[1] A. P. Kampf and J. R. Schrieffer, Phys. Rev. B 42, 7967 (1990).
[2] N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. 72, 705 (1994).
[3] P. W. Anderson, Physica B 199 & 200, 14 (1994).
[4] E. Dagotto, A. Nazarenko, and M. Bonisengi, Phys. Rev. Lett. 73, 728 (1994).
[5] S. Haas, A. Moreo, and E. Dagotto, Phys. Rev. Lett 74, 4281 (1995).
[6] R. Preuss, W. Hanke, and W. von der Linden, Phys. Rev. Lett. 75, 1344 (1995).
[7] M. Langer, J. Schmalian, S. Grabowski, and K. H. Bennemann, Phys. Rev. Lett. 75, 4508 (1995).
[8] A. V. Chubukov, Phys. Rev. B 52, 3840 (1995); A. V. Chubukov, D. K. Morr, and K. A. Shakhnovich, preprint.
[9] S. A. Trugman, Phys. Rev. B 37, 1597 (1988); E. Dagotto, R. Joynt, A. Moreo, S. Bacci, and E. Gagliano, Phys. Rev. B 41, 9049 (1990); G. Martines and P. Horsch, Phys. Rev. B 44, 317 (1991).
[10] R. Liu et al., Phys. Rev. B 46, 11056 (1992).
[11] B. O. Wells et al., Phys. Rev. Lett. 74, 964 (1995).
[12] Z. X. Shen and D. S. Dessau, Physics Reports 255, 1 (1995) and references therein.
[13] H. Romberg et al., Phys. Rev. B 42, 8768 (1990).
[14] B. Keimer et al., Phys. Rev. B 46, 14034 (1992).
[15] R. J. Birgenau et al., Phys. Rev. B 38, 6614 (1988).
[16] T. Imai, C. P. Slichter, K. Yoshimura, and K. Kosuge, Phys. Rev. Lett. 70, 1002 (1993).
[17] P. Aebi J. Osterwalder, P. Schwall, L. Schlappbach, M. Shimoda, T. Machiku, and K. Kadowaki, Phys. Rev. Lett. 72, 2757 (1994); ibid. 74, 1868 (1995).
[18] M. Langer, J. Schmalian, S. Grabowski, and K. H. Bennemann, Solid State Comm. 97, 663 (1996); Physics Letters A 212, 270 (1996); S. Grabowski, J. Schmalian, M. Langer, and K. H. Bennemann, to appear in Europhys. Lett.
FIG. 1. Momentum-dependence of \( \text{Im} \Sigma_k(0) \) demonstrating the strong increase of quasi particle scattering on the shadow of the Fermi surface for decreasing doping.

FIG. 2. Temperature dependence of the quasiparticle scattering rate \( \Gamma_k = -\text{Im} \Sigma_k(\omega = 0) \) for a \( k \)-value on the Fermi surface (solid squares) and on the shadow of the Fermi surface (open triangles), as indicated in the inset. Note the anomalous increase of \( \Gamma_k \) on the shadow for decreasing temperature.

FIG. 3. Doping dependence of \( n - n_{Lutt} \), with particle density \( n \) and volume of the Fermi surface \( n_{Lutt} \). For low doping concentration, a change of the FS-volume compared to \( U = 0 \) occurs. The agreement between the solid and dashed line demonstrates the applicability of Eq. 8 which relates the \( k \)-dependence of the scattering rate with the FS-volume. The results refer to a temperature \( T = 63 \) K and a value of the Coulomb repulsion \( U = 4t \) with nearest neighbor hopping element \( t = 0.25 \) eV. The inset shows the temperature dependence of \( \tilde{n}(T) - \tilde{n}_o \), which is smaller than the difference \( n - n_{Lutt} \), showing that the influence of Fermi function smearing on the violation of the LT can be neglected in our finite temperature calculation.
FIG. 4. (a) main Fermi surface (solid line), shadow of the Fermi surface (dashed line), and Fermi surface for $U = 0$ (dotted line), and (b) for the motion of holes within an antiferromagnetic background near half filling. While the change of the main FS-volume is rather small, in both cases additional states outside the FS are occupied. This leads near half filling to the formation of hole pockets around $(\pi/2, \pi/2)$ (shaded area).