Angle–Resolved Loss of Landau Quasiparticles in 2D Hubbard Model

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Abstract

The problem of weakly correlated electrons on a square lattice is studied theoretically. A simple renormalization group scheme for the angle–resolved weight $Z(\theta)$ of the quasiparticles at the Fermi surface is presented and applied to the Hubbard model. Upon reduction of the cutoff the Fermi surface is progressively destroyed from the van Hove points toward the zone diagonals. Due to the renormalized $Z(\theta)$, divergences of both antiferromagnetic and superconducting correlation functions are suppressed at the critical scale, where the interactions diverge.
Understanding of the one-particle spectrum of strongly correlated systems near the metal-insulator transition is an extremely difficult task, particularly if one wants to construct a microscopic theory. One standard example is the pseudogap regime of the HTC superconductors. ARPES measurements [1] showed that the Fermi surface is destroyed by correlations. This happens first near the van Hove points where the one-particle spectrum develops the characteristic 2-peak structure. Remaining parts of the Fermi surface, often called Fermi patches, get progressively narrower around Brillouin zone diagonals as the temperature decreases. Regions around van Hove points contain non-Fermi liquid with a pseudogap and other signatures of strong correlations such as flat bands [2]. In other words, the pseudogap has the form similar to the absolute value of the $d_{x^2-y^2}$-superconducting (SC) order parameter. This vision of the pseudogap is in agreement with STM results [3] as well, regardless of details on how these results are interpreted. The above experiments still do not reveal much on the origins of the pseudogap, namely whether it is simply the signature of a liquid of pre-formed pairs or something much richer in fluctuations. In fact it is known that the antiferromagnetic (AF) fluctuations are also strong in the pseudogap regime [4].

If we assume that AF and SC fluctuations are somehow together the major reason for the strong renormalization of the one-particle selfenergy, and for the consequent partial destruction of the Fermi surface, then a many-body analysis of the one-particle propagator can be done in a controlled way. In fact the weak coupling theory easily reproduces AF and SC fluctuations from particle–hole (p-h) and particle–particle (p-p) loop–logarithms. Even if the coupling in realistic HTC systems is of the order of Fermi energy (i.e. intermediate–to–strong), already the weak–coupling theory contains the observed two–particle correlations. In this paper I answer the question of how the angle–resolved quasiparticle weight $Z(\theta)$ is renormalized by strong and coupled AF and SC fluctuations, and of the main consequences of the renormalized $Z(\theta)$ to the characteristic angle–resolved two–particle correlation functions. The renormalization of the quasiparticle weight in 2D was recently studied by Kishine and Yonemitsu [5]. To calculate the renormalization of $Z$ resolved in the position on a flat Fermi surface they used a two–loop selfenergy expansion with the two–loop–renormalized vertex. The results show clearly that the flatness of the Fermi surface induces the suppression of the quasiparticle residue and that this effect is anisotropic. In the present work I consider the
whole square Fermi surface of the Hubbard model. For this purpose I employ the N–patch
renormalization group theory.

After recent theoretical studies from several groups it emerged that the N–patch model
describes in a systematic and controlled way weakly correlated electrons near half–filling,
and explains the major aspects of HTC-s.\[6, 7, 8, 9, 10, 11\] Until now the RG analysis of the
N–patch model has been done only on the level of the two–particle scattering amplitudes
or, in field–theoretical jargon, of the four–point vertex \(U(K_1, K_2, K_3)\). The analysis of the
renormalization group flow of \(U\) as a function of three patch indices \(i_1, i_2, i_3\) gave several
important results. Typically the amplitudes \(U(i_1, i_2, i_3)\) diverge at some interaction– and
doping–dependent critical energy scale \(\Lambda_c\). For the case of the Hubbard model, we distinguish
two main renormalization regimes \[8\], the parquet regime and the BCS regime.

In the parquet regime (\(|\mu| < \Lambda\)) both particle-particle and particle-hole propagators
have strong contributions to the beta–function due to the van Hove singularities and the
Fermi surface nesting. In this regime, provided \(\Lambda \rightarrow \Lambda_c\) and neglecting the selfenergy cor-
rections, both SC and AF tendencies are strong and build divergent correlation functions
\(\chi^{SC}\) and \(\chi^{AF}\). The dominant component of the antiferromagnetic susceptibility is of the
\(s\)–type and the dominant component of the superconducting one is of the \(d_{x^2−y^2}\)–type. Both
static compressibility \(\chi_c\) and homogeneous magnetic susceptibility \(\chi_s\) go to zero as the cut-
of approaches to its critical value \(\Lambda_c\).\[3, 4, 11\] Consequently \(\Lambda_c\) is the energy scale of the
crossover between the strange metal and the strongly correlated regime with gap or pseudogap. A question arising from already existing results on the Hubbard model \[3, 8\] and on its extensions \[9, 11, 11\] is the following: if one wants to interpret the critical scale \(\Lambda_c\)
(or temperature) as the energy (temperature) \(T^*\) for the onset of the pseudogap, why then
are all signatures of the pseudogap not seen? This means in particular that \(\chi^{AF}\) and \(\chi^{SC}\)
should be finite and not diverging. Emergent is the necessity to calculate the correlation
functions with the corrections due to the one–particle selfenergy.

At stronger doping (\(|\mu| > \Lambda\)) nesting properties get weaker so that eventually only re-
mainning renormalization channel is superconducting (p–p). This is the BCS regime. There
the superconductivity is simply BCS–like with the coupling constants and the angular pro-
file of the order parameter determined at higher scales by a parquet–like flow, where \(\Lambda\) was
larger than the chemical potential.

Equivalent to the RG approach is the fast parquet theory \[12, 13\], where \( \theta \) variable (continuum version of the patch index) is called the fast variable in addition to the cutoff logarithm called the slow variable. In two dimensions the parquet integro–differential equations always have mobile pole solutions, i.e. the AF and SC fluctuations decouple one from the other. This seems to be in disagreement with the RG results, where we detected only immobile poles, the type of solution in which all scattering amplitudes develop the pole at the same scale \( \Lambda_c \). The question of the consilience between the two theories is still controversial. However, the results of De Abreu and Douçot \[14\] indicate that the mobile pole solution is dominant only in the very vicinity of \( \Lambda_c \) and that the fixed pole solution is an intermediate solution, valid over several decades of energy scale. The width of the “very vicinity” characterized by the mobile poles depends on the coupling constant so that for reasonable and not too weak \( U_0 \) the final regime is so close to \( \Lambda_c \), that the couplings are already too strong and out of reach of a weak coupling theory. Consequently the real physical interpretation can be given only to the immobile pole regime. We will concentrate on this “intermediate” regime in which all fluctuations are coupled and at least behave as if having an immobile pole.

We suppose that the electronic Green function has the form

\[
G_l(K) = \frac{Z_l(\theta)}{i\omega - \xi(k)}.
\]

(1)

\( Z_l(\theta) \) is the angle–resolved scale dependent quasiparticle weight and \( \xi(k) \) is the tight–binding dispersion. The formalism keeps the notation introduced in the reference \[8\]. The form (1) contains two main approximations. The first one is to keep trace only of the renormalization of the coherent part of the propagator. The second approximation is to assume that the spectrum \( \xi(k) \) remains non–renormalized. This assumption implies that we ignore the flow of the Fermi surface (FS) and of the Fermi velocity. Because of the particle–hole symmetry the flow of the FS is zero at half–filling, where we can expect that our form of the Green function is closer to reality than in the imperfectly nested (non–half filled) case.

The flow equation for \( Z(\theta) \) is derived from the general and exact one–loop RG equation for the complete selfenergy \( \Sigma(K) \) given in \[8\]. Let us suppose that we are at some scale \( l \),
and that we know the propagator \( \Pi \). We integrate \( dl \) further and look at what is the effective two–point vertex \( \Gamma_2 \) in the effective action \( S(l + dl) \); it is

\[
\Gamma_2(l + dl) = Z_l^{-1}(\theta)(i\omega - \xi(k)) + d\Sigma_l(K) .
\]

(2)

To find \( Z_{l+dl} \) we expand \( d\Sigma_l(K) \) in first order in \( i\omega \) to obtain

\[
Z_{l+dl} = Z_l(1 - Z_l\partial_{i\omega}d\Sigma) .
\]

(3)

The differential equation for \( Z \) follows immediately

\[
\partial_lZ_l(\theta) = -Z_l^2(\theta)\partial_{i\omega}[\partial_l\Sigma(K)]|_{\xi=i\omega=0} .
\]

(4)

Only the terms of \( \partial_l\Sigma \) which are linear in energy contribute. These are just the terms which are marginal upon zeroth order scaling in Shankar’s sense.\[15\] We will look for these terms.

The equation for \( \partial_l\Sigma \) can be written as

\[
\partial_l\Sigma(\theta, \epsilon, \omega) = \frac{\Lambda}{(2\pi)^2} \int \frac{d\omega'}{2\pi} \sum_{\nu} \int J_\nu(\theta', \Lambda)d\theta' G_l(\theta', \omega', \nu\Lambda)D_l(K, K'_{\nu}) ,
\]

(5)

where \( D_l = 2F_l - \tilde{F}_l \); \( F_l \) and \( \tilde{F}_l \) are energy–momenta dependent forward and backward scattering processes at the scale \( l \), related to the effective interaction in a way that

\[
F_l(K_1, K_2) = U(K_1, K_2, K_1) \quad \text{and} \quad \tilde{F}_l(K_1, K_2) = U(K_1, K_2, K_2).
\]

\( J_\nu(\theta, \Lambda) \) is the angle–resolved density of states at energy \( \xi = \nu\Lambda \). There is another, approximate but physically justified way to decompose \( D \). In fact, we will suppose that \( D_l \) can be written as a sum of p-p and p-h terms:

\[
D_l(K, K') = D_{pp}^l(K + K') + D_{ph}^l(K - K') .
\]

(6)

The p-p part of the propagator \( D \) depends only on the total energy–momentum \( Q_{pp} = (\omega_{pp}, q_{pp}) \equiv K + K' \) while the p-h part depends only on the energy–momentum transfer \( Q_{ph} = (\omega_{ph}, q_{ph}) \equiv K - K' \). As usual we skip the marginal part of the dependence on \( q_{pp} \) and \( q_{ph} \). For that purpose we note that both momenta can be written in the form

\[
q = q^{(0)}(\theta, \theta') + q^{(1)}(\theta, \theta', \xi, \xi') ,
\]

(7)

where \( q \) stands either for \( q_{pp} \) or for \( q_{ph} \), \( q^{(0)}(\theta, \theta') \) is the value of \( q \) when both momenta \( k \) and \( k' \) are at the Fermi surface, while \( q^{(1)} \) is the correction due to non–zero energies \( \xi \) and
Using standard scaling arguments we can skip \( q^{(1)} \) in the limit \( \Lambda / \epsilon_F \to 0 \) because the cutoff is imposed to momenta. Similar argument cannot be used for \( \omega_{pp} \) and \( \omega_{ph} \) because the integral in (3) runs over all frequencies independently of the actual cutoff \( \Lambda(l) \). We are therefore left with the locally dispersionless phononic propagators

\[
D_{pp}^{i}(\theta, \theta', Q_{pp}) \approx D_{pp}^{i}(\theta, \theta', i\omega + i\omega') = 2F_{pp}^{i}(\theta, \theta', i\omega + i\omega') - \tilde{F}_{pp}^{i}(\theta, \theta', i\omega + i\omega') \quad (8)
\]

and

\[
D_{ph}^{i}(\theta, \theta', Q_{ph}) \approx D_{ph}^{i}(\theta, \theta', i\omega - i\omega') = 2F_{ph}^{i}(\theta, \theta', i\omega - i\omega') - \tilde{F}_{ph}^{i}(\theta, \theta', i\omega - i\omega') . \quad (9)
\]

In these expressions we made the same pp-ph decomposition of the forward and backward amplitudes as we did with \( D \) in eq.(6). The following step is to re-constitute the \( i\omega \) dependence from the cutoff dependence. This can be done with logarithmic precision simply replacing \( \Lambda \) with \( i\omega \). The derivatives over frequency in eq.(10) (acting only on \( F \)-parts) are then readily calculated

\[
\partial_{i\omega} F_{pp,ph}^{i}(\theta, \theta', i\omega \pm i\omega')|_{i\omega=0} = \pm \frac{1}{i\omega'} \partial_l F_{pp,ph}^{i}(\theta, \theta') , \quad (10)
\]

and equivalently for backward amplitudes \( \tilde{F}_{pp,ph}^{i} \). The frequency–independent quantities \( \partial_l F_{pp}^{i}(\theta, \theta') \) and \( \partial_l F_{ph}^{i}(\theta, \theta') \) are the p-p and p-h parts of the \( \beta \)-function of the N–patch model, with appropriate configurations of the external momenta:

\[
\begin{align*}
\partial_l F_{pp}^{i}(\theta, \theta') &= \beta_{pp}\{U, U\}(\theta, \theta', \theta) \\
\partial_l \tilde{F}_{pp}^{i}(\theta, \theta') &= \beta_{pp}\{U, U\}(\theta, \theta', \theta') \\
\partial_l F_{ph}^{i}(\theta, \theta') &= -[X\beta_{ph}\{XU, XU\}](\theta, \theta', \theta) \\
\partial_l \tilde{F}_{ph}^{i}(\theta, \theta') &= [2\beta_{ph}\{U, U\} - \beta_{ph}\{U, XU\} - \beta_{ph}\{XU, U\}](\theta, \theta', \theta') ,
\end{align*} \quad (11)
\]

where all \( \beta \)-functions are given in ref.[8], but for the moment with dressed Green functions (11). Notice that the forward scattering has finite p-h contributions only from the ZS’ channel (1=3) while only the ZS channel (1=4) contributes to the backward scattering. This means that we forget about the contributions at zero momentum transfer. They are somewhat tricky, but don’t have any logarithmic part so that we can forget them.

We can also get rid of the \( Z \) factors in beta–functions of the eq.(11) by rescaling the fermions at every step of the RG in a way that

\[
\bar{\Psi}(\theta)Z_{l}^{-1}(\theta)\Psi(\theta) \to \bar{\Psi}(\theta)\Psi(\theta) \quad (12)
\]
and re-defining the effective interaction

\[ U_l(1, 2, 3) \rightarrow [Z_l(1)Z_l(2)Z_l(3)Z_l(4)]^{-1/2}U_l(1, 2, 3) . \] (13)

After transformations (12) and (12) the calculations of the \( \beta \)-functions to the one–loop order are identical to the case with \( Z = 1 \). Performing \( \omega' \) integral to logarithmic precision, the flow equation for \( Z(\theta) \) becomes

\[ \partial_l \log Z_l(\theta) = \frac{1}{(2\pi)^2} \int d\theta' J_-(\theta', \Lambda) \eta_l(\theta, \theta') \equiv \eta_l(\theta) , \] (14)

where

\[ \eta_l(\theta, \theta') \equiv \partial_l \{ 2[F_{pp}^l - F_{ph}^l] - \tilde{F}_{pp}^l + \tilde{F}_{ph}^l \} \{ \theta, \theta' \} \]

with \( \partial_l F \)-terms given by eqs.(11) and calculated with the bare Green functions, as in ref.[8]. Generalization of eq.(14) to finite temperatures can be done simply by replacing \( J_\sigma \) with \( \sum_\nu (-\nu)J_\nu n_F(\nu \Lambda) \).

Taking 1D “limit” of the eq.(14) is simple and instructive: instead of \( N \) patches we now have 2 patches: \( \theta = R \) (right) and \( \theta = L \) (left). Independent scattering amplitudes at non-rational filling are \( F(RL) = g_2 = U(RLR) \) and \( \tilde{F}(RL) = g_1 = u(RLL) \). We skip \( g_4 = u(RRR) \) from considerations because it has no logarithmic renormalization. The \( \theta \)-integrals reduce to summation over two points so that it is easy to reproduce the well-known result \( \eta = -\frac{1}{4\pi \nu_F}(g_1^2 - g_4^2 + g_2^2) \) \[16\]. It is the Luttinger liquid exponent.

In two dimensions the angle resolved \( \eta_l(\theta) \) can also be associated with some non-Landau (non-Fermi liquid) behavior. We see that \( \eta \) becomes finite if the forward and backward amplitudes have some logarithmic flow over a wide range of \( \theta \)-space (\( \Delta \theta \sim 1 \)). Another possibility for having finite \( \eta \) is when the Fermi surface is close to the van Hove singularities. “Close” means that the distance between the Fermi level and the van Hove singularity is comparable or inferior to the scale \( \Lambda_c \) at which interactions start to flow strongly.

We will now calculate the renormalization of \( Z_l(\theta) \) in the 2D Hubbard model at half-filling, from the knowledge of the scale dependence of the patch-dependent interaction \( U_l(1, 2, 3) \). In the RG equations of the previous section the discretization of \( \theta \) is done in a way described in ref.[8]. In the present case the Fermi surface is square so that there are two mechanisms for the suppression of quasiparticle residues. Namely, both above mentioned
conditions are fulfilled: (i) forward and backward amplitudes have logarithmic flows for any configuration \((\theta, \theta')\) if the two angles are at opposite sides of the Fermi surface, so that the available phase space is indeed large; (ii) van Hove singularities are at the Fermi surface and are nested. In fact, one can alternatively imagine a Fermi surface with non-nested van Hove singularities and nested parts elsewhere. Such a model would be even closer to the realistic situation in some HTC compounds. For the sake of rigor, we will however remain limited to the Hubbard model.

![Graph](image)

**FIG. 1:** The evolution of the angle–resolved quasiparticle weight on the Fermi surface. The lines are for \(l \equiv \log (4t/\Lambda) = 3.; 4.; 4.4; 4.95; 5.11; 5.17; 5.20\). The critical scale is \(l_c \approx 5.204\).

The result is shown in fig [1]. The figure shows \(Z(\theta_i)\) with \(0 \leq \theta_i \leq \pi/2\) on 9 equidistant points. Different lines correspond to different values of the scaling parameter as it approaches its critical point, i.e. when couplings diverge. Settings are the same as in ref.[8]: the Fermi surface was discretized into 32 patches and the initial interaction is \(U_0/(4t) = 0.333\). One sees that the Fermi surface is first destroyed at the van Hove points and than the regions of the FS destroyed by correlations grow larger and larger. This kind of flow is compatible with the interpretation that \(\Lambda_c\) is not the critical temperature for some symmetry braking, but merely the scale at which coherent quasiparticle cease to exist at the Fermi surface giving place to a gapped or pseudogapped liquid. The magnitude of the (pseudo-)gap is largest in
van Hove points and smallest on the diagonals of the Brillouin zone. The whole gap function $\Delta(\theta)$ then scales as $\Lambda_c \times f(\theta)$, where $f(\theta)$ is a function with the symmetry of the absolute value of the $d_{x^2-y^2}$-harmonic. This is the angle-resolved (pseudo-)gap, responsible for the correlation-induced angle-resolved localization. In other words the electrons near the van Hove points get much less mobile than those near diagonals. The similar scenario has been proposed by the Zürich group [10] even without concrete calculations of the quasiparticle weight.

The question of antiferromagnetism and superconductivity remains to be clarified. Let’s discuss this problem taking into account the scale dependent $Z(\theta)$ in the flow equations for the susceptibilities $\chi^{AF}(\theta, \theta')$ and $\chi^{SC}(\theta, \theta')$. Following the procedure given in ref. [8] and dressing the electronic propagators with $Z$–factors we get

$$\dot{\chi}_l^\delta(\theta_1, \theta_2) = \frac{1}{Z_l(\theta_1)Z_l(\theta_2)} \int d\theta \tilde{z}_l^\delta(\theta_1, \theta) D_l^\delta(\theta) \tilde{z}_l^\delta(\theta, \theta_2) . \tag{15}$$

This equation has the same structure as the one in ref. [8], with two modifications. First, we skip the retardation effects, replacing $l_\delta$ simply by $l$, because we are at half–filling. Second, the quantity $\tilde{z}_l^\delta(\theta_1, \theta)$ that has the role of a triangular vertex is somewhat modified. Its flow writes:

$$[\partial_l - \eta(\theta_1) - \eta(\theta_2)] \tilde{z}_l^\delta(\theta_1, \theta_2) = - \int d\theta \tilde{z}_l^\delta(\theta_1, \theta) D_l^\delta(\theta) V_l^\delta(\theta, \theta_2) . \tag{16}$$

The meaning of $\tilde{z}_l^\delta(\theta_1, \theta_2)$ is that

$$\tilde{z}_l^\delta(\theta_1, \theta_2) \equiv Z_l(\theta_1) z_l^\delta(\theta_1, \theta_2) Z_l(\theta_2)$$

so that the initial conditions for $\tilde{z}_l^\delta$ and for $z_l^\delta$ are the same. After discretization we integrate numerically equations (15) and (16). Fig. 2 shows the flow of the dominant eigenvalues of susceptibilities $\delta = AF$ and $\delta = SC$ near the divergence of scattering amplitudes. The thin line represents both (degenerated) susceptibilities for $U = 0$. Including only the one–loop vertex renormalization we get the strong enhancement and, as far as my numerics can say, even divergences of both AF and SC susceptibilities. If we now include also the one–particle–weight renormalization, both susceptibilities are radically reduced and lose their divergent behavior. On the other hand, the flow of the compressibility $\chi_c$ and magnetic susceptibility
\( \chi_\sigma \) is not affected by \( Z \)-renormalization because of the Ward identities. All above results support the statement that what happens at energy scale \( \Lambda_c \) is a flow towards a state with spin– and charge–gap or pseudogap, insulating and without AF or SC ordering.

![Graph showing scale dependence of the dominant components of both antiferromagnetic and superconducting susceptibilities at half–filling. A: due to renormalized vertex only and B: due to renormalized vertex and quasiparticle weight. The thin line represents the bare susceptibility.](image)

**FIG. 2:** Scale dependence of the dominant components of both antiferromagnetic and superconducting susceptibilities at half–filling, A: due to renormalized vertex only and B: due to renormalized vertex and quasiparticle weight. The thin line represents the bare susceptibility.

We finish this discussion with a few words about the effects of doping. Two regimes, *parquet* and BCS, exist also in the scaling properties of \( Z_l(\theta) \). In the whole parquet regime we expect the behavior governed by the proximity to the half–filling situation, so that the present results can be applied at all energies larger than the chemical potential \(|\mu|\). Upon doping the nesting becomes more and more imperfect, the p-h logarithm loses its divergence, the critical scale is more and more suppressed and the p-h and p-p channels get progressively less coupled. Eventually at strong enough doping and low enough \( \Lambda \) one is in the BCS regime where the effective physics is described by the 2D BCS theory, with renormalized and \( \theta \)-dependent interaction and quasiparticle weight. The anomalous dimension \( \eta(\theta) \) goes to zero because (i) the range \( \Delta \theta \), over which the forward and the backward amplitude have strong flow due to BCS diagram, scales with the cutoff, and (ii) the van Hove singularities are outside of the cutoff. The critical temperature for the onset of the superconductivity is not affected by the renormalized \( Z \), but the magnitude and angular dependence of the
superconducting order parameter are dressed by $Z(\theta)$. The symmetry of the gap remains $d_{x^2-y^2}$.

To summarize, I proposed a simple renormalization group theory for the angle–dependent destruction of the Fermi surface in the Hubbard model. The results offer a theoretical comprehension of the angle–dependent Fermi surface truncation in the cuprate superconductors in terms of the scattering processes of the electrons on the low–energy collective excitations of both particle–particle and particle–hole types. The theory, based on the N–patch model, is in its essence a controlled weak–coupling procedure that keeps trace of the dependence of the effective interaction and one–particle spectral weight on the position of the particles at the Fermi surface. As one approaches the critical scale $\Lambda_c$, the quasiparticle weight goes to zero first near the van Hove points, and the effect progresses toward Brillouin zone diagonals as one lowers the temperature. Dressing the flow equations for AF and SC response functions with the one–particle weight factors results in dramatical reduction of correlations of both types. The strongly correlated state just below $\Lambda_c$ is gapped or pseudogapped and without any long–range–order. Critical scale $\Lambda_c$ is interpreted as the pseudogap temperature $T^*$ found in cuprate superconductors.

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