Breakdown of the Landau–Fermi liquid in Two Dimensions due to Umklapp Scattering

C. Honerkamp(1), M. Salmhofer(2), N. Furukawa(1,3), and T.M. Rice(1)
(1) Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland,
(2) Mathematik, ETH Zentrum, CH-8092 Zürich, Switzerland,
(3) Department of Physics, Aoyama Gakuin University, Setagaya, Tokyo 157-8572, Japan
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We study the renormalization group flow of the interactions in the two-dimensional $t$-$t'$ Hubbard model near half filling in a $N$-patch representation of the whole Fermi surface. Starting from weak to intermediate couplings the flows are to strong coupling with different character depending on the choice of parameters. In a large parameter region elastic Umklapp scatterings drive an instability which on parts of the Fermi surface exhibits the key signatures of an insulating spin liquid (ISL), as proposed by Furukawa et al., rather than a conventional symmetry-broken state. The ISL is characterized by both strong $d$-wave pairing and antiferromagnetic correlations, however it is insulating due to the vanishing local charge compressibility and a spin liquid because of the spin gap arising from the pairing correlations. We find that the ISL is a consequence of a Fermi surface close to the saddle points at the Brillouin zone boundaries which provides an intrinsic and mutually reinforcing coupling between pairing and Umklapp channels.

I. INTRODUCTION

The Landau theory is widely used to describe Fermi liquids even when the interactions are strong, but it cannot be justified ‘a priori’. The cuprate high-$T_c$ superconductors show clear deviations from Landau theory in the normal state and it has long been argued that the key to understanding these materials lies in the breakdown of Landau theory. One possible cause is a symmetry-breaking instability such as magnetic order. But in experiments on underdoped cuprates, the marked deviations from Landau theory, such as the onset of the spin gap and gaps in the ARPES spectra near the saddle points of the Fermi surface (FS), appear without an obvious symmetry-breaking. This raises the question whether a breakdown of Landau theory without symmetry-breaking is possible. Actually one example is well known and understood, the insulating spin liquid states of even-leg ladder systems at half-filling, which have only short range magnetic order and unbroken translational symmetry. The key to this behavior are elastic Umklapp scattering processes across the FS which open up a charge gap at half-filling in addition to the spin gap caused by the pairing instability. In this paper the role of these processes in a two-dimensional system will be carefully examined.

Renormalization group (RG) methods allow an analytical treatment and, although the one-loop approximation is in principle applicable only at weak coupling, we can hope to learn about possible instabilities at the strong to intermediate couplings that apply in the cuprates. Such methods have long been successfully applied to one-dimensional models. The first attempts to extend this analysis to two dimensions were made shortly after the discovery of high temperature superconductivity. They focussed on the dominant role of scattering processes involving the Fermi surface regions in the vicinity of van Hove singularities.

Limiting the two-dimensional FS to just two patches reduces the problem to the flow of a small number of coupling constants which can be handled analytically. For repulsive interactions there are two possible fixed points involving flows either to weak coupling or to strong coupling. The possible relevance of the latter to the cuprates was emphasized by three of the present authors. They showed that under certain conditions the local charge compressibility flowed towards zero, indicating that here too Umklapp scattering opened up a local charge gap.

A proper treatment requires that the flow of interactions involving the whole two-dimensional Fermi surface be included. Already several RG investigations using a discretization of the Fermi surface into $N$ patches with $N \lesssim 32$ have been made. Zanchi and Schulz studied the RG-flows of a 32-patch weak coupling Hubbard model with only nearest-neighbor (n.n.) hopping in the kinetic energy term. They found a crossover between an antiferromagnetic (AF) ordered groundstate to a $d_{x^2-y^2}$-paired superconducting (SC) groundstate as the electron density was lowered away from half-filling. Recent more extensive results by Halboth and Metzner have largely confirmed the Zanchi-Schulz results, extending them to the case where there is a small next-nearest-neighbor (n.n.n.) hopping as well and investigating possible incommensurate AF-orderings. Although in both these investigations Umklapp scattering was included, the possibility of a fixed point behavior which would be similar to that of the two-leg ladder was not explicitly considered.

In this paper we will use a one-loop RG method with a discretization of the FS into $N$-patches ($N = 32 - 96$) to examine the flow of the coupling constants and susceptibilities under various starting conditions. Throughout we take a substantial value for the n.n.n. hopping ampli-
tude, \( t' \). On the one hand this is a realistic value for the cuprates. Secondly it moves the critical density, where the saddle points are at the FS, away from half-filling so that the saddle point effects are not mixed with nesting effects on the zone diagonals, as occurs when one sets \( t' = 0 \). When \( t' \) is substantial, one can distinguish three density regions. The simplest is the strongly doped region where the saddle points lie above the Fermi energy and Umklapp scattering is unimportant. Here the leading instability is to \( d \)-wave SC — a form of Kohn-Luttinger instability, in agreement with previous studies. We call this the \textit{d-wave dominated regime}. A second relatively straightforward density regime is the weak doping regime close to half-filling, where the approximate nesting of FS segments near the zone diagonals dominates and an AF instability is favored — again in agreement with previous studies. We call this region the \textit{approximate nesting regime}.

The intermediate regime is most interesting and will be the focus of this work. In this case the saddle points lie slightly below the Fermi energy and Umklapp processes involving these FS regions are highly relevant. We call this density region the \textit{saddle point regime}. As in the case of the two-leg ladder these Umklapp processes act to reinforce \( d \)-wave pairing so that this channel competes strongly with the AF instability. If one looks only at these two instabilities in the one-loop RG, it is not possible to decide which dominates. In the case of the two-leg ladder the uniform (Pauli) spin susceptibility flows to zero indicating that pairing instability prevails — a result confirmed when bosonization methods are used to examine the strong coupling state below the critical scale in the one-loop scheme. Similarly we find in the present case that an examination of the uniform susceptibility favors an assignment of the strong coupling fixed point to the class of the two-leg ladder. Further the local charge compressibility defined for these FS segments appears to scale also to zero. Below we present a detailed examination of this saddle point regime. We argue that rather than the simple crossover between \( d \)-wave SC and AF order as the density varies, found by previous authors, an interpretation in terms of the formation of an insulating spin liquid (ISL) which truncates the FS segments near the saddle points is justified. This ISL can be viewed as a form of \( d \)-wave RVB (Resonance Valence Bond) state as in the case of the two-leg ladder. Such a state represents a clear violation of the Landau theory, which does not rely upon a translational symmetry breaking mechanism.

Clearly an instability that partially truncates the Fermi surface with a charge gap can be seen as a forerunner of the Mott insulating state which occurs for intermediate to strong interactions. Since our motivation is to understand better the phase diagram of the high-\( T_c \) cuprates, we are most interested in such instabilities. However we are aware that there are other instabilities which appear in a weak coupling theory driven by the diverging density of states (DOS) at the van Hove points. These are the Stoner instability to ferromagnetism and, as remarked by Halboth and Metzner, the Labbé-Friedel or Pomeranchuck instability from square to rectangular symmetry. These split the saddle points when the Fermi energy lies near the van Hove singularity. This is a drawback of using a weak coupling approach to describe an intermediate to strong coupling problem.

We will simply ignore these DOS-related instabilities in the forward scattering channel and concentrate on those which we believe are more relevant as weak coupling signatures of the intermediate to strong coupling problem.

Finally, a defect of our one-loop approximation is that it does not lead to a description of the strong coupling phase of the system which it predicts. There are many approaches in the literature which attempt to construct a theory of such a state that we can loosely call a lightly doped \( d \)-wave RVB state. Our aim here is rather different and seeks to complement these strong coupling theories by examining the approach from the strongly overdoped regime which behaves as a conventional Landau-Fermi liquid with an instability towards weak-coupling \( d \)-wave superconductivity. The question we seek to address is the form of the instability in a Landau-Fermi liquid which leads to this doped RVB state. How does it differ from a simple \( d \)-wave superconducting instability and how does the proximity to the Mott insulating state at half-filling manifest itself?

\section{II. THE MODEL AND ITS FERMI SURFACE}

The kinetic energy of the \( t-t' \) Hubbard model is given by the tight-binding dispersion

\begin{equation}
\epsilon(\vec{k}) = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu
\end{equation}

with nearest neighbor (n.n.) hopping \( t \), next nearest neighbor (n.n.n.) hopping \( t' \) and chemical potential \( \mu \). Typically we choose \( t' = 0.3t \) which yields a small convex curvature of the FS around \((\pi, \pi)\) at higher fillings. Another essential curve is the Umklapp surface (US) which connects the van Hove points with straight lines. If the FS crosses the line, two particles at the FS can be scattered from one side of the US to the opposite one in an elastic process. As we will see, these additional scattering channels then enhance the scale of the transition to a strong coupling regime.

The initial interaction is taken to be a simple on-site repulsion

\begin{equation}
H_U = U \sum_{\vec{x}} n_{\vec{x},\uparrow} n_{\vec{x},\downarrow},
\end{equation}

which is constant in \( k \)-space. The effective interaction will develop a pronounced \( k \)-space structure in the RG flow.

In recent years there have been several RG approaches to the 2D Hubbard model. Schulz and Lederer et al.
studied the RG flow of the processes connecting the saddle points emphasizing the divergence of both AF and \(d\)-wave pairing correlations. Dzyaloshinskii discussed the weak coupling non-Fermi liquid fixed point of such a model. Similar studies have been given by Alvarez et al. and Gonzalez et al. Later on, in a related formalism based on parquet equations, Zeleznjak et al. examined the interplay between critical scales and effects of the FS curvature for a quasi 2D model restricted to approximately flat FS faces close to half-filling. Another study of nesting effects between flat FS segments was given by Vistulo de Abreu and Doucot. Zanchi and Schulz discussed the wave pairing correlations. Dzyaloshinskii noted by

\[
\frac{\partial g_i}{\partial y} + 2 \frac{\partial g_i}{\partial y} = 2 \frac{\partial g_i}{\partial y} - 3 \frac{\partial g_i}{\partial y}.
\]

where \(\frac{\partial g_i}{\partial y} \geq 0\) and \(\frac{\partial g_i}{\partial y} \geq 0\). It is useful to briefly review the analysis of the two-patch model by Furukawa et al. The second term on the right hand side of Eq. (1) enhances the basin of attraction of the strong coupling fixed point. Starting from the onsite repulsion \(g_1 = g_2 = g_3 = g_4 = U\) given by Eq. (1), the coupling constants diverge at a scale \(\Lambda_c\): \(g_1 \to +\infty, g_2 \to -\infty\) and \(g_2 \to +\infty; \)

\[
\dot{g}_i = 2d_i g_i (g_2 - g_1),
\]

\[
\dot{g}_2 = \dot{d}_1 (g_2^2 + g_1^2),
\]

\[
\dot{g}_3 = -2d_0 g_3 g_4 + 2d_1 g_3 (2g_2 - g_1),
\]

\[
\dot{g}_4 = -\dot{d}_0 (g_2^2 + g_1^2).
\]

III. THE TWO-PATCH MODEL REVISITED

We start with a brief discussion of the dominant mechanisms for the case where the FS is at the saddle points. These are most transparent in the two-patch model, where only small phase space patches around the saddle points at \((\pi, 0)\) and \((0, \pi)\) are kept. Neglecting possible frequency dependence we can approximately describe the scattering processes within and between the two patches by four coupling constants, \(g_1 \ldots g_4\), depicted in Fig. 1.

![FIG. 1. The relevant scattering processes in the two-patch model. The gray semi-circles denote the phase space patches around the saddle points. The interactions are assumed to be spin-independent and constant over the patches. In this notation the spin of the initial and final particle connected by an arrow has to be the same.](image)

The main terms which drive the one-loop RG flow of these vertices are: a) the particle-particle loop \(d_0\) with zero total incoming momentum, which diverges like \(\log^2(\Lambda_0/\Lambda)\) with decreasing energy scale \(\Lambda \leq \Lambda_0\) due to the van Hove singularity in the density of states and b) the particle-hole loop with momentum transfer \((\pi, \pi)\) denoted by \(d_1\) which, in presence of a small but nonzero \(t'\), diverges like \(\log(\Lambda_0/\Lambda)\) with a large prefactor. Keeping only these two contributions, and denoting \(y = \log(\Lambda_0/\Lambda)\), so that decreasing \(\Lambda\) means increasing \(y\), we obtain the RG flow equations

\[
\dot{y}_1 = 2\dot{d}_1 \dot{g}_1 (g_2 - g_1),
\]

\[
\dot{y}_2 = \dot{d}_1 (g_2^2 + g_1^2),
\]

\[
\dot{y}_3 = -2\dot{d}_0 \dot{g}_3 \dot{g}_4 + 2\dot{d}_1 \dot{g}_3 (2g_2 - g_1),
\]

\[
\dot{y}_4 = -\dot{d}_0 (g_2^2 + g_1^2).
\]
pling regime. This form of ground state is already signaled in the RG calculation by the suppression towards zero in the uniform spin susceptibility and the charge compressibility. The ISL in the two-leg ladder at half-filling is a form of RVB (resonance valence bond) state with an approximate d-wave pairing symmetry, but without any explicit translational or gauge symmetry breaking.

IV. THE TECHNIQUE

For the N-patch analysis we use a Wilson RG flow for one-particle irreducible (1PI) vertex functions. The full RG flow associates to every energy scale Λ below the bandwidth Λ0 an effective interaction for the particles with energies ϵ(\vec{k}) below Λ, in a way that the generating functional for the Green functions remains independent of the scale Λ. Because of this exact invariance, the effective interaction is no longer just quartic but an infinite power series in the fields. The full RG can be expressed as an infinite hierarchy of differential equations for the 1PI m-point vertex functions. Here we study a truncation of this infinite system in which only the 2- and 4-point functions are kept. For a derivation of the flow equations and a discussion of this truncation see [2]. Here we just state the results, which are rather simple. Because our model is two-dimensional, continuous symmetries cannot be broken by long-range order at any positive temperature. Therefore the effective action must be gauge-invariant and invariant under spin rotations, hence the four-point function is determined by the function \( V_\Lambda(\omega_1, \vec{k}_1, \omega_2, \vec{k}_2, \omega_3, \vec{k}_3) \) which describes the scattering of two incoming particles \((\omega_1, \vec{k}_1, \sigma_1)\) and \((\omega_2, \vec{k}_2, \sigma_2)\) into two outgoing particles \((\omega_3, \vec{k}_3, \sigma_3)\) and \((\omega_4, \vec{k}_4, \sigma_4)\) where \(\sigma_1 = \sigma_3\) and \(\sigma_2 = \sigma_4\), \(\omega_4 = \omega_1 + \omega_2 - \omega_3\), and \(\vec{k}_4\) is given by momentum conservation as \(\vec{k}_4 = \vec{k}_1 + \vec{k}_2 - \vec{k}_3\) modulo reciprocal lattice vectors. Because the spin of particle 1 (first incoming) is the same as that of particle 3 (first outgoing), and similarly for 2 and 4, we may draw the vertex corresponding to \( V_\Lambda \) as in Fig. 2 where the solid fermion lines going through at the top and the bottom of the vertex indicate that spin is conserved along these lines.

\[
G_\Lambda(\vec{k}, i\omega_n) = \frac{\chi_\Lambda(\vec{k})}{i\omega_n - \epsilon(\vec{k}) - \chi_\Lambda(\vec{k})\Sigma_\Lambda(\vec{k}, i\omega_n)}
\]

where \(\chi_\Lambda(\vec{k}) = 1 - \{\exp(|\epsilon| - \Lambda)/(0.05\Lambda)\} + 1 \}$ cuts off energies below \(\Lambda\). The other line stands for a single-scale propagator, \(S_\Lambda\).

The contributions to the self-energy have the graphical representation shown in Fig. 4. Here the internal line stands for a single-scale propagator \(S_\Lambda\).

In the main part of this paper we will neglect self-energy corrections to the propagator. Then \(G(i\omega_n, \vec{k}) = \chi_\Lambda(\vec{k})(i\omega_n - \epsilon(\vec{k}))^{-1}\) and the single scale propagator is simply \(S_\Lambda = \partial G_\Lambda/\partial \Lambda\). In Appendix A we show some results for a flow with the real part of the selfenergy on the FS taken into account. A more complete study including selfenergy effects, in particular the effects of the wave function renormalization, is underway.

FIG. 2. The vertex corresponding to \( V_\Lambda(\vec{k}_1, \vec{k}_2, \vec{k}_3) \)

The contributions to the right-hand side of the RGDE. (a) the particle-particle term (b) the crossed particle-hole term (c) the direct particle-hole terms; the first of these three graphs gets a factor -2 because of the fermion loop.

FIG. 3.

FIG. 4. The contributions to the selfenergy
We want to emphasize that our RG method does not rely on any form of scale invariance or scaling ansätze. The RG we set up in Ref. 24 provides an exact rewriting of the generating functional in terms of the effective action. The approximations we make in the present paper are (i) we discard the 1PI $m$–point functions with $m \geq 6$, (ii) we project the four–point function to the Fermi surface and frequency zero (see the next section), and (iii) we neglect the selfenergy corrections. We discuss the justification of (i) and (ii) in detail in Ref. 24. The justification for (ii) is a standard RG argument, and the full momentum dependence can in principle be reconstructed by calculating susceptibilities and related quantities. The justification of (i) is less trivial but possible for curved Fermi surfaces and in a specific scale range. (iii) is an approximation on which we shall improve in a further paper.

In systems with a Cooper instability, the flow always tends towards strong coupling at a sufficiently low scale. This happens even in repulsive systems because of the Kohn–Luttinger effect. However, in repulsive, and initially weakly coupled systems, the flow stays in the weak coupling regime down to a very low scale which may never be reached because the temperature, which acts as a natural infrared cutoff, stops the flow before that (in the usual Kohn–Luttinger effect, this scale is at most of order $e^{-\text{const.}/U^2}$; see Refs. 22,23). In this case the system stays weakly coupled above a certain temperature, and components of the Fermi surface limits of the four-point function can be identified with the Landau interaction function $f(\vec{k},\vec{k})$.

When the four–point function flows to strong coupling, the critical scale $\Lambda_c$ where the coupling constants diverge gives an estimate for the scale where the quasiparticles will be strongly modified or entirely destroyed (e.g. for the superconducting transition, a gap opens up).

The general picture we find in this model is that the flow always tends to strong coupling, but that for fillings where Umklapp scattering is favored by the geometry of the Fermi surface, the critical scale is strongly enhanced.

We note that in our RG method the temperature $T$ is retained as a physical parameter and that the RG procedure of decreasing the scale $\Lambda$ is a priori not related to changing the temperature. The four–point vertex at scale $\Lambda$ is the effective interaction for the modes with energy below $\Lambda$, and at the same time it is the four–point function with infrared cutoff $\Lambda$. For $\Lambda \ll T$, one should use the second interpretation. Note that because we do not impose a scale-dependent cut-off on the frequencies the flow does not stop exactly at the point when $\Lambda$ decreases below the smallest fermionic Matsubara frequency, $\omega_1 = \pi T$.

V. NUMERICAL IMPLEMENTATION

Next we describe the practical implementation of this RG scheme for the 2D Hubbard model. First we define a phase space discretization following Zanchi and Schulz. The idea is to discretize the Brillouin zone (BZ) into $N$ segments centered around $N$ lines. Each line with index $k \in \{1 \ldots N\}$ starts from the origin ($\Gamma$-point) in a certain angular direction and from the $Y$ point ($\pm \pi, \pm \pi$) so that the lines meet at the Umklapp surface. All phase space space integrations with measure $d^2k/(2\pi)^2$ are performed approximately as sums over the lines and integrations over the radial direction. These imply Jacobians for polar coordinates with respect to the $\Gamma$– or the $Y$-point, respectively.

FIG. 5. The Brillouin zone, Fermi and Umklapp surface and the lines in the patch centers for $N = 32$.

The interaction vertex $V_\Lambda(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ depends on two incoming wavevectors $\vec{k}_1$ and $\vec{k}_2$ and one outgoing wavevector $\vec{k}_3$ lying in segments $k_1$, $k_2$ and $k_3$ respectively (here we have already projected the frequencies to zero). The fourth wave vector $\vec{k}_4$ is fixed by momentum conservation. In a next approximation we select a large but finite number of coupling constants representative for certain regions in the space spanned by $\vec{k}_1$, $\vec{k}_2$ and $\vec{k}_3$. We choose to take these wave vectors as the crossing points of the lines $k_1$, $k_2$ or $k_3$ with the Fermi surface (FS), i.e. $\vec{k}_F(k_1)$, $\vec{k}_F(k_2)$ and $\vec{k}_F(k_3)$, which lie at the centers of the corresponding FS patches. By Taylor expansion and power counting arguments, the leading part of the flow is given by the coupling functions on the Fermi surface and at zero frequency. Thus we approximate the function $V_\Lambda(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ by $V_\Lambda(\vec{k}_F(k_1),\vec{k}_F(k_2),\vec{k}_F(k_3)) = V_\Lambda(k_1,k_2,k_3)$ for all wave vectors $\vec{k}_i$ in the same patch $k_i$, where $i = 1, 2, 3$.

VI. PARAMETERS

The initial condition for the flow of the couplings is given by Hubbard interactions $V_\Lambda(k_1,k_2,k_3) = U$. For most results discussed here we take $U = 3t$. We choose
this rather strong initial interaction because we are interested in the breakdown of the Landau-Fermi liquid due to interaction effects and do not aim at a classification of possible weak coupling instabilities. For the most results shown here $t' = 0.3t$, which is in the range of the values reported for the cuprates.

We will vary mainly the temperature $T$ and the particle density near and below half filling via the chemical potential $\mu$. We considered values between $\mu = -0.7t$ and $\mu = -1.35t$ which corresponds to fillings between $\approx 99\%$ and $\approx 62\%$ of half-filling. The Van Hove filling, where the FS exactly touches the saddle points, is given by $\mu = -4t' = -1.2t$.

For a given $\mu$ the dependence of the average particle number on $T$ is weak and irrelevant for the results. Both parameters $\mu$ and $T$ change the effective phase space for the various scattering processes. In particular, increased temperature provides a larger phase space for particle-hole processes with momentum transfer $(\pi, \pi)$, which play an important role. This is similar to the quasi-1D organic conductors where above a certain temperature the band curvature due to interchain hopping becomes irrelevant and 1D nesting effects determine the behavior of the system.

Typically we start at energy scale $\Lambda_0 = 4t$ and integrate the flow down to the critical scale $\Lambda$, which we define as the scale where the first coupling reaches a high value like $50t$.

VII. COUPLINGS AND SUSCEPTIBILITIES

We will discuss the results of our numerical RG scheme by analyzing the interaction on the FS and susceptibilities. In the flow to strong coupling we will identify the most relevant, i.e. divergent couplings. In the absence of scale invariance we cannot expect to obtain simple expressions for the form of their divergence, therefore we use their numerical values as function of the scale to make a qualitative comparison.

Along with the interactions we calculate the $d$-wave pairing susceptibility $\chi_{dw}$ for zero pair momentum and the spin susceptibility $\chi_s(\vec{q})$ around $\vec{q} = (\pi, \pi)$. The method we use is described elsewhere. Typically both $\chi_{dw}$ and $\chi_s(\vec{q})$ grow strongly as the interactions flow to strong coupling. In general the ratio of these susceptibilities is a complicated, non-monotonic, function of the scale. Therefore we do not attempt to draw sharp boundaries between different cases.

As discussed earlier in Sec.I it is often useful to analyze also the response the coupling to uniform external charge and spin fields given by

$$H_{c/s} = \int \frac{d\vec{k}}{(2\pi)^2} h_{c/s}(\vec{k}) (c_{k,\uparrow}^\dagger c_{\vec{k}+\vec{q},\uparrow} \pm c_{k,\downarrow}^\dagger c_{\vec{k}+\vec{q},\downarrow}),$$

where the subscripts $c$ and $s$ stand for charge and spin respectively. The $\vec{k}$-independent bare couplings $h_{c/s}^0$ develop a $\vec{k}$-dependence due to vertex renormalizations depending on $\vec{k}$ leading to dressed vertex functions $h_{c/s}(\vec{k})$. We cannot directly incorporate these renormalizations of the uniform external fields in our present RG scheme with IR cut-off as they involve only excitations in a low energy region of width $T$ around the FS. Therefore we calculate $h_{c/s}(\vec{k})$ using the RPA for the effective theory below the IR cut-off $\Lambda$. This means that we use the scale-dependent interactions $V_\lambda(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ in the one-loop vertex corrections for the external couplings, which then can be summed up and solved for $h_{c/s}(\vec{k}, \Lambda)$ (see Appendix A).

VIII. RESULTS: THREE REGIMES

In the density range we examined, we always found a flow towards strong coupling at sufficiently low temperature. The character of this divergence of the coupling functions varies continuously with density and temperature. However we can identify three qualitatively different regimes, which we will call the $d$-wave dominated regime, the saddle point regime and the approximate nesting regime, as illustrated in Fig. 8. Our analysis does not allow us to draw sharp boundaries between the different regions. Rather, the character of the strong coupling flow changes in a crossover–like fashion as one moves from one region into the other.

In order to show the main features we examine the flow for three densities typical for each regime. The Fermi surfaces and locations of the patch centers that label our coupling constants are displayed in Fig. 8. In Figs. 7 and 8 we show snapshots of the couplings at the scale where the largest coupling have exceeded the order of the bandwidth: we plot the dependence of the coupling $V_\lambda(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ with the first outgoing wave vector $\vec{k}_3$ fixed at point 1 closest to the saddle points or at point 3 closer to the BZ diagonal. In Fig. 8 we compare the flow of several relevant couplings as a function the RG scale and in Fig. 11 we plot the behavior of the $d$-wave pairing susceptibility $\chi_{dw}$ and the AF susceptibility $\chi_s(\pi, \pi)$. In the following we describe the three regimes in detail.

![Figure 6](image_url)  
**FIG. 6.** Fermi surfaces and the 32 points for the three different chemical potentials discussed in the text. $\langle n \rangle$ denotes the average particle number per site, i.e. $\langle n \rangle = 1$ corresponds to half-filling. The dots on the FS (solid line) indicate the patch centers with patch indices given by the numbers. The dashed line denotes the Umklapp surface (US).
a. The d-wave dominated regime: At band fillings around the van Hove filling $\mu = -1.2t$ and low temperature $T = 0.01t$ (see right plots in Figs. 3, 8, and 9), the divergence of the coupling functions only occurs at a low scale and the d-wave pair scatterings are by far the most strongly divergent couplings. In Fig. 3, they appear as red and blue features along the lines with patch numbers $|k_1 - k_2| = N/2$ (on these lines, the incoming pair momentum is zero). Other couplings like Umklapp and forward scatterings (the red, violet and black lines in Fig. 9) grow, too, but are much smaller than the Cooper couplings. This is the typical flow to strong coupling in the lightly shaded regions in Fig. 13. At low temperatures it extends also to densities slightly higher than the van Hove density.

A closer analysis shows that the d-wave component in the pair scattering is generated at intermediate scales by the particle-hole processes with momentum transfer $(\pi, \pi)$ corresponding to the second term in Eq. (5). This type of flow to strong coupling can be considered as a Kohn-Luttinger-type Cooper instability where the repulsive scattering in the particle-hole between the saddle points first generates a sizable initial value for the d-wave pair scattering and is then gradually cut off at lower scales because the phase space for the $(\pi, \pi)$-particle-hole processes decreases due to the shape of the FS.

The dominance of the d-wave Cooper scattering is also seen in the comparison of the susceptibilities: the d-wave pairing susceptibility $\chi_{dw}$ grows much faster than the AF susceptibility $\chi_s(\mathbf{q})$ (see Fig. 10). The uniform charge susceptibility $\kappa$ is somewhat suppressed at intermediate scales but very close to the instability the attractive Cooper scatterings in the forward scattering channel start to dominate the vertex corrections to the charge coupling and cause a pole in the RPA-like expression (see Eq. (3)) for $h_c(\mathbf{k})$ for $\mathbf{k}$ near the saddle points. This is then the reason of a sharp upturn in $\kappa$ (see Fig. 10) as also observed by Halboth et al. [4]. At low scales the uniform spin susceptibility $\chi_s(0)$ is suppressed to zero by the strong attractive $g_2$ couplings favoring singlet formation. However at higher scales, which are not related to the flow to strong coupling, the naive Stoner criterion for ferromagnetism is fulfilled due the large DOS around the van Hove filling. As discussed in the introduction, we ignore this effect.

b. The saddle point regime: Next we increase the temperature to $T = 0.04t$ and choose a band filling slightly above the van Hove filling such that the FS crosses the US (chemical potential $\mu = -t$). Now the scale where the couplings reach the order of the bandwidth is strongly enhanced. In Fig. 9 we observe that next to the d-wave pair scatterings new features have developed. The strongly repulsive interactions, for instance $(k_1, k_2) \approx (24, 25) \rightarrow (k_3, k_4) \approx (1, 17)$, correspond to $g_3$-type Umklapp scatterings which now diverge together with the repulsive Cooper couplings. The forward scatterings of $g_2$-type also show a strong increase towards the divergence. In addition there is a general increase for couplings with momentum transfer $(\pi, \pi)$ due to the enhanced influence of the particle-hole channel with this momentum transfer. On the other hand we also observe strongly attractive couplings emerging e.g. $(k_1, k_2) \approx (16, 17) \rightarrow (k_3, k_4) \approx (1, 18)$. These processes correspond to Umklapp $g_4$ processes of pairs with both incoming particles at the same saddle-point and outgoing particles on opposite sides of the FS. Since these pairs have small total momentum they couple into the Cooper channel and are driven to strong attraction along with the attractive Cooper couplings with zero pair momentum. This clearly demonstrates that Umklapp and Cooper channel are strongly coupled. For this choice of parameters the AF susceptibility grows considerably towards the divergence and is as large as the d-wave pairing susceptibility.

We call this the saddle point regime because the flow to strong coupling is dominated by the saddle point regions. Here, as we will show, we find the key signatures of the ISL and the basic mechanism of the two-patch model described in Sect. III is at work: the diverging $g_4$-type Umklapp scattering between the saddle point regions drives the forward scattering of $g_2$-type to strong repulsion, correspondingly the coupling $h_c(\mathbf{k})$ of external charge fields to these FS parts and thus their contribution to the charge compressibility $\kappa$ is increasingly suppressed as we approach the instability. This can be seen in Figs. 11 and 12. In contrast to the FS near the saddle points regions, which tends to incompressible i.e. insulating behavior, for $\mathbf{k}$ in the BZ diagonal the charge coupling $h_c(\mathbf{k})$ is more or less unchanged. Therefore one can expect that at wave vectors near $(\pi/2, \pi/2)$ gapless charge excitations will remain while near the saddle points the FS will be truncated. We use this particular behavior of the $\mathbf{k}$-space local charge compressibility to define the saddle point regime (darker gray regions in Fig. 13). Here the charge couplings around the saddle points continue to go to zero if we integrate the flow far out of the perturbative range without any indication of the upturn in $\kappa$ that we found in the d-wave dominated regime. However we repeat that in this analysis the border between saddle point and d-wave dominated regime is a continuous cross-over.

The uniform spin susceptibility exhibits a similar albeit somewhat more isotropic suppression (see Figs. 13 and 12) when we approach the instability in this saddle point regime. On the one hand this is plausible because the rapid growth of the d-wave susceptibility signals strong singlet pairing tendencies. On the other hand the AF susceptibility $\chi_s(\pi, \pi)$ seems to diverge as well, from which one might expect long range AF order, i.e. a strong coupling state with nonzero $\chi_s(0)$. 

FIG. 7. (color) Snapshot of the couplings $V_{\Lambda}(k_1, k_2, k_3)$ with first outgoing wave vector $k_3$ fixed at point 1 (see Fig. 6) when the largest couplings have exceeded the order of the bandwidth for the three different choices of chemical potential and temperature discussed in the text. The colorbars indicate the values of the couplings.

FIG. 8. (color) Snapshot of the couplings $V_{\Lambda}(k_1, k_2, k_3)$ with first outgoing wave vector $k_3$ fixed at point 3 (see Fig. 6) when the largest couplings have exceeded the order of the bandwidth for the three different choices of chemical potential and temperature discussed in the text. The colorbars indicate the values of the couplings. For $k_3 = 22$, $\vec{k}_2 - \vec{k}_3 \approx (\pi, \pi)$ for $\vec{k}_2, \vec{k}_3$ close to the US.

FIG. 9. (color) Flow of the couplings for 32-patch system: $d$-wave Cooper (blue dashed lines), $g_3$ Umklapp (e.g. $V_{\Lambda}(24, 24, 1), V_{\Lambda}(23, 23, 2)$, solid red lines), $g_2$ forward (e.g. $V_{\Lambda}(24, 1, 24), V_{\Lambda}(23, 2, 23)$, black dashed dotted lines), $g_4$ Umklapp couplings (e.g. $V_{\Lambda}(16, 17, 1)$, solid violet lines) and Umklapp scatterings $V_{\Lambda}(21, 21, 4)$ in the BZ diagonal (green) for the three different choices of chemical potential and temperature discussed in the text.
Here we argue that for the saddle point regime the more likely candidate is a spin liquid state with strong short range AF correlation but nonzero spin gap. As explained, the flow to strong coupling in this regime is caused by the coupling and mutual reinforcement of the \( d \)-wave pairing and the Umklapp processes between the broad saddle point regions. Therefore the strong coupling state should feature the singlet pairing of the \( d \)-wave channel and a strong enhancement of \( \chi_s(q) \) for \( q \approx (\pi, \pi) \). This is exactly what we observe for \( \chi_{dw} \) and \( \chi_s(q) \). Moreover due to the extension of the saddle point regions the peak of \( \chi_s(q) \) is very broad around \((\pi, \pi)\) and does not sharpen significantly in the flow. Therefore we expect a rather short AF correlation length of 2-3 lattice spacings. This is in contrast to the half filling, where we find sharp peaks in \( \chi_s(q) \) developing around \( q = (\pi, \pi) \) and where one would expect AF long range order at \( T = 0 \).

c. The approximate nesting regime: The plots on the left in Figs. 6 and 7 show the flow for a higher filling (\( \mu = -0.8t \)). In this case the leading interactions are Umklapp couplings between the BZ regions where the FS intersects the US (see red features in Fig. 6) while the importance of the vicinity of the saddle points decreases. We call this the approximate nesting regime. The dominating FS regions are now further away from the saddle points due to the higher filling. As a consequence the coupling between Umklapp and pairing channel decreases and the \( d \)-wave pairing processes become less relevant. This can be seen best from the weaker flow of the attractive Cooper couplings in Fig. 7. Now the AF susceptibility clearly exceeds the \( d \)-wave pairing susceptibility. This signals increasing AF ordering tendencies which are in accordance with sharper \((\pi, \pi)\) features in the interactions (see Fig. 8), decreasing suppression of \( \chi_s(0) \) relative to its initial value (see Fig. 9), and a sharper peak of \( \chi_s(q) \) around \((\pi, \pi)\). The charge susceptibility is also suppressed like in the saddle point regime, however the FS regions with smallest charge couplings stay fixed to the US and therefore move towards the BZ diagonal if we increase the filling.

We emphasize that in our RG treatment the next nearest neighbor hopping \( t' \) is important for the existence of a sizable saddle point regime. For zero or very small \( t' \) the FS is closer to the US in the BZ diagonals and the \((\pi, \pi)\) scattering between the rather flat FS faces dominates even more strongly than in our approximate nesting regime with more FS curvature. If we now decrease the band filling, at some point, as pointed out by Zheleznyak et al. and explicitly shown for the 2D case by Zanchi and Schulz, these processes are cut off at low scales and can only serve as generators of an attractive \( d \)-wave initial condition. With \( t' \) very small the system crosses rather sharply from a nesting regime into a \( d \)-wave dominated regime without going through a saddle point regime in between.

![Figure 10](image1.png)

**FIG. 10.** \( d \)-wave (heavy solid line) and AF susceptibility (heavy dashed line) for the three different choices of chemical potential and temperature discussed in the text. The thin lines denote the flow of the bare susceptibilities without vertex corrections. The mark at the \( \Lambda \)-axis indicates the scale, where the largest coupling reaches 10\( t \).

![Figure 11](image2.png)

**FIG. 11.** a) Flow of the charge compressibility \( \kappa \) normalized to their initial values of quasi-particles with wave vector \( \vec{k} \) on the FS as the electronic interactions flow to strong coupling from a 96 point calculation at \( \mu = -t \) and \( T = 0.04t \). The different lines are for points close to the saddle points (solid lines), and points closer to the BZ diagonal (dashed lines). We emphasize that in our RG treatment the next nearest neighbor hopping \( t' \) is important for the existence of a sizable saddle point regime. For zero or very small \( t' \) the FS is closer to the US in the BZ diagonals and the \((\pi, \pi)\) scattering between the rather flat FS faces dominates even more strongly than in our approximate nesting regime with more FS curvature. If we now decrease the band filling, at some point, as pointed out by Zheleznyak et al. and explicitly shown for the 2D case by Zanchi and Schulz, these processes are cut off at low scales and can only serve as generators of an attractive \( d \)-wave initial condition. With \( t' \) very small the system crosses rather sharply from a nesting regime into a \( d \)-wave dominated regime without going through a saddle point regime in between.
Apart from the suppression of the total charge compressibility described above there are other potential instabilities in the forward scattering channel. For example, as pointed out by Halboth and Metzner, there appears to be a strong tendency towards Labbé-Friedel or Pomernacki FS deformations which break the square symmetry. These are mainly rectangular deformation modes which split the degeneracy of the saddle points. However we will ignore those tendencies for the reasons discussed above. We have checked that a moderate deformation of the FS that breaks the square symmetry and leads to saddle point splittings of the order of the critical scale \( \sim 0.1t \) does not invalidate the results described above.

A difference to the two-patch analysis of Sec.III is that the saddle point regime, where we observe the ISL signature in our \( N \)-patch calculation, is found at positive temperatures and densities slightly higher than the van Hove density assumed in the two-patch analysis. The reason for the latter is that in the \( N \)-patch flow the FS parts away from the saddle points reinforce mainly the Cooper channel. Only if the FS really crosses the US there is sufficient low energy phase space for the Umklapp processes which then act together with the Cooper processes leading to the unusual strong coupling flow. For similar reasons nonzero temperature is needed for the saddle point regime. Moderate \( T \) smears out the FS and provides additional phase space for both the particle-particle processes with small total momentum and the particle-hole processes with momentum transfer \((\pi, \pi)\). Especially due to the latter there is a certain temperature range where this thermal phase space gain outweighs the ordinary decrease of the one-loop contributions for increasing \( T \) and the critical scale \( \Lambda_c \) is enhanced with respect to its \( T = 0 \) value.

IX. DISCUSSION AND CONCLUSIONS

We have presented an \( N \)-patch renormalization group analysis of the 2D Hubbard model and found indications that the path from a Fermi liquid-like state to the Mott insulating state may pass through a spin liquid phase with partially truncated FS and incompressible regions around the saddle points. Certainly the above results have to be interpreted with care and are only qualitative as they are an attempt to learn about possible strong coupling states from extrapolating weak–coupling flows. However they demonstrate that the breakdown of a Fermi liquid through an ISL state with partially truncated FS seems to be a viable concept, because in the saddle point regime the qualitative features of the ISL, e.g. spin and charge gaps, are visible as tendencies in our weak coupling approach. The essential phenomenon which can be identified as the cause for the ISL in the two-patch model, namely the coupling of Umklapp and pairing channel, is found to exist in a sizable temperature and density range also in our improved RG calculation, which includes the entire Fermi surface. We believe that this behaviour is robust because it only requires sufficiently large low energy phase space around the saddle points but does not rely on further details of the interaction or dispersion relation. What remains to be clarified is when this interplay between pairing and Umklapp processes, which frustrates symmetry-breaking tendencies and thus leads to an ISL, indeed represents an energetically favorable situation for the system. Another interesting and related aspect is the question of the precise conditions for which the overlap between the channels becomes too small, such that at \( T = 0 \) the system can still undergo a transition into a symmetry-broken state with presumably renormalized properties. In our calculation such symmetry-broken states are suggested on either side of the saddle point regime, e.g. in the \( d \)-wave dominated phase or closer to half-filling in the approximate nesting regime.

Our approach certainly bears some appealing features when compared to the high-\( T_c \) cuprates. However note that especially very close to half filling, in the approximate nesting regime, our description will be much too simple, as interaction effects which are not taken into account will become large. On the other hand further away from half filling in the saddle point regime we can hope to give a reasonable qualitative description of the driv-
ing forces for the breakdown of the Landau-Fermi liquid. Due to the mutual reinforcement between Cooper and Umklapp channel d-wave pairing correlations appear in a natural way at an enhanced scale on the threshold to the Mott state. If the insulating tendencies are strong enough they will lead to the ISL formation around the saddle points.

The stabilization of the ISL in the vicinity of the saddle points opens up a novel channel to enhance Cooper pairing on the remaining open parts of the FS. A similar mechanism was recently proposed by Geshkenbein et al.\textsuperscript{[10]} who examined a model with infinite mass preformed pairs existing at higher temperatures also in the vicinity of the saddle points. Let us assume that the ISL has formed in a region (called the A region) around the saddle points at an energy scale $\Lambda_{\text{ISL}}$. Then the dominant coupling between the ISL and the open FS parts (called the B regions) will occur through the exchange of zero momentum hole pairs in the Cooper channel. Further it will occur in the d-wave pairing channel. We denote by $V_{AB}$ the pair scattering matrix element between the ISL in the A-regions and the open B regions of the FS at the scale $\Lambda_{\text{ISL}}$ and by $\epsilon_A$ the energy relative to the chemical potential to add a hole pair to the ISL. Then, at energy scales $\Lambda \ll \Lambda_{\text{ISL}}$, an additional attraction $V_{BB}$ is generated between pairs in the open B regions, which has a pole at

$$\Lambda_{BB}^p = \Lambda_{\text{ISL}} \exp \left( -\frac{\epsilon_A}{N_{AB}} \right) , \quad (9)$$

$$N_{AB} = n_A \int_{\text{B-FS}} \frac{dk}{(2\pi)^2} \frac{V_{AB}^2(k)}{v_F(k)} .$$

Here the integral is over the Fermi surface of the B regions and $n_A$ denotes the number of intermediate states with two additional particles in the A regions per lattice site.

Although we do not have a full theory of the strong coupling phase, it is plausible to assume that in the A-regions a charge gap spreads out along the US in analogy to ladder systems which when lightly doped show simultaneously channels with and without charge gap.\textsuperscript{[11]} Then the open B-region of the FS will enclose an area measured from the US, determined by the hole density and so the superfluid density will be given by the hole density in the saddle point regime. Also there will be two energy scales, a higher one determining the onset of the ISL in the A regions, and a lower scale setting the transition temperature to superconductivity, $T_c$. These features are in nice qualitative agreement with the observations in the underdoped cuprates. However a full microscopic theory of the strong coupling phase and also the crossover to the more conventional d-wave superconductivity in the lower electron density d-wave regime remains to be worked out. Note that in the latter regime Umklapp scattering is irrelevant at low energy scales and the superfluid density is determined by the electron density, not the hole density.

Finally we note that the ISL concept might provide a microscopic basis for understanding the ARPES results on the cuprates which clearly show the truncation of the FS around the saddle points\textsuperscript{[12]} and also for phenomenological models\textsuperscript{[13]} which have proven to be plausible descriptions of the transport properties of the normal state of the underdoped high-$T_c$ cuprates.

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**APPENDIX A: THE ONE-LOOP SELF-ENERGY AND THE FERMI SURFACE SHIFT**

Here is a short overview of the results for the RG flow of the Fermi surface with fixed particle number. In order to obtain the FS flow we calculate in every RG step the change of the one-loop self-energy given by the contributions in Fig.\textsuperscript{[14]}\textsuperscript{a}. Due to the approximations made for the couplings this self-energy is constant over a single patch and only yields a patch-dependent shift of the Fermi surface. In order to keep the particle number fixed we adjust the chemical potential after each step. Quite generally we find that the FS parts which have the strongest repulsive scatterings with momentum transfer close to $(\pi, \pi)$ develop positive self-energies and are therefore are shifted inwards during the RG flow. The reason for that becomes clear if one considers a model interaction which is sharply peaked and repulsive at $\tilde{Q} = (\pi, \pi)$. For the self energy $\Sigma(\tilde{k})$ of a particle with wave vector $\tilde{k}$ on the FS one primarily has to examine the Hartree term (first term in Fig.\textsuperscript{[14]}\textsuperscript{b}) which is the main contribution for the typical divergence of the couplings. This diagram contains a propagator with a differentiated cut-off function and gives a positive contribution if the state $\tilde{k}$ is occupied for $\tilde{Q} = (\pi, \pi)$ and zero contribution otherwise. After subtraction of the FS average of $\Sigma(\tilde{k}_F)$ (or more precisely a constant which keeps the particle number fixed) this yields a positive selfenergy $\Sigma(\tilde{k}) > 0$ for particles outside the US (because then in general the state $\tilde{k} + \tilde{Q}$ is occupied for a FS with the densities and $\tilde{t}$ values we are interested in) and a negative shift $\Sigma(\tilde{k}) < 0$ for states inside the US. In our case the interaction only has a broad peak around $(\pi, \pi)$, therefore in general also FS points inside the BZ can be pushed inwards provided they are more affected by this repulsion than the average FS (this happens in the overdoped $\mu = -1.34$ case). The flow of the selfenergies with fixed FS close to the instability is shown in Fig.\textsuperscript{[14]}\textsuperscript{b} for different positions on the FS; for...
the FS points near the saddle points $\Sigma(\vec{k})$ flows to positive values, while for $k_F$ in the BZ diagonal it becomes negative. The resulting movement of the FS points if we include $\Sigma(\vec{k})$ in the dispersion, i.e. allow the FS to move, can be seen in Fig. 14 (a). It reveals the tendency of the FS to become flat, thus remaining in the vicinity of the Umklapp surface. In both cases the density is kept fixed at $\langle n \rangle \approx 0.88$ per site. Our RG results are in qualitative agreement with calculations using a model interaction due to AF spin fluctuations and the FLEX approximation.

FIG. 14. Left: Initial (open circles) and final (squares) FS for $t' = 0.3t$ and $\langle n \rangle \approx 0.88$ per site. Right: Flow of the self-energy on the FS (solid line: point closest to the saddle points, dotted line: point closest to BZ diagonal). The flow was stopped when the largest coupling reached the bandwidth $8t$.

APPENDIX B: CALCULATION OF THE UNIFORM SUSCEPTIBILITIES

The uniform ($\vec{q} \to 0$) susceptibilities describing the response to external charges and magnetic fields cannot be calculated successively by lowering the IR cut-off as they only involve degrees of freedom very close to the FS (the width of this region is given by the temperature). Therefore we determine these responses for the effective theory below the cut-off $\Lambda$ with the interactions at this scale as the effective interactions renormalizing the coupling to the external fields via vertex corrections. More precisely we calculate the effective couplings $h_i(\vec{k})$ ($i = c$ for charge and $i = s$ for spin) of quasiparticles on the FS, occurring in the Hamiltonian as

$$\langle \frac{d\vec{k}}{2\pi^2} h_{c/s}(\vec{k}) (c_{\vec{k},\uparrow}^\dagger c_{\vec{k},\uparrow} + c_{\vec{k},\downarrow}^\dagger c_{\vec{k},\downarrow}) \rangle$$

Denoting the bare coupling as $h_{c/s}^0$, we can express the effective coupling as

$$h_i(\vec{k}) = h_{c/s}^0(\vec{k}) + \langle \frac{d\vec{k}'}{(2\pi)^2} h_i(\vec{k}') \Phi(\vec{k}') V_i(\vec{k}', \vec{k}) \rangle$$

where $V_c(\vec{k}, \vec{k}') = (-V_A(\vec{k}, \vec{k}', \vec{k}) + 2V_A(\vec{k}, \vec{k}', \vec{k}))$ for the charge and $V_s(\vec{k}, \vec{k}') = -V_A(\vec{k}, \vec{k}', \vec{k})$ for the spin coupling. Diagrammatically this equation is shown in Fig. 15.

FIG. 15. Diagrammatic expression for the renormalization of the couplings $h_{c/s}(\vec{k})$ to external charge or magnetic fields.

In absence of an instability the coupling functions for zero momentum transfer $V_A(\vec{k}, \vec{k}', \vec{k}) - \frac{1}{2} V_A(\vec{k}, \vec{k}', \vec{k})$ and $-\frac{1}{2} V_A(\vec{k}, \vec{k}', \vec{k})$ would converge to the Landau interaction functions $f_c(\vec{k}, \vec{k}')$ and $f_s(\vec{k}, \vec{k}')$, respectively, and the expressions for the susceptibilities obtained with the above scheme reduce to the results from Fermi liquid theory.

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Below an energy scale determined by $t'/t$ and $\mu$, these terms become small compared to $\delta_0$, which then dominates the flow. However if the initial coupling is not very weak, the coupling constants diverge already above that scale.

We have also calculated the flow including a radial dependence of $V_s$, by keeping three radial points in each patch (inside, on, and outside of the FS, i.e. $(32 \times 3)^3$ coupling constants). The main conclusions are the same as the ones without radial dependence.

In the $t' = 0$ case close to half filling the states in the BZ diagonal are slightly more affected by the strong $(\pi, \pi)$-repulsion than the states at the saddle points. Therefore the FS expands towards the saddle points, although the trend is weaker than for $t' = 0.3t$.

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