Strong correlations and formation of “hot spots”
in the quasi-one-dimensional Hubbard model at weak coupling

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We study the anisotropic two-dimensional Hubbard model at and near half filling within a functional renormalization group method, focusing on the structure of momentum-dependent correlations which grow strongly upon approaching a critical temperature from above. We find that a finite nearest-neighbor interchain hopping is not sufficient to introduce a substantial momentum dependence of single-particle properties along the Fermi surface. However, when a sufficiently large second-nearest neighbor inter-chain hopping is introduced, the system is frustrated and we observe the appearance of so-called “hot spots”, specific points on the Fermi surface around which scattering becomes particularly strong. We compare our results with other studies on quasi-one-dimensional systems.

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I. INTRODUCTION

The one-band Hubbard model serves as a minimal model for various correlated electron systems, since it is capable of capturing a number of non-trivial phenomena which are due to the interplay between kinetic and potential energy. In one dimension, numerous theoretical methods are available which have led to a thorough understanding of the low-energy physics\cite{1}. In higher dimensions, however, rigorous statements are scarce and many controversies remain. It is therefore natural to ask the question how the cross-over from one to two or higher dimensions takes place. Furthermore, since the discovery of quasi-one-dimensional organic conductors and superconductors we have access to materials which are realizations of this physical situation. In these compounds many interesting observations were made during the last two decades, some of which are still calling for a conclusive theoretical description\cite{2}.

In this work we will consider the evolution of a model system near half-filling, upon increasing the dimensionality via an increase in the perpendicular kinetic-energy coupling between one-dimensional chains. To tackle this question, we employ a functional renormalization group (fRG) technique, which provides a rigorous framework for the computation of low-energy properties starting from a microscopic model\cite{3}. While this method reduces to the well-known gology RG in one dimension, it has been applied successfully to the two-dimensional case, where the angular dependence of the coupling function along the Fermi surface needs to be taken into account\cite{4}. By allowing for anisotropic hopping parameters we are in principle able to access the complete region from the one-dimensional to the two-dimensional case. In this work we will fix the degree of anisotropy and study the behavior of the system as a function of other parameters.

The dimensional cross-over in quasi-one-dimensional systems (and the intimately related phenomenon of “deconfinement”, i.e the Mott insulator to metal transition induced by increasing the inter-chain kinetic energy) have been investigated in recent years within several theoretical approaches. There is consensus on some aspects, but some disagreements between these studies do remain (mainly due to the different theoretical tools which have been employed, and the different regimes of parameters which have been investigated). The issue as such was raised by experimental studies on Beechgard salts. In particular, the optical spectroscopy experiments of Vescoli et al. revealed an insulator-to-metal transition as a function of increasing interchain hopping parameter, which changes with chemical composition\cite{5}. At the same time, Bourbonnais and Jérôme discussed these results within a scenario where a one-dimensional Mott insulator evolves into a metallic state when the inter-chain hopping reaches the order of the Mott gap\cite{6}.

Subsequently, several model calculations where made to substantiate and verify this concept. Biermann et al. employed an extension of dynamical mean-field theory (DMFT), the so-called chain-DMFT, which replaces the original problem by a chain self-consistently coupled to a bath, while taking into account the full intra-chain momentum dependence \cite{7}. They do indeed find a transition from an insulating to a metallic state when the interchain hopping is increased, as well as a crossover from a Luttinger liquid to a Fermi liquid at fixed interchain hopping, when the temperature is decreased. Essler and Tsvelik considered this problem starting from a one-dimensional Mott
insulator and using a resummed expansion in the inter-chain hopping. Using this approach, they suggested that the metallic phase does not develop immediately with a large Fermi surface resembling the non-interacting one. In contrast, close enough to the Mott insulating phase, Fermi surface pockets appear in specific locations, while large parts of the would-be Fermi surface remain gapped due to the influence of the one-dimensional Mott gap. The location of these pockets is such that the neighbourhood of the point \( k_a = k_b = \pi/2 \) (with \( k_a \) the momentum along the chain direction and \( k_b \) perpendicular to it) is gapped out and not part of the Fermi surface. This point thus corresponds to a “hot spot”, at which the scattering rate is very large (and can even lead to a complete suppression of quasiparticles at this point). While the chain-DMFT studies of Ref. 12 did not observe this phenomenon (perhaps because of the range of coupling or temperature), more recent studies of an anisotropic spinless model using chain-DMFT did observe a partial destruction of the Fermi surface with hot spots at the same location.

From the weak-coupling standpoint, early calculations suggested the occurrence of hot spots from a simple perturbative calculations of the scattering rate. Within a renormalization group treatment, Duprat and Bourbonnais found that for a finite and fixed value of the interchain hopping the influence of strong spin-density-wave fluctuations can lead to anisotropic scattering rates along a quasi-one-dimensional Fermi surface, leading to the emergence of hot spots. However, the locations of cold and hot regions are exactly exchanged with respect to the findings by Essler and Tsvetlik, with the hot spots found at \( k_b = 0 \) and \( k_b = \pm \pi \) in Ref. 12. It should be noted that these results were obtained for a system away from half filling, meaning that umklapp processes are suppressed in the RG treatment. In the present work, we focus on the half-filled case or its immediate vicinity, and use a functional RG technique which does take umklapp processes into account.

Thus, there exists a consensus that “hot spots” might form in quasi one-dimensional systems, but the various treatments do not agree on their location. It is tempting to speculate that this simply reflects the different locations of these hot regions in the weak and strong coupling limits. At any rate, there are some compelling experimental indications for strongly anisotropic scattering rates in quasi one-dimensional organic conductors, as pointed out early on in Ref. 14 and dicussed further in the conclusion.

### II. Model

We consider the one-band Hubbard model:

\[
H = \sum_{j,j'} \sum_{\sigma} t_{jj'} c_{j\sigma}^\dagger c_{j'\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow},
\]

with a local repulsion \( U > 0 \) and hopping amplitudes \( t_{jj'} = -t_a \) between nearest neighbors in the \( a \)-direction along the chains, \( t_{jj'} = -t_b \) between nearest neighbors in the \( b \)-direction perpendicular to the chains, and \( t_{jj'} = -t'_b \) between second-nearest neighbors in the \( b \)-direction. The corresponding dispersion relation reads

\[
\epsilon_k = -2t_a \cos k_a - 2t_b \cos k_b - 2t'_b \cos 2k_b.
\]

At half-filling and \( t'_b = 0 \) the non-interacting Fermi surface is perfectly nested. The introduction of a finite \( t'_b \) will allow us to study the effects of deviation from this perfect nesting condition. It is important to note that we do not linearise the dispersion in the chain direction, as is commonly done in RG treatments originating from the 1d g-ology setup. Therefore, the Fermi surface is perfectly nested only at half filling. Away from half filling perfect nesting is destroyed, even without a finite value of \( t'_b \). In the following all energies are given in terms of \( t_a \) which we set to unity.

### III. Method

In direct analogy to the technique applied in reference 12, we use the Wick-ordered version of the fRG to compute the one-loop flow of the interaction vertex and the two-loop flow of the self energy, as depicted in Fig. 1. The internal lines without slash in the Feynman diagrams correspond to the bare propagator

\[
D^\Lambda(k) = \frac{\Theta(\Lambda - |\xi_k|)}{ik_0 - \xi_k},
\]

where \( \xi_k = \epsilon_k - \mu \) and \( \Lambda > 0 \) is the cutoff; the lines with slash correspond to \( \partial_\delta D^\Lambda \), which is proportional to \( \delta(\Lambda - |\xi_k|) \).

We parametrize the interaction vertex \( \Gamma \) by its static values on a reduced number of points/patches on the non-interacting Fermi surface, as illustrated in Fig. 2. It is thus parametrised by a momentum-dependent singlet (triplet) component \( \Gamma_{s(t)}(k_1,k_2,k_3) \), where the \( k_i \) constitute a discrete set of momenta on the Fermi surface. We stress that this does not correspond to treating a
\[ \partial_\Lambda \Sigma = \Gamma \]

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FIG. 1: Flow equations for the self energy \( \Sigma^\Lambda \) and the two-particle vertex \( \Gamma^\Lambda \), respectively; the internal lines without slash correspond to the bare propagator \( D^\Lambda \), the lines with a slash to its \( \Lambda \)-derivative \( \partial_\Lambda D^\Lambda \).

In the present work, we do not directly compute the flow of the self-energy, but rather infer from the properties of the two-loop diagram what the influence of a strongly renormalized vertex function on the self energy will be. In the case of the two-dimensional Hubbard model this calculation has been done explicitly, giving us confidence with respect to this reasoning.

finite system, since internal integrations are done in the thermodynamic limit.

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\[ \Pi = (\pi, \pi) \]

FIG. 2: Patching scheme for \( N = 28 \).

IV. RESULTS

A. \( t'_b = 0 \) - perfect nesting

At \( t'_b = 0 \) and \( \mu = 0 \) the non-interacting Fermi surface is perfectly nested with nesting vector \( \Pi = (\pi, \pi) \) and defines the so-called Umklapp surface as illustrated in Fig. 3. For \( t'_b = 0 \) the problem reduces to the one-dimensional half-filled Hubbard model. In this case the divergence of Umklapp couplings at low energies signals the onset of the Mott insulating phase. When we analyze the one-loop flow of the interaction vertex for finite values of the interchain hopping \( t_b \), we find that the divergence of Umklapp processes persists at all finite values of \( t_b \), which we chose to be \( t_b = 0.1 t_a \) throughout this work. Namely the one-dimensional Umklapp couplings connect to two-dimensional Umklapp processes of the type \((k_F, k'_F) \rightarrow (k_F + \Pi, k'_F - \Pi)\) with momentum transfer \( \Pi = (\pi, \pi) \). The crucial point is that this divergence is nearly perfectly homogeneous along the Fermi surface. Due to the feedback of the interaction onto the self energy via the two-loop diagram, this implies that there are no isolated hot spots at which the dominant scattering processes are dominant compared to other regions on the Fermi surface. Instead, the whole Fermi surface is "hot". Along with Umklapp processes, the interaction develops divergences in the Cooper channel, also owing to the importance to scattering with wave vector \( \Pi = (\pi, \pi) \). The behavior of the coupling function illustrates this very clearly. In the left plot of figure 4 we display the singlet com-
eventually lead to a phase where all one-particle states along the Fermi surface exhibit a pseudogap. Since we look at a system at half filling it is essential to consider Umklapp processes, as mentioned above. We therefore extend the analysis offered in reference [12] and show in figure 4 in the right plot the interaction function $\Gamma_S(k_b^R, k_b^L, k'_b)$ on the Fermi surface in the so-called twin-Umklapp channel, meaning that both incoming momenta are identical, and $k_b^L(k_b^L)$ are momenta corresponding to right (left) movers in the standard terminology familiar from the one-dimensional case. We see that along the lines $k_b^L = k_b^R - \pi$ and $k_b^L = k_b^R + \pi$ the coupling function in this channel is also homogeneously peaked, confirming the conclusion drawn on the basis of the Cooper channel. We recall that in contrast to the one-dimensional case the system will eventually undergo a transition into an antiferromagnetic state at zero temperature. Here, however, we are concerned with finite-temperature precursor effects, which may legitimately be compared.

These results are distinct from those obtained in other RG calculations[12]. There, perfect nesting is artificially introduced due to a linearization of the dispersion in the chain direction, and Umklapp processes are neglected. The divergent couplings are then found only in the Peierls section of the Cooper channel for sufficiently small $t_b'$, leading to isolated hot spots at $k_b = 0$ and $k_b = \pm \pi$.

B. $t_b' \neq 0$ - effects of frustration

1. $\mu = 0$ - half filling

A finite second-nearest neighbor hopping $t_b'$ will destroy the nesting condition for all wave vectors on the Fermi surface, except for a few special points. We set the chemical potential to $\mu = 0$ and use $t_b = 0.1$ and $t_b' = 0.1t_b$. In this case the non-interacting system essentially remains half filled and the frustrated Fermi surface intersects the Umklapp surface at $k_b = \pm \pi/4$ and $k_b = \pm 3\pi/4$, as shown in Fig. 5. Then, at arbitrarily low energies Umklapp scattering of the type $(k_F, k_F) \rightarrow (k_F + Q, k_F - Q)$ is possible if and only if $k_F$ is located at the intersection between the non-nested Fermi surface and the Umklapp surface. The resulting RG flow of the interaction vertex shows a dominant divergence of the couplings corresponding to exactly these processes. This can best be seen in figure 6 where the coupling function is shown in analogy to figure 4. In contrast to the case $t' = 0$ the coupling function in both channels shows a strongly peaked behavior which is not homogeneous along the Peierls lines,

FIG. 4: Left: Singlet Vertex in the Cooper channel on the Fermi surface as a function of $k_b$ and $k'_b$. Right: Singlet Vertex in the Twin-Umklapp channel on the Fermi surface as a function of $k_b^R$ and $k_b^L$. Here $t_b = 0.1$, $t_b' = 0$, $T = 0.011$, $\mu = 0$, $U = 2.45$ (All energies in units of $t_b = 1$). In this case the Fermi surface is essentially perfectly nested.

ponent of the interaction function $\Gamma_S(k, -k, -k')$ on the Fermi surface as a function of $k_b$ and $k'_b$ at the end of the flow, in direct analogy to the analysis presented in reference [12]. The bare interaction is chosen in such a way that the temperature is slightly above the pairing temperature, at which the flow of the vertex function diverges. The interaction is homogeneously peaked along the lines $k'_b = \pi - k_b$ and $k'_b = -\pi - k_b$. We name these lines "Peierls lines" since they correspond to scattering processes in which a momentum $Q$ is exchanged between the two incoming particles and $Q$ is the generalization of $2k_F$ in one dimension at half filling and perfect nesting.

We thus see that all points on the Fermi surface are equally strongly affected by strong correlations appearing in the Cooper channel, which may
but which is peaked at the points where the Fermi surface intersects the Umklapp surface. This is reminiscent of a scenario in which there exist so-called hot spots, that is special points at which the scattering rate is particularly large or a pseudogap may appear in the spectral function, in analogy to the case of a two-dimensional system. Note that for the frustrated system the Peierls lines defined above in the plots of the vertex function correspond to scattering processes with wave vector $Q$ only at hot spots. Elsewhere the momentum transfer on the Fermi surface is incommensurate.

2. $\mu \neq 0$ - slightly doped system

Upon changing the chemical potential the hot spots mentioned above move along the Fermi surface. When $\mu$ is increased, the two points in each quadrant eventually merge until the Fermi surface touches the Umklapp surface at $(\pm \pi/2, \pm \pi/2)$. In figure 7 we show plots for the vertex function in analogy to figures 4 and 6. Indeed, the vertex function along the Peierls lines in both Umklapp and Cooper channel exhibits a strong increase in the diagonal region, corroborating the identification of the hot spots as originating from the points where the Fermi surface intersects the Umklapp surface. For even larger values of the chemical potential these points do not exist anymore and thus Umklapp processes will not feed back into the self energy. Similarly, upon decreasing $\mu$ the eight hot spots move towards the axis and eventually merge to form four hot spots located at $k_b = 0$ and $k_b = \pi$. Once more the structure of the vertex function reflects this, as can be seen in figure 8, although for the parameters chosen here the variation along the Fermi surface is somewhat weaker. For small enough values of $\mu$ the hot spots will again disappear.

V. DISCUSSION AND CONCLUSION

In summary, we have studied a quasi one-dimensional model of coupled chains at and near half-filling, using an fRG technique and focusing on the appearance of “hot” regions on the Fermi surface. In the presence of perfect nesting, we have found that the whole Fermi surface is hot. In contrast, in the presence of frustration ($t'_{tb} \neq 0$), isolated hot spots appear. The mechanisms for the formation of these hot spots is that the effective...
FIG. 7: Same as Figure 6 but here $\mu = 0.02$, $U = 3.126$. In this case the Fermi surface touches the Umklapp surface at $(\pi/2, \pi/2)$.

couplings (vertex functions) in the various channels become large in an anisotropic manner. The location of the hot spots corresponds to the intersection of the Umklapp surface with the Fermi surface. In general, there are eight hot spots, i.e. two in each quadrant of the Brillouin zone. Their precise location depends on the doping level and on the ratio $t'/t_b$. These results are perfectly consistent with previous weak-coupling fRG studies of the frustrated two-dimensional case. The location of these hot spots do not agree however with a previous weak-coupling RG study of a quasi one-dimensional model. As we have seen, a proper treatment of Umklapp processes, which are a key ingredient to the mechanism described in the present work, is essential. Because Ref. was motivated by the strongly metallic regime, it did not explicitly include these processes in the RG treatment, besides a mere renormalisation of the forward scattering amplitude.

There are naturally also some limitation to our fRG calculation. First, it is valid only in the weak-coupling regime. Second, the argument that a strongly peaked interaction can create hot spots on the Fermi surface relies on the low-dimensional properties of the model, the reason being that with increasing dimension the feedback of the interaction onto the one-electron self-energy via the two-loop diagram weakens and is eventually washed out. The method does take transverse Umklapp processes into account, which is essential to the main mechanism and observed features. This can already be achieved by a much simpler RPA calculation. However, the fRG not only provides an exact starting point relying on rigorous statements, it also modifies the RPA results. The critical scales are lower and in contrast to RPA the properties in Cooper and Umklapp channels are different at equal momentum transfer.

A different location of the hot spots was also found by strong-coupling techniques, such as the resummation of the expansion in the inter-chain
hopping of Ref. 9,10 and the recent chain-DMFT treatment of Ref. 11. This is less surprising, and it is tempting to speculate that the hot spot location may be determined by the regions in momentum space where the effective couplings are big in the weak coupling limit, while it is associated with regions in which the inter-chain kinetic energy is small in the strong coupling limit. Future studies at intermediate coupling are needed in order to elucidate this point and provide a consistent picture of how the location of the hot spots evolve from weak to strong coupling.

The possibility that electron-electron Umklapp scattering may account for the emergence of hot spots along a quasi-1d Fermi surface was first suggested by Chaikin in order to explain magic angles in the magnetoresistance data of Beechgaard salts. 14 Here we have shown on the basis of a microscopic model and a functional renormalization group approach how such a situation may arise. Angular dependent magnetoresistance oscillations experiments only provide indirect evidence for the formation of hot spots however, through a momentum dependence of the scattering rate on the Fermi surface which requires theoretical modelisation. Obviously, direct angular-resolved spectroscopy experiments (e.g photoemission), although very difficult to perform on quasi one-dimensional organic conductors, would be highly desirable in order to probe these effects experimentally.

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