Magnetic and superconducting instabilities of the Hubbard model at the van Hove filling

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We use a novel temperature–flow renormalization group technique to analyze magnetic and superconducting instabilities in the two-dimensional $t$-$t'$ Hubbard model for particle densities close to the van Hove filling as a function of the next-nearest neighbor hopping $t'$. In the one-loop flow at the van Hove filling, the characteristic temperature for the flow to strong coupling is suppressed drastically around $t'_c \approx -0.33t$, suggesting a quantum critical point between $d$-wave pairing at moderate $t' > t'_c$ and ferromagnetism for $t' < t'_c$. Upon increasing the particle density in the latter regime the leading instability occurs in the triplet pairing channel.

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In recent years the two-dimensional (2D) Hubbard model has mainly served as an idealized model in the efforts to understand the Mott-insulating, antiferromagnetic (AF), superconducting (SC) and more exotic properties of the high-$T_c$ cuprates, like the pseudo-gap or stripe phases. While the latter phenomena are still under current debate and the Mott-insulating state is generically restricted to larger onsite repulsion $U$, the AF and $d$-wave SC ground states in the Hubbard model can be understood, at least qualitatively, by calculations at weak or moderate $U$. Here, besides diagrammatic approaches taking into account subclasses of diagrams, like ladder summations and the fluctuation-exchange approximation, one-loop renormalization group (RG) methods restricted to the saddle point regions and more recently taking into account the whole Fermi surface have become a popular method to study the interplay between magnetism and superconductivity in the Hubbard model. They indicate that for small nearest-neighbor hopping $t'$ and close to half-filling, the weakly coupled state is unstable with respect to AF fluctuations, while at smaller or larger electron densities the RG flow exhibits a Cooper instability in the $d_{x^2-y^2}$-wave channel. For $t' \approx -0.25t$ to $-0.3t$ on the hole-doped side, the change from AF to $d$-wave instability leads over an intermediate regime, the saddle point regime of Ref. \textsuperscript{2}.

Originally the Hubbard model was introduced by Hubbard, Gutzwiller, and Kanamori with a somewhat different motivation, namely as a model to describe the metallic ferromagnetism in the transition metals. Since then several attempts have been undertaken to clarify the conditions for itinerant ferromagnetism within the Hubbard model and related systems. For several classes of one-dimensional and higher-dimensional models, spin polarized ground states can be proven to exist, and also in the limit of infinite dimensions a number of clear results exist. For the 2D $t$-$t'$ Hubbard model at large $U$ Becca and Sorella recently found numerical evidence for a Nagaoka phase close to half-filling. At weak to moderate $U$ however the situation is more involved. Hartree-Fock treatments and more recently $T$-matrix approximation calculations combined with Quantum Monte Carlo and parquet approaches indicated that for larger absolute values of the next-nearest neighbor hopping $t'$ the ground state should be ferromagnetic (FM) in a certain density range around the van Hove-filling where the Fermi surface is near the saddle points of the band dispersion. A one-loop scaling analysis restricted to the saddle-point regions indicated similar tendencies. Nonetheless, one-loop RG calculations derived from exact RG equations and covering the full FS have so far not indicated any FM ground states. Moreover the competition between FM and SC ground states remains an open problem.

In this Letter we reinvestigate possible instabilities of the 2D $t$-$t'$ Hubbard model towards magnetic and superconducting phases from the weak-coupling perspective. The microscopic Hamiltonian we study is

$$H = -t \sum_{\text{n.n.n.s}} c_{i,s}^\dagger c_{j,s} - t' \sum_{\text{nn.n..s}} c_{i,s}^\dagger c_{j,s} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

with onsite repulsion $U$ and hopping amplitudes $t$ and $t'$ between nearest neighbors (n.n.) and next-nearest neighbors (n.n.n.) on the 2D square lattice. We apply a novel one-loop RG scheme covering the full FS which we call the temperature-flow ($T$-flow) RG scheme. Like the approaches in Refs. it is derived from an exact RG equation. However, no infrared cutoff is used, and instead the temperature $T$ itself is the flow parameter. This new feature allows for the first time an unbiased comparison between AF and FM tendencies, whereas RG schemes with a flowing infrared cutoff artificially suppress particle-hole excitations with low wavevectors. A detailed discussion of this issue and a derivation of the $T$-flow RG equations are given in Ref. \textsuperscript{4}. Using the RG formalism, we obtain a hierarchy of differential equa-
utions for the one-particle irreducible $n$-point vertex functions $\Gamma_T^{(n)}$ as functions of the temperature. Integration of this system gives the $T$-flow. We pose the initial condition that at a higher temperature $T_0$ the single-particle Green’s function of the system is described by $G_0(i\omega, \vec{k}) = [i\omega - \epsilon(\vec{k})]^{-1}$ and the interaction vertex is given by a local repulsion $U$. This is justified if $T_0$ is large enough. We truncate the infinite system of equations by dropping all $\Gamma_T^{(n)}$ with $n > 4$. In the present treatment we also neglect self-energy corrections and the frequency dependence of the vertex functions. This restricts the scheme to a one–loop equation for the spin–rotation invariant four-point vertex $\Gamma_T^{(4)}$. Starting with weak to moderate interactions, we follow the flow of $\Gamma_T^{(4)}$ as $T$ decreases.

$\Gamma_T^{(4)}$ is determined by a coupling function $V_T(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ [3]. For the numerical treatment, we define elongated phase space patches around lines leading from the origin of the BZ to the $(\pm \pi, \pm \pi)$-points, and approximate $V_T(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ by a constant for all wave vectors in the same patch. We calculate the RG flow for the subset of interaction vertices with one wavevector on the FS representative for each patch, with initial condition $V_T(\vec{k}_1, \vec{k}_2, \vec{k}_3) = U$. Most calculations were performed using 48 patches. Further we calculate several static susceptibilities, as described in Ref. [3]. Here we focus on the most divergent ones, namely $d_{x^2-y^2}$-wave and $p$-wave pairing susceptibilities, the AF susceptibility $\chi_s(\vec{q} = (\pi, \pi))$ and the FM susceptibility $\chi_s(\vec{q} \to 0)$. This way we analyze which classes of coupling functions and which susceptibilities become important at low $T$. For a large parameter range, we observe a flow to strong coupling. The approximations mentioned above fail when the couplings get too large. Therefore we stop the flow when the largest coupling exceeds a high value larger than the bandwidth, e.g. $V_{T,\text{max}} = 18t$. This defines a characteristic temperature $T_c$ of the flow to strong coupling. Because breaking of continuous symmetries is impossible in 2D at $T > 0$, we interpret $T_c$ as an estimate for the temperature where ordering occurs when a small additional coupling in the third spatial direction is included.

Here we describe the results for the RG flow of the coupling function for the 2D Hubbard model with initial interaction $U = 3t$ and varying value for the next-nearest neighbor hopping amplitude $t'$ from a 48-patch calculation (the crosses show data for 96 patches). The chemical potential is fixed at the van Hove value $\mu = 4t'$. $T_c$ is defined as temperature where the couplings reach values larger than $18t$. As criterion for the distinction between antiferromagnetic, $d_{x^2-y^2}$-wave pairing and ferromagnetic regime we use the temperature derivatives of the susceptibilities at the scale where the couplings become larger than $10t$.

Lin and Hirsch [3] analyzed the Hartree-Fock phase diagram for the $t$-$t'$ Hubbard model and found the FM state to be stable against the AF state for $t' < -0.24t$. Since they used the bare Hubbard repulsion, the $d_{x^2-y^2}$-wave phase is absent. The critical $t'$-value from Hartree-Fock is practically equivalent to the critical $t'_c \approx -0.33t$ from the RG treatment. On the other hand in Hartree-Fock one would find a first order transition at $t'_c$, while in the RG the characteristic temperature gets suppressed to lowest values, hinting at a quantum critical point. A $T$-

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matrix approximation (TMA) applied by Hlubina et al. indicated a stable fully polarized FM state beyond a critical $t' \approx -0.43t$. The screening in the particle-particle channel of the TMA is included in our $T$-flow scheme, which gives a somewhat larger window for a FM state with nonzero polarization at the VH filling. The density range around the VH filling where FM dominates gets more and more narrow as $t'$ is decreased towards $t'_0$. Recently Irkhin et al. applied a parquet scheme with a simplified dispersion and found indications for FM at the VH filling for very similar values of $t'$.

A crucial feature of models where large-spin ground states have been found is a sharp peak of the density of states (DOS) at the bottom of the band. This property is shared by the 2D $t$-$t'$ Hubbard model for $t' \approx -0.5t$, but at the van Hove filling, the DOS is also peaked at the Fermi level. In our RG calculation the DOS at the Fermi level, and not that at the bottom of the band, is essential for the FM tendencies: they also exist, and dominate, for smaller $|t'|$ in the range described above, and they are strongly reduced when the Fermi level is raised above the VH energy (see below). This sensitivity of the FM regime to the FS location points to another effect which is not included in the present calculation. It is probable that the inclusion of selfenergy effects in the flow will shift the FS and alter the low energy DOS such that the actual FM regime might be shifted, or changed more strongly. The analysis of these effects is left for future work.

FIG. 2. Flow of the AF (dashed line), $d$-wave pairing (solid line) and FM (dotted line) susceptibilities in the AF nesting regime (left plot, $\mu = -0.01t$), $d$-wave regime (middle plot, $\mu = -t$) and FM regime (right plot, $\mu = -1.8t$). The crosses (triangles) on the horizontal axes denote the temperatures where the largest couplings reach 5$t$ (10$t$). The insets show the Fermi surfaces and the 48 points in the Brillouin zone for which the coupling function is calculated.

Next we investigate the flow to strong coupling for densities away from the VH filling. The RG flow for smaller $|t'|$ is very similar to the flow found with the momentum-shell techniques which has been extensively discussed in Refs. Therefore we now focus on the case $t' < -0.33t$ corresponding to the FM regime at the VH filling and search for SC tendencies when the band filling is varied. In the 2D Hubbard model the occurrence of triplet pairing in vicinity of a FM phase has been proposed by several authors. Our approach allows a more detailed analysis of this interplay.

The Cooper pair scattering $V_T(\vec{k}, -\vec{k}, \vec{k'})$ transforms according to one of the 5 irreducible representations of the point group of the 2D square lattice. Among those there is the one-dimensional representation with $d_{x^2-y^2}$-symmetry important for smaller $|t'|$ and the two-dimensional representation transforming like $p_x$ and $p_y$.

In a solution of the BCS gap equation, components belonging to different representations do not mix, while e.g. within the $p$-representation components $p_x \propto \cos \theta$ and $p_y \propto \sin \theta$ and corresponding higher harmonics $\propto \cos 3\theta$ and $\propto \sin 3\theta$ (also called $f$-wave) will occur together.

As shown in the right plot of Fig. 3 for $t' = -0.45t$, the critical temperature drops by several orders of magnitude when we increase the particle density per site from the VH value $\langle n \rangle \approx 0.47$ at $\mu = -1.8t$ to $\langle n \rangle \approx 0.58$ at $\mu = -1.7t$. Further upon moving away from the VH filling, the growth of the FM susceptibility gets cut off and the $p$-wave triplet SC susceptibilities with symmetry $p_x \propto \cos \theta$ or $p_y \propto \sin \theta$ diverge at low temperature. Higher order harmonics $\propto \cos 3\theta$ and $\sin 3\theta$ diverge in a weaker fashion. The pair scattering at low $T$ in this parameter range is shown in Fig. One nicely observes that the pair scattering involving particles close to the saddle points is suppressed as the odd-parity nature of the $p$-wave pairing requires an opposite sign of the pair scattering $V_T(\vec{k}, -\vec{k}, \vec{k'})$ e.g. for $\vec{k'} \approx (0, \pi)$ and $\vec{k'} \approx (0, -\pi)$. Comparing the temperature derivatives of FM and SC susceptibilities when the leading couplings become larger than $12t$, the transition from the FM to the $p$-wave SC regime occurs at a particle density $\langle n \rangle \approx 0.52$ per site or $\mu = -1.76t$. Again, just as in the interplay between AF and $d_{x^2-y^2}$ SC fluctuations for small $|t'|$, our one-loop flow to strong coupling exhibits a smooth evolution from the FM dominated to the $p$-wave dominated instability. This suggests a transition between the two types of ordered states as a function of the band filling provided that symmetry-breaking at $T > 0$ becomes possible in a three-dimensional environment. From our analysis the transition appears to be first order, but additional interaction effects beyond our one-loop calculation could change that.

With our method we cannot calculate the SC gap function directly, but we can use the pair scattering obtained from the RG flow as a pair potential in the BCS gap equation. In our case, it is plausible to assume that the SC gap function will be a nodeless superposition of the two components with symmetries $p_x$ and $p_y$, e.g. given by $\Delta(\vec{k}) = \Delta_0(\vec{k}) (k_x + i k_y)$, which maximizes the condensation energy. The real–valued prefactor $\Delta_0(\vec{k})$ takes care of the anisotropy within symmetry-related FS parts. The direction of the Cooper pair spin remains indeterminate in the absence of spin-orbit coupling. The strongly angle-dependent gap function calculated with the rescaled pair
scattering taken from the RG flow is shown in Fig. 4. A similar SC order parameter is under debate for the superconducting state of Sr$_2$RuO$_4$ [22]. In this quasi-2D system one of the three Fermi surfaces has a similar shape as the case studied above. It will be interesting to investigate the RG flow and the SC properties suggested by that in a more realistic three-band model.

FIG. 3. Left: Flow of ferromagnetic (solid lines) and $p_x$-wave (dashed lines) susceptibilities for $t' = -0.45t$ at $\mu = -1.78t$ (thick lines) and $\mu = -1.74t$ (thin lines). Right: Characteristic temperature $T_c$ where the largest couplings reach $18t$ versus chemical potential $\mu$.

FIG. 4. Left plot: Pair scattering $V(\vec{k}, -\vec{k}, \vec{k}_3)$ with $\vec{k}$ varying around the Fermi surface for $t' = -0.45t$ and $\mu = -1.71$ at $T = 1.1 \cdot 10^{-6}t$. For the solid line $\vec{k}_3$ is fixed close to the saddle point ($-\pi, 0$) while for the line with the dots, $\vec{k}_3 \approx (-1.06, -0.86)$ is near the zone diagonal. Middle plot: Real and imaginary part of the SC gap function obtained from the solution of the BCS gap equation with the rescaled pair scattering from the RG flow. Right plot: gap magnitude.

In conclusion, using the new temperature-flow RG scheme, we have given a comprehensive analysis of the flow to strong coupling for the 2D $t$-$t'$ repulsive Hubbard model on the square lattice. The flow to strong coupling close to half-filling for small next nearest neighbor hopping $t'$ with its AF and $d_{x^2-y^2}$-pairing regimes is qualitatively similar to the RG flow known from the momentum-shell techniques [3]. For larger absolute values of $t'$ beyond a quantum critical point at $t' \approx -0.33t$ the flow to strong coupling is dominated by FM fluctuations. This has not been found with the momentum-shell schemes used previously [3] for the reasons explained in Ref. [2]. Finally, for larger $|t'|$, when the electron density is increased slightly above the VH density, the FM tendencies get cut off at low T and the flow to strong coupling is dominated by triplet SC correlations suggesting a highly anisotropic energy gap.

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