Functional renormalization group study of superconductivity in the two-dimensional Hubbard model

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The cuprate high-temperature superconductors attracted a lot of research interest since their discovery more than a quarter of a century ago. The reason is not only the high critical temperature for superconductivity, but also the competition of instabilities and the intriguingly rich phase diagrams. The latter include antiferromagnetic or d-wave superconducting phases and more exotic behavior like the so-called pseudogap. In these materials, fluctuation effects are particularly strong due to the reduced dimensionality that is caused by the layered crystal structure. This gives rise to enhanced spin as well as charge fluctuations and a strong renormalization of electronic quasiparticles.

The two-dimensional Hubbard model is believed to capture the essential physics of these materials. It is defined by the Hamiltonian

$$H = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where $c^{(\dagger)}_{i\sigma}$ creates (annihilates) an electron with spin projection σ on site i and $n_{i\sigma}$ is the density of electrons with spin projection σ on site i. t_{ij} describes the hopping between lattice sites and is restricted to nearest neighbor hopping with amplitude t and next-nearest neighbor hopping with amplitude t'. U is the strength of the on-site repulsion. In this model, d-wave superconductivity is difficult to detect with numerical methods due to finite size and temperature restrictions. The reason is that superconductivity emerges only on energy scales that are much smaller than the bare ones like the hopping amplitudes or the interaction.

We used the functional renormalization group method (for a recent review, see [1]) to study the ground state of this model. The method is unbiased, treats all interaction channels on equal footing and copes with hierarchies of relevant energy scales over several orders of magnitude. The method proved very successful for the classification of weak-coupling instabilities of the Hubbard model and unambiguously established the formation of d-wave superconductivity at least at weak-coupling. However, these instability analyses were not able to study the properties of the symmetry broken phases.

Our work allowed to continue the renormalization group (RG) flow into the symmetry broken state in case the leading instability is towards d-wave superconductivity. We studied the structure of the Nambu two-particle vertex in a singlet superconductor and identified its important singular dependences on external momenta and frequencies. This allowed for a decomposition of the vertex in interaction channels and their efficient parametrization as boson-mediated interactions. Extending ideas by Husemann and Salmhofer [2] to the case of symmetry breaking in the Cooper channel, we derived channel-decomposed renormalization group equations for the effective interactions in the channels. These equations isolate the singular dependence on external momenta and frequencies in one variable per equation, thus proving a good starting point for the formulation of approximations for the vertex and its efficient computation [3]. We also applied the channel-decomposition scheme for the vertex and the renormalization group equations to the two-dimensional attractive Hubbard model at zero temperature, which can be seen as a good testing ground for new approximation schemes. For the weak-coupling regime of this model, we obtained results for the superconducting gap that are in good agreement with values reported in the literature and gained a comprehensive understanding of the Nambu two-particle vertex in an s-wave superconductor.

For the repulsive Hubbard model, we parametrized the effective interactions in the density, magnetic and pairing channels as boson-mediated interactions with exchange propagators for the s- and d-wave channels. Below the critical scale, the pairing channel describes the amplitude and phase mode of the superconducting gap. As an example, the effective interaction describing the amplitude mode of the gap was approximated as

$$A^\Lambda_{\boldsymbol{k}\boldsymbol{k}'}(\boldsymbol{q}) = A^\Lambda_s(\boldsymbol{q}) + A^\Lambda_d(\boldsymbol{q}) f_d(\boldsymbol{k}) f_d(\boldsymbol{k}'),$$

where A^Λ_s and A^Λ_d describe the s- and d-wave components, respectively, and $f_d(\boldsymbol{k}) = \cos k_x - \cos k_y$ is a form factor of d-wave symmetry. Similar ansätze were used for the other channels, too. Λ is the RG scale that is introduced in order to organize the integration over fermionic modes in a scale-separated way, proceeding from high to low energy scales. So far, the frequency dependence of the vertex and the self-energy were neglected. This framework of approximations was used to compute the critical scales for antiferromagnetism and d-wave superconductivity as well as the d-wave superconducting gap as a function of the interaction strength U, the next-nearest neighbor hopping t' and the fermionic density n at zero temperature.

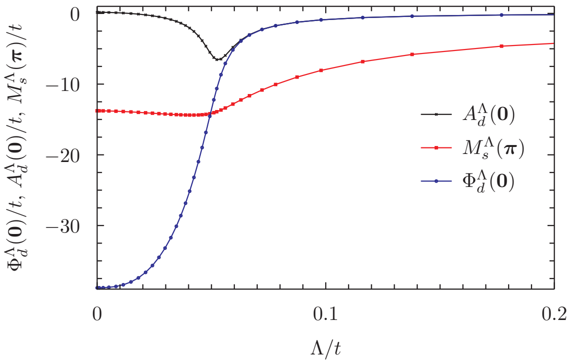

Figure 1: Renormalization group flow of the antiferromagnetic coupling $M_s^\Lambda(\boldsymbol{\pi})$, the amplitude mode $A_d^\Lambda(\mathbf{0})$ and the phase mode $\Phi_d^\Lambda(\mathbf{0})$ of the superconducting gap. The phase mode is finite at the end of the flow due to the presence of a finite external pairing field. The parameters are $U = 3$, $t' = -0.25$, $n = 0.85$, $\Delta_{(0)} \approx \Delta^{\Lambda=0}(0,\pi)/200 \approx 3 \cdot 10^{-4}$.

Figure 1 shows a representative example for a renormalization group flow into the d-wave superconducting phase for $U = 3t$, $t' = -0.25t$, $n = 0.85$ and a small external pairing field $\Delta_{(0)}$. The latter triggers the symmetry breaking and fixes the phase of the superconducting order parameter. It was chosen roughly two orders of magnitude smaller than the final value of the gap, so that it does not influence the latter significantly. The figure shows the flow of the antiferromagnetic coupling $M_s^\Lambda(\boldsymbol{q} = \boldsymbol{\pi})$ together with that of the d-wave amplitude $A_d^\Lambda(\boldsymbol{q} = \mathbf{0})$ and phase $\Phi_d^\Lambda(\boldsymbol{q} = \mathbf{0})$ modes. For this intermediate value of t', antiferromagnetic fluctuations are strong, but do not diverge. At intermediate scales, they generate an attractive interaction in the d-wave pairing channel that starts to grow quickly at low scales. Former instability analyses had to be stopped roughly at the scale where $(-A_d^\Lambda(\mathbf{0}))$ is maximal. At this scale, the d-wave pairing interaction promotes the external pairing field to sizeable values. This can be seen in Fig. 2 that shows the flow of the d-wave superconducting gap, which is parametrized as $\Delta^\Lambda(\boldsymbol{k}) = \Delta^\Lambda f_d(\boldsymbol{k})$, for $\boldsymbol{k} = (0,\pi)$. The increase of the gap suppresses the amplitude mode below the critical scale, while the phase mode grows until the end of the flow. In the limit where the external pairing field vanishes, the phase mode becomes the Goldstone degree of freedom of the symmetry broken state.

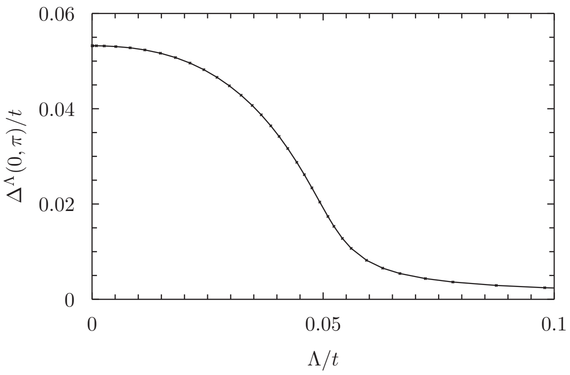

Figure 2: Renormalization group flow of the maximum of the d-wave superconducting gap at $\boldsymbol{k} = (0,\pi)$. The parameters are the same as in Fig. 1.

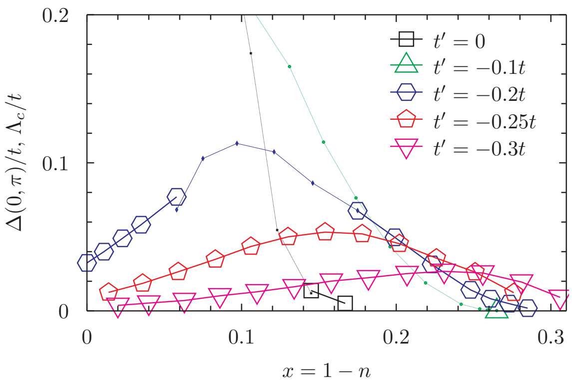

Figure 3: Phase diagram for $U = 3$ and various values of t' showing the critical scale Λ_c in case the leading instability is towards antiferromagnetism (lines with small symbols) and the d-wave superconducting gap at the end of the flow $\Delta^{\Lambda=0}(0,\pi)$ (lines with large symbols) in case the leading instability is towards d-wave superconductivity. In the latter case, for the chosen regulator the critical scale equals $\Delta^{\Lambda=0}(0,\pi)$ to a very good approximation.

Figure 3 shows the dependence of the critical scale and the d-wave superconducting gap on the hole doping away from half-filling $x = 1 - n$ for $U = 3t$ and various values of the next-nearest neighbor hopping t'. For the smallest values of $-t'$, the leading instability is mostly towards antiferromagnetism and only small superconducting regions are found with tiny values of the gap. The approximate nesting of the weakly curved Fermi surface favors (incommensurate) antiferromagnetism close to half-filling. For larger dopings, the coupling of incommensurate antiferromagnetic fluctuations to the d-wave pairing channels becomes worse and the pairing gaps small. Slightly increasing $-t'$ favors superconductivity because the antiferromagnetic channel becomes more frustrated but antiferromagnetic fluctuations are nevertheless strong. For $-t' > 0.25t$, antiferromagnetic fluctuations are so strongly frustrated due to the increasing curvature of the Fermi surface that the critical scales and gaps for d-wave superconductivity decrease. Our results therefore suggest the existence of an optimal value of t' for superconductivity. Besides, it is interesting to note that the largest gaps appear for densities somewhat above van Hove filling due to the amplification of antiferromagnetic fluctuations by umklapp scattering, which in turn enhances the attractive interaction in the d-wave pairing channel.

References:

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[2] *Husemann, C. and M. Salmhofer.* Phys. Rev. B **79**, 195125 (2009).

[3] *Eberlein, A. and W. Metzner.* Prog. Theor. Phys. **124**, 471–491 (2010).