Competing order in correlated electron systems made simple: Consistent fusion of functional renormalization and mean-field theory

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We derive an efficient and unbiased method for computing order parameters in correlated electron systems with competing instabilities. Charge, magnetic and pairing fluctuations above the energy scale of spontaneous symmetry breaking are taken into account by a functional renormalization group flow, while the formation of order below that scale is treated in mean-field theory. The method captures fluctuation driven instabilities such as $d$-wave superconductivity. As a first application we study the competition between antiferromagnetism and superconductivity in the ground state of the two-dimensional Hubbard model.

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Competing order is a ubiquitous phenomenon in two-dimensional interacting electron systems. A most prominent example is the competition between antiferromagnetism and high temperature superconductivity in cuprate and iron pnictide compounds. Some of the ordering tendencies are fluctuation driven, and can therefore not be captured by mean-field (MF) theory. Numerical simulations of correlated electrons are still restricted to relatively small systems.

For weak and moderate interaction strengths, the functional renormalization group (fRG) has been developed as an unbiased and sensitive tool to detect instabilities toward any kind of order in interacting electron models. 3 In that method, effective interactions, self-energies, and susceptibilities are computed from a differential flow equation, where the flow parameter $\Lambda$ controls a scale-by-scale integration of fields in the underlying functional integral. Instabilities are signalled by divergences of effective interactions and susceptibilities at a critical energy scale $\Lambda_c$. To complete the calculation and compute, for example, the size of the order parameters, one has to continue the flow below the scale $\Lambda_c$, which requires the implementation of spontaneous symmetry breaking. This can be done either in a purely fermionic framework 2 or by introducing bosonic order parameter fields. 3 Both approaches have been applied already to interacting electron models, such as the two-dimensional Hubbard model with repulsive and attractive interactions.

The flow in the symmetry-broken regime ($\Lambda < \Lambda_c$) is complicated considerably by the presence of anomalous interaction vertices. In complex problems, such as systems with several competing and possibly coexisting order parameters, or in multi-band systems, it can therefore be mandatory or at least desirable to simplify the integration of the scales below $\Lambda_c$. A natural possibility is to treat the low-energy degrees of freedom (below $\Lambda_c$) in mean-field theory. The generation of instabilities and also the possible reduction of the critical scale of spontaneous symmetry breaking is not affected by such a simplification. In the ground state, fluctuations below the critical scale are expected to influence the size of order parameters only mildly. This has been confirmed for the attractive and repulsive Hubbard model by several previous fRG studies. 3–5, 7 A combination of an fRG flow for $\Lambda > \Lambda_c$ with a mean-field treatment of symmetry-breaking has been formulated and applied already for a particular fRG version based on Wick ordered generating functionals. 3 However, for calculations beyond the lowest-order truncation, another fRG version, which is based on the effective action, turned out to be more efficient, as it avoids one-particle reducible contributions, and self-energy feedback can be implemented easily.

In this paper we derive a consistent combination of the one-particle irreducible fRG with MF theory for symmetry breaking. The resulting scheme differs from the naive idea of plugging the effective interaction at scale $\Lambda_c$ (or slightly above) into the mean-field equations. We demonstrate the performance of the combined fRG + MF theory by computing antiferromagnetic and superconducting order parameters in the ground state of the repulsive two-dimensional Hubbard model, including the possibility of coexistence of both orders.

To see how a mean-field treatment of symmetry breaking can be linked to the fRG flow, we consider the case of superconductivity as a prototype. Fermionic fRG flow equations for spin-singlet superfluids have been already derived and studied in detail. 9–12 In a one-loop truncation with self-energy feedback the flow is determined by two coupled flow equations for the self-energy $\Sigma^\Lambda$ and the two-particle vertex $\Gamma^\Lambda$, respectively. Both quantities contain anomalous components in the symmetry-broken regime.

The flow equation for the self-energy (normal and anomalous) is given by 11

$$
\frac{d}{d\Lambda} \Sigma_{s_1 s_2}^\Lambda(k) = \sum_{s'_1 s'_2} \int_{k'} \Gamma_{s_1 s'_2 s'_1 s_2}^\Lambda(k, k', k', k) S_{s'_2 s'_1}^\Lambda(k'),
$$

where $S^\Lambda = \frac{d}{d\Lambda} G^\Lambda|_{\Sigma^\Lambda \text{ fixed}}$ is a scale-derivative of the full propagator $G^\Lambda$ which acts only on its bare part $G_0^\Lambda$. The variable $k = (k_0, k)$ comprises momentum and Matsub-
ara energy, \( f \) is a short hand notation for \( T \sum_{k} \int \frac{d^3k}{(2\pi)^3} \), and \( s_i = \pm \) are indices labeling the two components of Nambu spinors. \( \Sigma_{\pm} = \pm \Sigma_0 \), \( \Sigma_0(k) = -\Sigma_{\pm}(k) = \Sigma_{\pm}(k) \) is the normal self-energy, and \( \Sigma_{\pm}(k) = \Sigma_{\pm}(k) = -\Delta^2(k) \) the (sign-reversed) gap function. Note that the vertex enters only with a special choice of momenta corresponding to zero total momentum (Cooper channel) or zero momentum transfer (forward scattering).

The flow of the vertex is given by a sum of three distinct one-loop contributions. It was shown previously that in mean-field models with reduced interactions, such as the reduced BCS model, only the channel which generates the instability contributes to the vertex flow. Hence, the other two channels describe fluctuations. Our strategy is thus to take all contributions to the vertex flow into account above the scale for symmetry breaking, but discard the fluctuation channels below. For a singlet superfluid, discarding the fluctuation terms in the flow equation for the vertex leads to a simplified flow equation for the relevant vertex components \( \Gamma_{s_1s_2s_3s_4}(k,k') = \Gamma_{s_1s_2s_3s_4}(k,k',k',k) \),

\[
\frac{d}{d\Lambda} \Gamma_{s_1s_2s_3s_4}(k,k') = \sum_{s'_i} \int_\nu \Gamma_{s_1s_2s_3s_4}(k,p) \Pi_{s_1's_2's_3's_4'}(p) \Gamma_{s_1's_2's_3's_4'}(p,k') ,
\]

where \( \Pi_{s_1s_2s_3s_4}(p) = G_{s_1s_2}(p)G_{s_3s_4}(p) \), and the dot denotes a \( \Lambda \)-derivative.

We denote the scale at which we switch from the full \( \text{fRG} \) to the mean-field treatment by \( \Lambda_{\text{MF}} \). Typically \( \Lambda_{\text{MF}} \) will be chosen slightly above the critical scale \( \Lambda_c \). The full \( \text{fRG} \) flow for \( \Lambda > \Lambda_{\text{MF}} \) yields \( \Sigma_{\text{MF}} \) and \( \Gamma_{\text{MF}} \), which pose the initial condition for the remaining (mean-field) flow for \( \Lambda < \Lambda_{\text{MF}} \). The coupled equations (1) and (2) for the self-energy and vertex describing the mean-field flow for \( \Lambda < \Lambda_{\text{MF}} \) can be integrated with arbitrary initial conditions at \( \Lambda = \Lambda_{\text{MF}} \). The resulting vertex is determined by a Bethe-Salpeter-type integral equation

\[
\Gamma_{s_1s_2s_3s_4}(k,k') = \Gamma_{s_1s_2s_3s_4}(k,k') + \sum_{s_i} \int_\nu \Gamma_{s_1's_2's_3's_4'}(k,p) \Pi_{s_1's_2's_3's_4'}(p) \Gamma_{s_1's_2's_3's_4'}(p,k') ,
\]

and the self-energy by a Hartree-type equation of the form

\[
\Sigma_{s_1s_2}(k) = \Sigma_{s_1s_2}(k) + \sum_{s_i} \int_\nu \tilde{\Gamma}_{s_1's_2's_3's_4'}(k,k') [G_{s_1's_2'}(k') - G_{s_2's_1'}(k')] .
\]

The vertex \( \tilde{\Gamma}_{\text{MF}} \) on the right hand sides is the irreducible part of \( \Gamma_{\text{MF}} \), which can be determined from the latter via Eq. (3) at \( \Lambda = \Lambda_{\text{MF}} \). Contributions which are two-particle reducible in the symmetry breaking channel are removed in \( \Gamma_{\text{MF}} \). The computation of \( \Sigma_{\text{MF}} \) from Eq. (4) does not require a computation of the vertex for \( \Lambda < \Lambda_{\text{MF}} \).

To obtain the physical self-energy and vertex, with all degrees of freedom integrated, it suffices to solve Eqs. (3) and (4) for \( \Lambda = 0 \). Choosing \( \Lambda_{\text{MF}} > \Lambda_c \), the vertex \( \Gamma_{\text{MF}} \) and its irreducible part \( \tilde{\Gamma}_{\text{MF}} \) have no anomalous components, which simplifies the computation considerably. In particular, the equation for the gap function becomes

\[
\Delta(k) = -\int k' \tilde{V}_{\text{MF}}(k,k') F(k') ,
\]

where \( F(k) \) is the anomalous propagator, and \( \tilde{V}_{\text{MF}}(k,k') \) is the irreducible part of the spin-singlet component of the normal two-particle vertex\(^{13} \) in the Cooper channel,

\[
V_{\text{MF}}(k,k') = \frac{1}{2} \Gamma_{\text{MF}}(k,-k_1,k_1,k') - \int_p \tilde{V}_{\text{MF}}(k,p) G_{\text{MF}}(p) G_{\text{MF}}(-p) V_{\text{MF}}(p,k') .
\]

To compute \( \Delta \), one first computes \( V_{\text{MF}} \) from the \( \text{fRG} \) flow, then solves the linear integral equation for \( \tilde{V}_{\text{MF}} \), and finally the gap equation. The \( \text{fRG} + \text{MF} \) procedure described above solves mean-field models exactly, by construction. For mean-field models, the irreducible vertex \( \Gamma_{\text{MF}} \) is just the bare vertex for any \( \Lambda_{\text{MF}} \). The integration over momenta and frequencies on the right hand side of the equation for \( \Sigma_{\text{MF}} \) is not restricted by \( \Lambda_{\text{MF}} \). This differs from the Wick ordered \( \text{fRG} + \text{MF} \) scheme\(^{12} \) where integrations are restricted by \( \Lambda_{\text{MF}} \) as an upper cutoff. On the other hand, in that approach the full vertex \( \Gamma_{\text{MF}} \) enters, not only its irreducible part. However, that scheme, and also its analogue for the one-particle irreducible \( \text{fRG} \)\(^{12} \) suffers from systematic errors even for mean-field models. In particular, the order parameter obtained from solving the mean-field equations with the full vertex exhibits an artificial divergence when \( \Lambda_{\text{MF}} \) approaches \( \Lambda_c \), due to an overcounting of contributions.

The generalization of the above \( \text{fRG} + \text{MF} \) procedure to other instabilities is straightforward. The crucial point is that the irreducible part \( \tilde{\Gamma}_{\text{MF}} \) of the relevant vertex component has to be inserted as effective interaction in the mean-field equation for the order parameter. The computation of \( \tilde{\Gamma}_{\text{MF}} \) from \( \Gamma_{\text{MF}} \) is done for each instability channel separately, even in cases of coexistence of order in different channels.

To illustrate the performance of the \( \text{fRG} + \text{MF} \) theory in a situation of competing instabilities, we now present an application to the two-dimensional Hubbard model. The model is well-known for its intriguing competition between antiferromagnetism and superconductivity. Indeed the \( \text{fRG} \) flow of the vertex generically diverges either
in the antiferromagnetic or in the $d$-wave pairing channel in that model. Hence we allow for antiferromagnetic and superconducting order, including the possibility of coexistence. Although the antiferromagnetic wave vector may deviate from $(\pi, \pi)$, we consider only the case of conventional Néel order for simplicity.

The effective interaction for singlet pairing is given by Eq. (6), and its irreducible part by Eq. (7). Similarly, the effective interaction triggering antiferromagnetism is given by

$$U^{\text{MF}}(k, k') = \sum_{\sigma' = \uparrow, \downarrow} s_{\sigma'} \Gamma^{\text{MF}}_{\sigma' \sigma}(k+Q, k', k+Q, k),$$

where $s_{\uparrow}, s_{\downarrow} = \pm 1$, and $Q = (0, Q)$ with the antiferromagnetic wave vector $Q = (\pi, \pi)$. Its irreducible part is obtained from the integral equation

$$U^{\text{MF}}(k, k') = \bar{U}^{\text{MF}}(k, k') + \int_p \bar{U}^{\text{MF}}(k, p) G^{\text{MF}}(p) G^{\text{MF}}(p + Q) U^{\text{MF}}(p, k').$$

So far, the formalism allows for dynamical (frequency dependent) effective interactions and order parameters. In this first application, we will discuss only the static mean-field theory obtained from the static (zero frequency) effective interactions $U_{kk'}^{\text{MF}}$ and $V_{kk'}^{\text{MF}}$. We will also discard normal self-energy contributions. The superconducting and antiferromagnetic order parameters are then defined as gap functions in the usual form

$$\Delta_k^{\text{SC}} = \int_{k'} \bar{V}_{kk'}^{\text{MF}}(p_{k'}),$$

$$\Delta_k^{\text{AF}} = \frac{1}{2} \int_{k'} \bar{U}_{kk'}^{\text{MF}}(m_{k'}),$$

where $p_k = a_{k\uparrow} a_{-k\downarrow}$ is the Cooper pair annihilation operator, $m_k = a_{k\uparrow} a_{k\uparrow} + a_{k\downarrow} a_{-k\downarrow}$ is the operator for staggered magnetization, and $\int_{k'}$ is an abbreviation for $\int \frac{d^2 p'}{2\pi}$. We choose the phase of the superconducting order parameter such that $\Delta^{\text{SC}}_k$ is real. A mean-field decoupling of the effective interactions yields the mean-field Hamiltonian

$$H_{\text{MF}} = H_0 + \int_k \Delta_k^{\text{AF}} (m_k - \frac{1}{2} \langle m_k \rangle)$$

$$+ \int_k \Delta_k^{\text{SC}} (p_k + p_k^\dagger - \frac{1}{2} \langle p_k + p_k^\dagger \rangle),$$

where $H_0 = \int_k \epsilon_k n_k$ is the kinetic energy. For the Hubbard model with nearest and next-to-nearest neighbor hopping on a square lattice, the dispersion relation is $\epsilon_k = -2t(\cos{k_x} + \cos{k_y}) - 4t'\cos{k_z}\cos{k_y}$.

The mean-field Hamiltonian can be diagonalized by a Bogoliubov transformation and the resulting gap equations can be solved numerically by iteration. Occasionally two distinct locally stable solutions of the gap equations are found. One then has to compute the corresponding free energies to discriminate globally stable from metastable states. In case of coexistence of antiferromagnetism and superconductivity, an additional triplet pairing with pair momentum $(\pi, \pi)$ is generically generated. However, its feedback on the main order parameters is very weak so that we can safely discard this additional order parameter in the computation of $\Delta^{\text{AF}}_k$ and $\Delta^{\text{SC}}_k$.

We now show and discuss results for the magnetic and superconducting order parameters in the ground state of the hole-doped Hubbard model with a small next-to-nearest neighbor hopping $t' / t = -0.15$ and a moderate Hubbard interaction $U/t = 3$. The RG flow has been computed with a static vertex parametrized via a decomposition in charge, magnetic and pairing channels, with $s$-wave and $d$-wave form factors as described in Ref. [5]. The scale $\Lambda_0$ was fixed by the condition that the modulus of one of the coupling functions parametrizing the vertex reaches the maximum value 50$t$. With this criterion $\Lambda_0$ is typically less than 10 percent above $\Lambda$. For the computation of $\Gamma^{\text{MF}}$ and the solution of the gap equations, the momentum dependence was discretized by partitioning the Brillouin zone in 100 patches.

In Fig. 1 we show results for the amplitudes of the antiferromagnetic and superconducting gap functions, $\Delta^{\text{AF}} = \max_k \Delta^{\text{AF}}_k$ and $\Delta^{\text{SC}} = \max_k \Delta^{\text{SC}}_k$, as a function of the electron density. The coupled solution of both gap equations exhibits an extended region where magnetic and superconducting order coexist. In the major part of that region the pairing gap is smaller than the magnetic gap. Here superconductivity is a secondary instability within the antiferromagnetic phase, which naturally occurs as a Cooper instability of electrons near the reconstructed Fermi surface confining hole pockets in the antiferromagnetic state. The pairing gap decreases rapidly
as the pockets shrink upon approaching half-filling. Magnetic order vanishes at a critical density \( n_{c}^{AF} \) situated slightly above Van Hove filling. Below that density the state is purely superconducting. The magnetic transition is continuous such that \( n_{c}^{AF} \) is a quantum critical point.\(^9\) Fig. 1 also shows results for the gap amplitudes as obtained from solutions of the individual gap equations with either magnetic or superconducting order. A comparison with the coupled solution confirms that the two order parameters compete with each other. In particular, superconductivity is strongly suppressed by antiferromagnetism. In the absence of superconductivity, the antiferromagnetic regime extends to lower densities and terminates at a first order transition accompanied by a density jump, which opens a density window where no homogeneous solution exists.

For densities below \( n = 0.95 \), the two-particle vertex diverges actually at incommensurate wave vectors, indicating a leading instability toward incommensurate antiferromagnetic order.\(^7\) The resulting ground state is probably an incommensurate spin density wave state coexisting with superconductivity. Such states can also be treated by the fRG + MF theory. Since mean-field equations for incommensurate magnetic order are more involved, we leave this extension for future studies. For parameters where pairing is the leading instability, the results for \( \Delta^{SC} \) are very close to those from a full fRG calculation,\(^5\) which indicates that the fluctuations below the scale \( \Lambda_{k} \) have indeed limited impact on the size of the ground state order parameter.

The momentum dependence of the gap functions is shown in Fig. 2. The antiferromagnetic gap \( \Delta^{AF} \) exhibits only a moderate modulation around a constant. The superconducting gap \( \Delta^{SC} \) obeys the expected \( d_{x^2-y^2} \) symmetry, but with visible deviations from the simple \( \cos k_x - \cos k_y \) form. In the coexistence regime the (global) extrema of \( \Delta^{SC} \) are shifted away from the axial directions, as a natural consequence of the Fermi surface truncation in the antinodal region.

The above results for the gap functions agree qualitatively with those obtained previously from the Wick ordered fRG + MF theory.\(^9\) However, the suppression of \( \Delta^{SC} \) by antiferromagnetic order was stronger in that work. A relatively broad coexistence of antiferromagnetism and superconductivity as found here has also been obtained at stronger interactions by embedded quantum cluster methods.\(^24\) The results for the order parameters depend to some extent on the precise choice of \( \Lambda_{MF} \), but much less than in the Wick ordered fRG + MF approach.

In summary, we have derived an efficient and unbiased method for computing order parameters in correlated electron systems with competing instabilities. Charge, magnetic and pairing fluctuations above the energy scale of symmetry breaking are taken into account by an fRG flow, while the formation of order below that scale is treated in mean-field theory. The effective interaction entering the mean-field equations is given by the irreducible part of the two-particle vertex. The method captures fluctuation driven instabilities such as \( d \)-wave superconductivity in two-dimensional electron systems. It can deal with any order parameter based on a bilinear fermionic expectation value. As a first application we have studied the competition between antiferromagnetism and superconductivity in the two-dimensional Hubbard model. An interesting extension would be the computation of incommensurate magnetic order, in possible coexistence with superconductivity, which is very hard to study by other methods. More generally, competing instabilities in complex multi-band systems offer a wide field of fruitful applications for the fRG + MF theory.

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