Fermionic renormalization group flow at all scales: breaking a discrete symmetry

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Abstract. We extend the functional renormalization group technique in a modification of the one-particle irreducible scheme to study discrete symmetry breaking at finite temperature. As an instructive example, we employ the technique to access both the symmetric and the symmetry-broken phase of a charge-density wave mean-field model. We study the half-filled case, and thus the breaking of a discrete symmetry, at finite temperature. A small external symmetry-breaking field allows us to access the symmetry-broken state without encountering any divergence in the flow. We show diagrammatically that our method is equivalent to an exact resummation treatment. We numerically study the dependence of the flow on the external field and on temperature.

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INTRODUCTION

Renormalization group flows are a standard method to study the interplay of competing symmetry breakings, despite the fact that the actual symmetry-broken phase is not accessible to most of these flows. The fermionic renormalization group (fRG) presents one of the least biased approaches in this field. It starts from an infinite hierarchy of differential equations. This hierarchy arises from the expansion of the effective action in powers of the fermionic fields. The coefficients of this expansion are functions of the system's degrees of freedom (momenta, frequencies, and spins) and are determined by the hierarchy. They are closely related to the *n*-particle Green's functions, and the differential equations for the two-point function and the four-point function can be reformulated in terms of the effective interaction and the self-energy. Frequently, the flow is approximated by truncating the hierarchy beyond the equations for the four-point function by setting the six-point function to zero. For most systems of physical interest, only approximate treatments based on such a truncation of the hierarchy are available. These treatments are unable to deal with flows to a strong effective interaction. However, in the case of the spontaneous breaking of a symmetry of the original Hamiltonian, a divergence of the flow of the effective interaction occurs, making it impossible to describe the full system using only the fRG. One way around this problem is to stop the flow at a finite cutoff value and to treat the effective theory thus obtained with an alternative method (see [1, 2]).

In this work, we study the flow of the fRG in a variation of the one-particle irreducible scheme [4] proposed by Katanin [3], employing a small external symmetry-breaking field to prevent the divergence of the flow [5] and access the symmetry-broken phase. In contrast to the truncation described above, a part of the contribution of the six-point function to the flow of the four-point function is taken into account in this variation. The model under study, chosen for its instructiveness, is the reduced charge-density wave model of spinless fermions at half-filling in arbitrary dimension. We thus employ the Katanin-scheme fRG to study the breaking of a discrete symmetry at finite temperature, in contrast to previous work [5], where the breaking of a continuous symmetry at zero temperature was studied. We first determine analytically the effective interaction and the self-energy in the thermodynamic limit by means of a resummation of all orders of perturbation theory. We show that the equations obtained from the resummation are equivalent to the fRG equations in the Katanin scheme. We present numerical results for the flow at temperatures above and below the critical temperature to study the typical shapes of the flow and to determine the effective interaction strengths encountered.

This paper is organized as follows. In the second section, we present the reduced charge-density wave model. The resummation is outlined in the third section. The flow equations are related to the resummation equations in the fourth section. Numerical results for the flow are shown in the following section. We present conclusions and an outlook in the last section.

MODEL

In this section, we will describe the model for which we will study the fRG flow in later sections. We will specify the space on which our model lives and introduce a kinetic energy operator, which we will diagonalize by Fourier transformation. Next, we will introduce a particle-particle interaction with a particularly simple momentum structure. Lastly, we will couple the system to an external symmetry-breaking field.

The model under study has been chosen for its simplicity and instructiveness. It is defined on a hypercubic lattice in d dimensions and contains particles that can hop between nearest-neighbor sites. This process is represented in the kinetic part of the Hamiltonian

$$H_{\text{kin}} = -t \sum_{\vec{x},\vec{n}} (c^\dagger_{\vec{x}} c_{\vec{x}+\vec{n}} + h.c.), \tag{1}$$

where $c^\dagger_{\vec{x}}$ and $c_{\vec{x}}$ are fermionic operators which create and annihilate, respectively, a particle at lattice site $\vec{x}$. Fourier-transforming the operators according to

$$c_{\vec{x}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\vec{x}} c_{\vec{k}}, \tag{2}$$

we obtain

$$H_{\text{kin}} = -2t \sum_{\vec{k}} \left(\sum_{j=1}^{d} \cos(k_j) \right) c^\dagger_{\vec{k}} c_{\vec{k}}. \tag{3}$$

We add an infinite-range density-density interaction with oscillating sign in the following sense. We split the lattice into two sublattices so that all nearest neighbors of any site of one sublattice are part of the other sublattice. A particle on one sublattice is attracted by all other particles on the same sublattice and repelled equally strongly by the particles on the other sublattice. Writing $\vec{Q} = (\pi, \pi, \dots)$, we see that the interacting part of the Hamiltonian reads

$$H_{\text{int}} = \frac{V_0}{N} \sum_{\vec{k}_1, \vec{k}_2} c^\dagger_{\vec{k}_1} c_{\vec{k}_1 - \vec{Q}} c^\dagger_{\vec{k}_2} c_{\vec{k}_2 + \vec{Q}}. \tag{4}$$

The infinite range of the interaction ensures that a mean-field treatment of the model yields exact results in the thermodynamic limit.

We furthermore add an external field that modifies the energy of particle-hole pairs with a momentum difference of $\vec{Q}$. Formally, this is accomplished by the term

$$H_{\text{ext}} = \sum_{\vec{k}} \Delta_{\text{ext}} c^\dagger_{\vec{k}} c_{\vec{k} + \vec{Q}}. \tag{5}$$

Adding this term favors a commensurate modulation of the charge density energetically, as can be seen by Fourier-transforming $\langle c^\dagger_{\vec{k}} c_{\vec{k}+\vec{Q}} \rangle$ with respect to both momentum variables separately.

The full Hamiltonian to be considered in the following now reads

$$H = H_{\text{kin}} + H_{\text{ext}} + H_{\text{int}}. \tag{6}$$

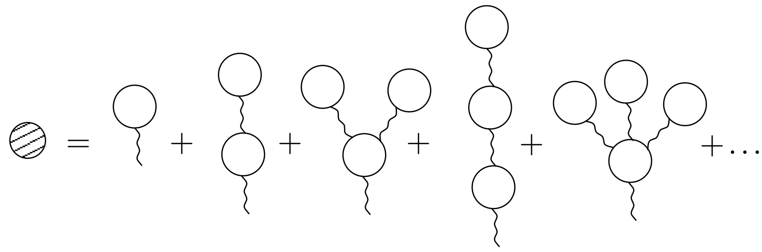
RESUMMATION TREATMENT

In this section, we will solve the Hamiltonian (6) analytically by resumming the perturbation expansions for the self-energy and the effective interaction. This is possible because, in the thermodynamic limit, only a subclass of all possible diagrams remains nonzero. We will then study the effect of the external field (5).

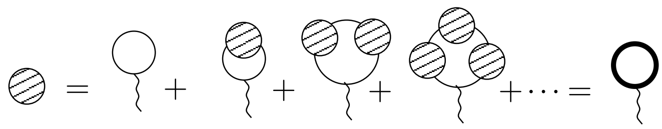
In the following, we first fix our diagrammatic conventions. The bare interaction is represented by a wiggly line, the effective interaction by a hatched rectangle, the self-energy by a hatched circle, bare propagators are drawn as lines, and full propagators are distinguished from bare ones by using heavy lines. Propagator lines without arrows imply that one has to sum over normal ($\langle c^\dagger_{\vec{k}} c_{\vec{k}} \rangle$) and anomalous ($\langle c^\dagger_{\vec{k}} c_{\vec{k}+\vec{Q}} \rangle$) contributions when evaluating the diagram.

The simplification of the diagrammatic perturbation expansion which allows us to resum all orders is based on the observation outlined below. Every internal propagator line carries one summation over all degrees of freedom by standard Feynman diagram evaluation rules. There are $O(N)$ degrees of freedom. However, from (4) follows that every interaction line carries a factor $1/N$ and the constraint that the momentum transfer through the interaction line must exactly equal $\vec{Q}$. Therefore, each closed loop of propagator lines only contributes a factor of $O(N)$, as all except one of the internal momentum variables of the loop are fixed by the constraint. Other contributions are of $O(1)$. Thus, if n is the number of interactions lines and l is the number of loops, a diagram's contribution is of order N^{l-n}. In the thermodynamic limit $N \to \infty$, only diagrams of the highest order in N have to be taken into account. These have maximal $l - n$ among all diagrams.

For the self-energy, the above argument entails that only diagrams of cactus type, for which $n = l$, contribute in the thermodynamic limit:



This can be resummed to read



Clearly, the full propagator in the final tadpole or Hartree diagram must be of anomalous type to satisfy the constraint that a momentum of $\vec{Q}$ must be carried by the interaction line. The full Green's function is obtained from the Dyson equation

$$G^{-1} = G_0^{-1} - \Sigma, \tag{7}$$

where the self-energy has been denoted by Σ. Including the external field (5) in the bare propagator, matrix inversion yields

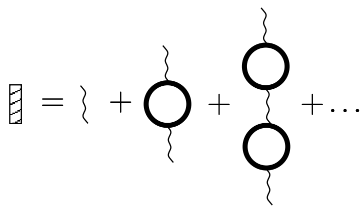
$$G(\vec{q}, i\omega_n) = \frac{1}{\omega_n^2 + \varepsilon(\vec{q})^2 + \Delta_{\text{ext}}^2} \begin{pmatrix} -i\omega_n - \varepsilon(\vec{q}) & \Sigma \\ \Sigma & -i\omega_n + \varepsilon(\vec{q}) \end{pmatrix}, \tag{8}$$

where $\omega_n = (2n+1)\pi T$ are fermionic Matsubara frequencies, $\varepsilon(\vec{q}) = -2t\sum_{j=1}^{d}\cos(q_j)$, and the external field has been included in the self-energy. Using (8), the gap equation is determined from the diagrammatics. After Matsubara summation, it reads

$$\Sigma - \Delta_{\text{ext}} = V_0 \Sigma \int_0^W \mathrm{d}\varepsilon \rho(\varepsilon) \frac{\tanh(E/2T)}{E}, \tag{9}$$

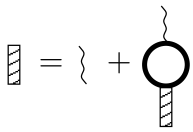
where $E = \sqrt{\varepsilon^2 + \Delta^2}$, $\rho(\varepsilon)$ is the density of states, and $2W$ is the bandwidth.

The effective interaction can be calculated in a similar fashion. Considering the above observation about the thermodynamic limit, we conclude that only chains of full-propagator loops contribute in the thermodynamic limit:



Branching of the chain is excluded for the following reasons. Consider any of the above loop chain diagrams. It is of $O(N^{-1})$. We refer to the chain in this diagram as the main chain. We will now attach further chains to the main chain and see that the resulting diagram is either already included or that it is of lesser order than $O(N^{-1})$. If a branch were connected to only one propagator of the main chain, it would constitute a self-energy correction, all of which are already included in the full propagators. Instead, we now study a branch which is connected to two different propagators of the main chain. Such a diagram can be constructed from the original diagram by taking a chain of loops ($O(N^{-1})$) and gluing the interaction lines at its two ends to two different propagators of the main chain. Since this process creates no additional fermionic loops, the resulting diagram is of $O(N^{-2})$ and does not contribute in the thermodynamic limit. Thus, we have seen that we only have to take the above diagrams into account.

The loop chain series can be resummed in the following way:



The Bethe-Salpeter equation,

$$V = \frac{V_0}{1 - V_0 \int_0^W \rho(\varepsilon) \frac{\mathrm{d}\varepsilon}{E^2} \left[\frac{\Sigma^2}{2T} \cosh^{-2}\left(\frac{E}{2T}\right) + \frac{\varepsilon^2}{E} \tanh\left(\frac{E}{2T}\right) \right]}, \tag{10}$$

is obtained by evaluating the above diagrams and employing the residue theorem to carry out the Matsubara summation.

(9) and (10) can be solved numerically. The effect of the external field on the temperature dependencies of the self-energy and the effective interaction is exhibited in Fig. 1. The introduction of the external field regularizes the singularity of the effective interaction at the critical temperature T_c. The discontinuity of the temperature derivative of the self-energy at the same point is lifted.

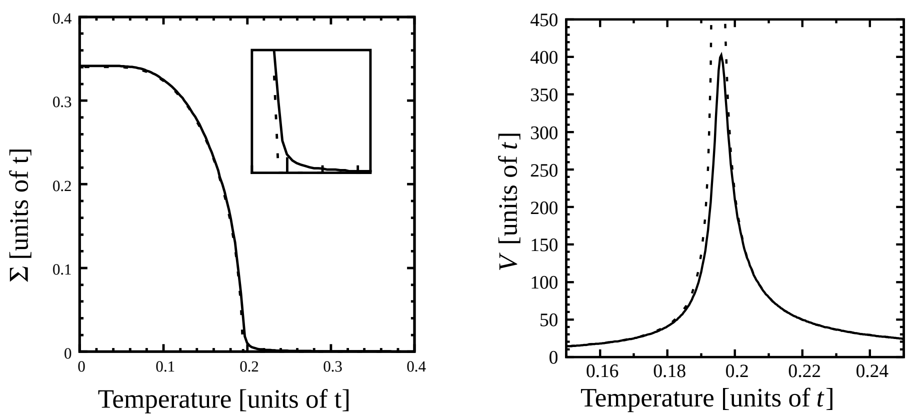


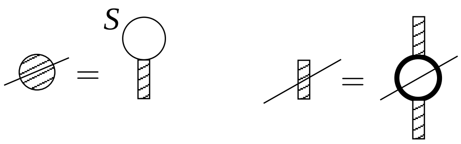
FIGURE 1. Effect of the external field on the self-energy and the effective interaction, $U = 2t$. Full: $\Delta_{\text{ext}} = 10^{-4}t$, dashed: no external field. In this calculation, a one-dimensional density of states was used.

In summary, we have seen how to solve the Hamiltonian (6) analytically. We have resummed the perturbation expansions for the self-energy, obtaining the gap equation (9), and the effective interaction, obtaining the Bethe-Salpeter equation (10). We have graphically studied the effect of the external field on the self-energy and the effective interaction.

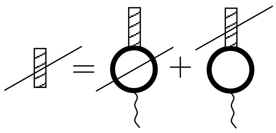
RESUMMATION EQUATIONS FROM FLOW EQUATIONS

In this section, we show that the Katanin-scheme fRG treatment of the Hamiltonian (6) is exact. We will first introduce the fRG flow equations. We will then show that the flow equation for the vertex is a derivative of the Bethe-Salpeter equation and that the flow equation for the self-energy is a derivative of the gap equation. The proofs will proceed largely diagrammatically.

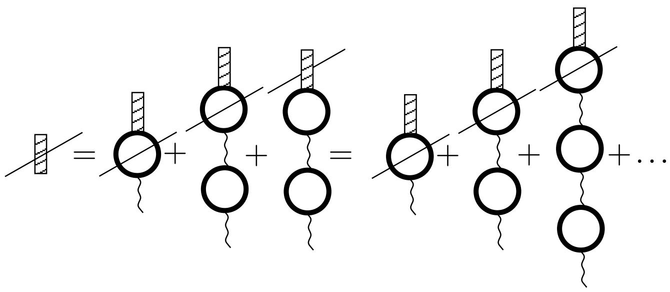
We introduce a momentum cutoff by multiplying the inverse quadratic part of the action by a sharp cutoff function, $\Theta(|\varepsilon(\vec{q})| - \Lambda)$. The fRG flow equations in the Katanin scheme are given in [5]. Using the additional conventions that (i) slashed lines correspond to Λ-derivatives and (ii) $S := -G(dG_0^{-1}/d\Lambda)G$ (all depending on Λ), the flow equations in the thermodynamic limit read:



The arguments of the preceding sections that lead to the resummations of the perturbation expansions for the self-energy and the effective interaction also hold if a cutoff is introduced as above. We can therefore take the derivative with respect to Λ of the diagrammatic form of the Bethe-Salpeter equation for the system including the cutoff:

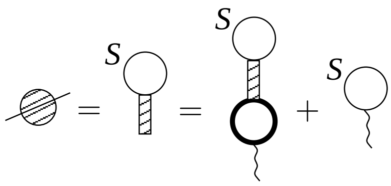


On the right-hand side, we have applied the product rule. We repeatedly replace the scale-differentiated effective interaction on the right-hand side with the full right-hand side to obtain:

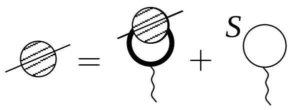


We identify the sum of loop chains that we resummed in the derivation of (10) and thus recover the right-hand side of the flow equation for the effective interaction. Since the solution of the corresponding initial-value problem is unique, the solution of the fRG flow equations satisfies the Bethe-Salpeter equation from which we started. This shows the equivalence of the effective interaction flow equation and the Bethe-Salpeter equation.

We now study the flow equation for the self-energy. Replacing the effective interaction on the right-hand side with the right-hand side of the diagrammatic form of the Bethe-Salpeter equation yields:



The flow equation for the self-energy allows us to substitute the cutoff-differentiated self-energy for the tadpole part of the diagram including the effective interaction:



Symbolically, the loops of the two tadpole diagrams read:

$$G\left(\frac{d}{d\Lambda}\Sigma\right)G - G\left(\frac{d}{d\Lambda}G_0^{-1}\right)G = -G\left(\frac{d}{d\Lambda}G^{-1}\right)G = \frac{d}{d\Lambda}G. \qquad (11)$$

This shows that the fRG flow equation for the self-energy is the derivative of the gap equation for the system including the cutoff. Since the solution of the corresponding initial-value problem is unique, the solution of the fRG flow equations is also a solution of the gap equation. This concludes the proofs.

NUMERICAL RESULTS

In this section, we will study the solutions of the flow equations for various parameters. First, we will observe the change in the $T = 0$ flow when varying the magnitude of the external field. Then, we will analyze the dependence of the flow on temperature for a small external field.

Fig. 2 shows the dependence of the fRG flow at zero temperature on the external symmetry-breaking field Δ_{ext}, see (5). The value of Δ_{ext} decreases exponentially from top to bottom in the self-energy diagram and vice versa in the effective interaction diagram. Clearly, the final value of the self-energy flow saturates for small Δ_{ext}. The dependence of the $\Lambda = 0$ self-energy on the external field strength is relatively weak: while the external field varies over two orders of magnitude, the self-energy changes by only $\approx 15\%$. However, the dependence of the height of the effective interaction flow peak on the external field is strong. It is strongly suppressed by increasing the strength of the external field. A more thorough investigation of these relationships can be found in [6].

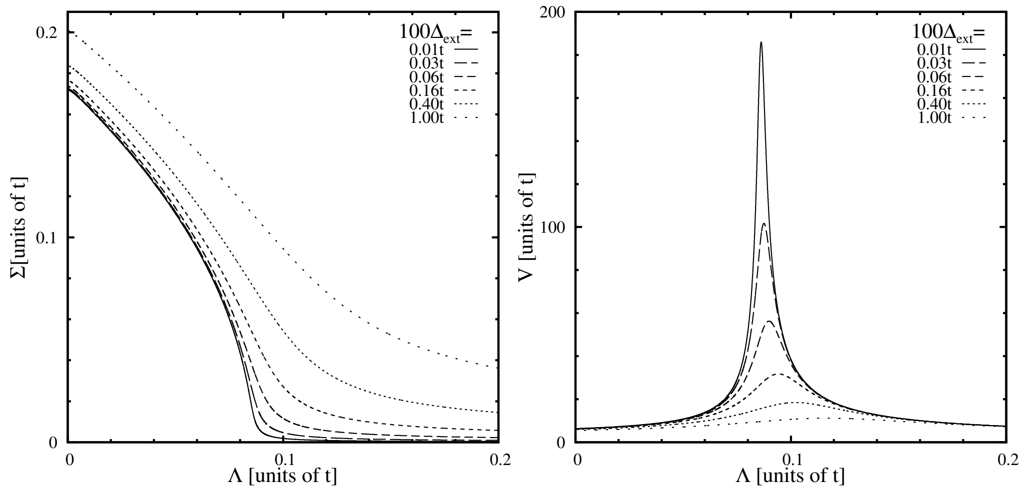


FIGURE 2. fRG flows of the self-energy and the effective interaction at $T = 0$. In contrast to Fig. 1, a constant density of states of $1/2\pi$ was used.

Fig. 3 shows how the flow of the self-energy and the effective interaction changes when the temperature is varied around T_c. The shape of the effective interaction flow barely varies. However, the graph is shifted to lower values of the cutoff by an increase in temperature; this can be most clearly seen by observing the position of the peak for the various graphs. The flow of the self-energy is shifted likewise. A more thorough examination of the temperature dependence of the flow can be found in [6].

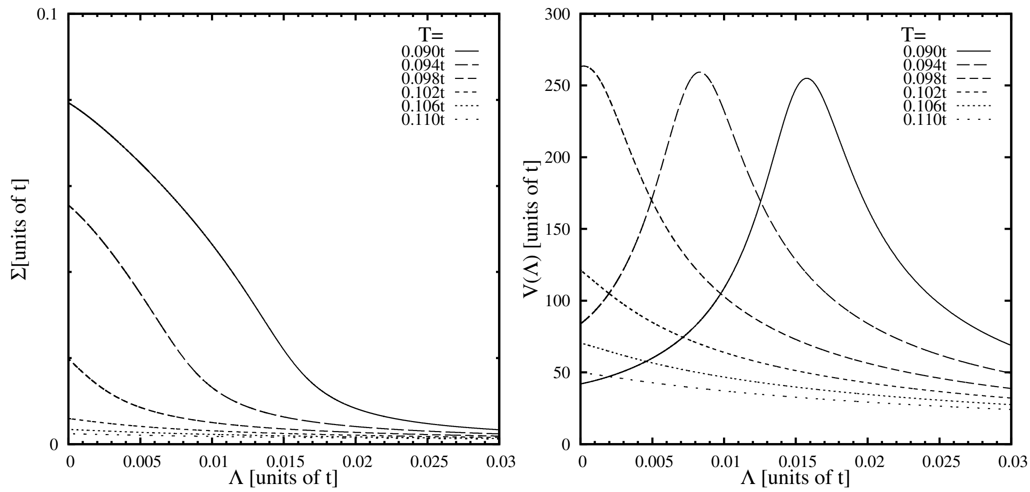


FIGURE 3. fRG flows of the self-energy and the effective interaction at various temperatures close to T_c. Δ_{ext} is set to $10^{-4}t$ here. In contrast to Fig. 1, a constant density of states of $1/2\pi$ was used.

CONCLUSIONS AND OUTLOOK

We have studied the fRG in the Katanin scheme for the example of a reduced charge-density wave model with a small symmetry-breaking external field. In the thermodynamic limit, we have obtained the exact self-energy and the exact effective interaction by means of a resummation of all orders of perturbation theory. We have shown that the fRG equations are the cutoff derivatives of the equations obtained by the resummations. We have briefly studied the temperature dependence of the numerically obtained flow of the self-energy and the effective interaction. At $T = 0$, we have seen that the flow of the self-energy does not depend strongly on the external field, but that the flow of the effective interaction does. In this paper, it has become clear at least at $T = 0$ that the flow of the effective interaction can be suppressed by increasing the strength of the external field. Although it was not shown here, this is also true for $T > 0$.

Future studies will include the investigation of models which cannot be solved exactly by resummation. For these models, the right-hand side of the effective interaction flow equation will have to be truncated at some order of the effective interaction. The fRG will thus become perturbative in the effective interaction, which therefore must remain small compared to the bandwidth in the flow to produce meaningful results. As we have studied more closely in [6], in the reduced charge-density wave model this implies employing a relatively large external field, which changes the physical situation to an extent depending on the proximity to the critical temperature. However, in a model encompassing many interaction channels, large effective interactions would most likely only occur in a small number of channels. Due to the thus limited phase space, effects from feedback into other channels may be small and meaningful results for quantities of physical interest may be obtainable even if the strength of the large effective interactions exceeds the bandwidth.

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