Interacting fluctuations and the two-loop order parameters of the strong-coupling negative-U Hubbard model

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Abstract

The effective field theory that describes the interaction of fluctuations of the attractive Hubbard model in the strong-coupling limit is formulated and applied to obtain the two-loop results for the order parameters of the model at low temperatures and in the leading singularities near two dimensions. Starting from a Grassmann functional integral representation of the strong-coupling model on the restricted fermionic Hilbert space, which corresponds to the anisotropic spin-1/2 Heisenberg quantum antiferromagnet, we derive the effective field theory up to fifth order in the bosonic fluctuation fields. The loop-corrections of the order parameters for superconductivity and charge-ordering and of the chemical potential are evaluated including both the singular planar phase fluctuations and the out-of-plane fluctuations, which become soft at half band-filling. The results are in agreement with the scaling behaviour expected from the corresponding XY and Heisenberg limits of the $O(n)$ nonlinear σ-model.

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1 Introduction

The Hubbard model with attractive on-site (negative-U) interaction [1, 2] is the simplest effective model of strongly correlated electron systems in which the local electronic degrees of freedom are coupled to quasiparticles which mediate an attractive interaction mechanism overweighing the Coulomb repulsion [3]. Besides its immediate physical applications in a variety of such systems with an effective short-ranged attractive interaction of electrons [4, 5, 6] the strong-coupling limit of the negative-U Hubbard model is of interest in its own right, since it provides several simplifications of the original model which make it accessible to more rigorous field theoretic techniques [7, 8] than in the case of general coupling strength.

In the strong-coupling limit [9, 10], the negative-U Hubbard model is equivalent to a spin-1/2 anisotropic quantum Heisenberg model in an external field, with an attractive XY-like pair interaction and a repulsive coupling in the pseudo-spin Ising sector, and where the total pseudo-magnetization is given by the band-filling. This equivalence is related to a constraint of the local fermionic Hilbert space which can be modelled exactly by the Popov-Fedotov technique [11], leading to a conventional representation of the model in Grassmann fields, albeit involving a modification of the fermionic Matsubara frequency spectrum. Utilizing such a representation, and applying usual fermionic field theoretic and diagrammatical methods, a number of previously unaccessible results for this quantum model have been derived, which include the one-loop corrections for the local singlet-superconductivity order parameter [12] and for the velocity of the Bogoliubov-Anderson backflow mode [13] in the superconducting low-temperature phase of the model. In this previous work, the leading singular contributions near two dimensions have been obtained at one-loop level, considering only the soft XY-like order parameter phase fluctuations, while fluctuations in the Ising-sector have been neglected due to their irrelevance away from half band-filling. As a particular finding, the one-loop expression for the superconducting order parameter could be identified with the corresponding scaling result for the classical abelian nonlinear σ-model.

In the present work, a field theoretic representation for the strong-coupling negative-U Hubbard model is formulated and applied, which fully takes into account both the planar and out-of-plane fluctuations of the Heisenberg quantum pseudo-spins. At half band-filling, a partial particle-hole transformation maps the Hubbard model with negative U on the positive-U case and reflects the full $O(3)$ symmetry of the isotropic pseudo-spin Heisenberg model, while away from half filling the nonvanishing chemical potential suppresses the singular out-of-plane fluctuations and causes a crossover to XY-like behaviour. Starting from the Grassmann representation of the model on the restricted fermionic Hilbert space, the effective theory for the bosonic order parameter pair fields is derived. This allows to include all possible types of fluctuations on the lattice and thus does not have to rely on the peculiar assumptions [14, 15] related to the derivation of a corresponding quantum nonlinear σ-model, whose scaling behaviour near $d = 2$ is however reproduced. In particular, it is not necessary to invoke the large-spin limit or to restrict the fluctuations to low momenta. While in the case of the nonlinear σ-model the fields are subject to a "fixed length" constraint which restricts the fluctuations to soft ones and in this way generates higher powers of the fields in the action, in our theory higher order contributions are naturally obtained from the expansion of the effective action. Both soft and massive modes are contained in this action on an equal footing, since our approach does not require to impose any restricting conditions on the fields. As a consequence, also in the limit of zero frequency and momentum, quantum fluctuations are still present in the theory. The field theoretic formulation presented in this paper can therefore also be put in a broader perspective in relation to the description of quantum spin models.

The effective lattice action is derived up to fifth order in the fluctuation fields, which is sufficient to obtain the two-loop contribution to the order parameters for low temperatures and in the leading dimensional singularities. Compared to a many-body theoretical expansion in the fermionic one-particle operators, this field theoretical approach simplifies the calculations significantly. While at two-loop order the diagrammatical expansions of both the superconducting and charge-density order parameters involve several thousand contractions of the fermionic variables, in our effective field theory only eight different diagram types need to be evaluated. In the diagrammatical expansions in the fermionic variables a n-orbital generalization of the Hubbard model was used for the systematic classification of diagrams [12, 13], whereas in our field theoretic approach we exploit the equivalence of the loop-expansion with an expansion in powers of the temperature. Since such a classification breaks down for temperatures which are not small on the scale of the pseudo-spin coupling, we have to restrict our calculations to a region well below the critical temperature.

2 Effective field theory and fluctuations

We consider the Hubbard Hamiltonian with attractive on-site interaction $U < 0$, the chemical potential μ, and hopping t between neighboring lattice sites,

$$\mathcal{H} = t \sum_{\langle ij \rangle \sigma} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}, \tag{1}$$

where $c^{+}_{j\sigma}$ creates an electron with spin σ at site j. In the strong-coupling limit, $t \ll |U|$, the well-known t/U-expansions for the Hubbard model [9, 10] lead to a mapping of this Hamiltonian on the anisotropic quantum Heisenberg model,

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \left(-A^{+}_{i} A_{j} + N_i N_j \right) - 2\mu \sum_{i} N_i, \tag{2}$$

with the nearest-neighbor coupling constant $J_{ij} = J = 2t^2/|U|$ and the pseudo-spin pair operators $A_j = c_{j\downarrow} c_{j\uparrow}$ and $N_j = n_{j\uparrow} n_{j\downarrow} = \frac{1}{2} \sum_{\sigma} n_{j\sigma}$. This last identification allows to absorb the Hubbard interaction term into the chemical potential by the shift $\mu \to \mu - U/2$. It is permissible in the limit $t \ll |U|$, which imposes the constraint that the local fermionic Hilbert space contains only pair states, i.e. single occupancy of sites is ruled out. This constraint is modelled exactly by a spin-dependent Popov-Fedotov potential [12]. The identity $\langle N \rangle = \frac{1}{2} \sum_{\sigma} \langle n_{\sigma} \rangle$ imposes a further condition, relating the total pseudo-magnetization to the band-filling. The partition function of the model (2) can then be written as a functional integral over Grassmann fields,

$$Z = \int \prod_{i\sigma\tau} \mathcal{D}\overline{\psi}_{i\sigma}(\tau) \mathcal{D}\psi_{i\sigma}(\tau) \, \exp \mathcal{S}\{\overline{\psi}_{i\sigma}(\tau), \psi_{i\sigma}(\tau)\}, \tag{3}$$

with the action

$$\mathcal{S}\{\overline{\psi}_{i\sigma}(\tau), \psi_{i\sigma}(\tau)\} = \frac{1}{\hbar} \int_0^{\beta\hbar} \mathrm{d}\tau \left[\sum_{i\sigma} \overline{\psi}_{i\sigma}(\tau) \left(\hbar \partial_{\tau} + \mu \right) \psi_{i\sigma}(\tau) \right.$$

$$+J\sum_{\langle ij\rangle}\left(\overline{\psi}_{i\uparrow}(\tau)\overline{\psi}_{i\downarrow}(\tau)\psi_{j\downarrow}(\tau)\psi_{j\uparrow}(\tau)-\frac{1}{4}\sum_{\sigma\sigma'}\overline{\psi}_{i\sigma}(\tau)\psi_{i\sigma}(\tau)\overline{\psi}_{j\sigma'}(\tau)\psi_{j\sigma'}(\tau)\right)\Bigg]. \quad (4)$$

As a consequence of the elimination of the unphysical fermionic states which are not related to a pseudo-spin state, the Grassmann fields obey the modified periodicity conditions $\psi_{j\sigma}(\beta\hbar)=i\sigma\psi_{j\sigma}(0)$, which correspond to the spin-dependent Matsubara frequencies $z_{n\sigma}=\frac{\pi}{\beta\hbar}(2n+1+\frac{\sigma}{2})$, with $\sigma=\pm1$.

We now introduce the local Hubbard-Stratonovitch order parameter pair fields Δ_i and X_i, with $\langle\Delta_i\rangle=\sum_j J_{ij}\langle c_{j\downarrow}c_{j\uparrow}\rangle$ and $\langle X_i\rangle=\frac{1}{2}\sum_{j\sigma}J_{ij}(-1)^j\langle c^+_{j\sigma}c_{j\sigma}\rangle$, and transform to momentum and Matsubara frequency space. The action (4) is then decoupled into bilinear products of Grassmann variables which are integrated out to yield the effective action for the pair fields,

$$\mathcal{S}\{\Delta_{q,m},X_{q,m}\}=-\beta\sum_m\int \mathrm{d}^dq\frac{1}{J_q}\left(\overline{\Delta}_{q,m}\Delta_{q,m}+X_{q,m}X_{-q,-m}\right)+\sum_j\ln\det\mathbf{M}_j, \quad (5)$$

where $J_q=J_0\gamma_q=J\sum_{l=1}^d 2\cos(q_la)$ is the momentum dependent pseudo-spin coupling on the simple cubic lattice. The bilinear kernel $\mathbf{M}_j$ which enters into the fermion determinant is given by

$$\beta^{-1}(\mathbf{M}_j)_{n+m,n}=(i\hbar z_{n\sigma}\,\rho_z+\mu\,\rho_0)\delta_{m,0}+(-1)^jX_{j,m}\,\rho_0-\Delta_{j,m}\,\rho_++\overline{\Delta}_{j,-m}\,\rho_-, \quad (6)$$

with the Pauli matrices ρ.

In order to extract the saddle-point solutions $\langle\Delta_{0,0}\rangle^{(0)}$ and $\langle X_{0,0}\rangle^{(0)}$ from the effective action (5), $\mathcal{S}$ is now divided into a static and homogeneous part $\mathcal{S}_0$ and the fluctuation contribution $\mathcal{S}_{\rm fl}$. In the following we choose $\langle X_{0,0}\rangle^{(0)}\equiv0$, which is always a solution of the saddle-point equations that follow from (5), and which corresponds to purely planar ordering of the pseudo-spins in the low-temperature phase. Since in the saddle-point solution charge-ordering (with $\langle X_{0,0}\rangle^{(0)}\neq0$) is suppressed for nonzero chemical potential, only at half band-filling this choice is a restriction of the full symmetry of the saddle-point manifold, which in this case is restored by singular out-of-plane fluctuations.

In this way one finds

$$\mathcal{S}_0=-\frac{\beta\Delta^2}{J_0}+\ln\cosh\beta\sqrt{\mu^2+\Delta^2}, \quad (7)$$

which immediately leads to the self-consistency equation for the superconducting order parameter $\Delta=\langle\Delta_{0,0}\rangle^{(0)}$,

$$\frac{\tanh\beta\sqrt{\mu^2+\Delta^2}}{2\sqrt{\mu^2+\Delta^2}}=\frac{1}{J_0}. \quad (8)$$

The saddle-point equations also allow for a nonzero $\langle X_{\pi,0}\rangle^{(0)}$ which corresponds to the band-filling; this simply reflects a shift of the chemical potential, which can be viewed as the order parameter related to the pair occupation number. Choosing $\langle X_{\pi,0}\rangle^{(0)}\equiv0$, one obtains in the superconducting phase

$$\mu=J_0(\nu-\frac{1}{2}), \quad (9)$$

where $\nu = \langle n_\uparrow n_\downarrow \rangle$ is the band-filling. For $T = 0$, this implies $\Delta = J_0|\alpha_0| = J_0\sqrt{\nu(1-\nu)}$.

We now introduce the local (fermionic) propagator matrix $\mathbf{G} = (\mathbf{M}_0)^{-1}$, where $\mathbf{M}_0$ is the saddle-point value of the kernel (6), and the fluctuation fields

$$\beta^{-1}(\Phi_j)_{n+m,n} = (-1)^j X_{j,m}\,\rho_0 + \phi_{j,m}\,\rho_+ - \overline{\phi}_{j,-m}\,\rho_-, \tag{10}$$

which allow the separation $\mathbf{M}_j = \mathbf{M}_0 + \Phi_j$. The (spin-dependent) propagator $\mathbf{G}$ describes lattice fermions with infinite mass,

$$\beta(\mathbf{G})_{n+m,n} = \frac{\delta_{m,0}}{(\hbar z_{n\sigma})^2 + \mu^2 + \Delta^2}\left(-i\hbar z_{n\sigma}\,\rho_z + \mu\,\rho_0 + i\Delta\,\rho_y\right). \tag{11}$$

Inserted in (5), this results in the effective action that describes the fluctuations, $\mathcal{S}_{\rm fl} = \mathcal{S}_2 + \mathcal{S}_{\rm int}$. Its free part is given by

$$\begin{aligned}
\mathcal{S}_2 &= -\beta\sum_m \int \mathrm{d}^d q \frac{1}{J_q}\left(\overline{\phi}_{q,m}\phi_{q,m} + X_{q,m}X_{-q,-m}\right) - \frac{1}{2}\sum_j \mathrm{Tr}(\mathbf{G}\Phi_j)^2 \\
&= -\frac{\beta}{J_0}\sum_m \int \mathrm{d}^d q \frac{1}{C_m\gamma_q}\chi^T_{q,m}\mathbf{A}_{q,m}\chi_{-q,-m},
\end{aligned} \tag{12}$$

where $C_m = \mu^2 + \Delta^2 + \frac{1}{4}(\hbar\omega_m)^2$, and the new basis $\chi^T_{q,m} = (\phi^+_{q,m}, i\phi^-_{q,m}, X_{\pi+q,m})$ with the components $\phi^\pm_{q,m} = \frac{1}{2}(\overline{\phi}_{-q,-m} \pm \phi_{q,m})$ has been introduced. For $q \approx 0$, the fields ϕ^- correspond to the soft transversal phase fluctuations of the complex order parameter Δ, while the massive longitudinal ones are related to ϕ^+. The structure of the inverse propagator for the fluctuation fields is given by the matrix

$$\mathbf{A}_{q,m} = \begin{pmatrix} C_m - \mu^2\gamma_q & -\frac{1}{2}\mu\hbar\omega_m\gamma_q & -\mu\Delta\gamma_q \\ \frac{1}{2}\mu\hbar\omega_m\gamma_q & C_m - (\mu^2+\Delta^2)\gamma_q & \frac{1}{2}\Delta\hbar\omega_m\gamma_q \\ -\mu\Delta\gamma_q & -\frac{1}{2}\Delta\hbar\omega_m\gamma_q & -C_m - \Delta^2\gamma_q \end{pmatrix}. \tag{13}$$

In the static limit, $\omega_m \equiv 0$, the soft planar fluctuations ϕ^- decouple from the massive ones, ϕ^+ and X. For vanishing chemical potential, also the massive in-plane and out-of-plane modes are decoupled. Away from half band-filling, however, all components are coupled dynamically. The excitation spectrum related to these fluctuations then immediately follows from the condition $\det\mathbf{A} = 0$, which by analytical continuation $i\omega_m \to \omega$ yields the dispersion relation of the possible modes,

$$\frac{1}{4}(\hbar\omega)^2 = \mu^2(1-\gamma_q)^2 + \Delta^2(1-\gamma_q^2). \tag{14}$$

This energy spectrum encapsulates two massless modes, whose leading components at half band-filling are $\phi^-_{q,m}$ for $q \approx 0$, and $X_{\pi+q,m}$ for $q \approx \pi$. These excitations correspond to the Bogoliubov-Anderson mode of the superconducting phase, and alternating charge-density fluctuations which become soft at half band-filling, respectively. In the massless case, both are described by the linear dispersion $\omega = ck$, with the velocity $c = 2\Delta a/\hbar\sqrt{d}$. Due to the coupling of the planar modes to the out-of-plane fluctuations, this result modifies the value for the velocity c obtained in previous work [12, 13].

The higher order terms of the fluctuation expansion contribute to the interacting part of the effective action,

$$\mathcal{S}_{\rm int} = \sum_j \sum_{k=3}^{\infty} \frac{(-1)^{k+1}}{k}\mathrm{Tr}(\mathbf{G}\Phi_j)^k. \tag{15}$$

To evaluate the two-loop corrections of the order parameters and of the chemical potential consistently, it is sufficient to obtain $\mathcal{S}_{\rm int}$ up to fifth order in the fluctuation fields, if we restrict ourselves to the contributions which are leading *both* in T for low temperature and in the dimensional singularities near $d=2$. For small T, the loop-expansion corresponds to an expansion in powers of the temperature [16], but due to the existence of massive modes and nonsingular quantum corrections partially nonsingular diagrams of higher order in T may still contribute to a lower order in the singularities. To make the expansion well controlled, we neglect these non-leading terms. This also implies to consider only diagrams related to *static* internal propagators, therefore we may set $\omega_m=0$ in the free bosonic Matsubara sums. For higher temperature $T\approx T_c$, the loop expansion is no longer equivalent to an expansion in powers of T, and this classification of diagrams can not be applied. Since the interacting part of the action mixes singular and nonsingular modes, at a given order of the singularities arbitrarily high loop-orders contribute, which makes the loop-expansion completely uncontrolled. Therefore, our calculations are restrained to the low-temperature case, keeping only the leading singularities and powers in T. This is in contrast to the fermionic diagram theory based on the n-orbital generalization of the model, which provides an independent classification of diagrams in orders of $1/n$.

Introducing the new fields λ, with $J_0\lambda_{q,m}=\mu X_{\pi+q,m}-\Delta\phi^+_{q,m}$, we find for the interacting part of the effective action, $\mathcal{S}_{\rm int}=\mathcal{S}_3+\mathcal{S}_4+\mathcal{S}_5$, the explicit low-temperature results

$$\mathcal{S}_3=\frac{\beta}{J_0^2}\sum_j\left[16\,\lambda_{j,0}^3-4\,\lambda_{j,0}(\chi_{j,0}^T\chi_{j,0})\right], \tag{16}$$

$$\mathcal{S}_4=\frac{\beta}{J_0^3}\sum_j\left[-80\,\lambda_{j,0}^4+24\,\lambda_{j,0}^2(\chi_{j,0}^T\chi_{j,0})-(\chi_{j,0}^T\chi_{j,0})^2\right], \tag{17}$$

and

$$\mathcal{S}_5=\frac{\beta}{J_0^4}\sum_j\left[448\,\lambda_{j,0}^5-160\,\lambda_{j,0}^3(\chi_{j,0}^T\chi_{j,0})+12\,\lambda_{j,0}(\chi_{j,0}^T\chi_{j,0})^2\right], \tag{18}$$

which complete the derivation of the fluctuation part of the effective action. In accordance with the leading behaviour, in these expressions we have considered only the static contributions, and in the prefactors terms which are exponentially small in the temperature have been neglected.

In the original fields ϕ_j^+, ϕ_j^-, and X_j, the effective action derived in this section corresponds to an interacting theory with six different types of 3-point vertices, nine types of 4-point vertices, and twelve different 5-point vertices, which are encapsulated in the fluctuation contributions (16-18). It is apparent from this result for $\mathcal{S}_{\rm int}$ that the fluctuations do not decouple into soft and massive ones, but are described by interactions mixing the singular and nonsingular modes.

3 Results in one-loop order

In this section we show that the one-loop results for the order parameters and the chemical potential, which partly have been obtained in earlier work by many-body theoretical expansions [12], can be easily rederived and extended in our field theoretic approach. The loop-corrections of the saddle-point value for these quantities involve the calculation of the related 1-point functions, i.e. the expectation value for the corresponding fluctuation fields, $\langle\phi^+_{0,0}\rangle^{(1)}$, $\langle X_{0,0}\rangle^{(1)}$, and $\langle X_{\pi,0}\rangle^{(1)}$, respectively. Since the transversal planar fluctuations are soft, they are coupled to the massive modes only dynamically and therefore do not contribute, $\langle\phi^-_{0,0}\rangle^{(1)} = 0$. This can be verified directly by inspection of the propagator matrix derived from (13) and the interaction terms (16-18).

At one-loop level, for the fluctuation contribution to the 1-point functions only one diagram related to $\mathcal{S}_3$ has to be evaluated (see fig. 1), compared to 20 possible fermionic contractions [12]. Since the effective 1-point vertex cannot carry a total momentum $q = \pi$, one immediately finds

$$\langle X_{0,0}\rangle^{(1)} = 0, \tag{19}$$

which is a consequence of the choice of the corresponding saddle-point value, $\langle X_{0,0}\rangle^{(0)} = 0$. From the action $\mathcal{S}_3$ and the structure of the propagator that follows from (13), it is also easily seen that for $\langle X_{\pi,0}\rangle$ only nonsingular contributions are obtained. Therefore, in our approximation,

$$\langle X_{\pi,0}\rangle^{(1)} = 0, \tag{20}$$

which implies that the one-loop contribution to the chemical potential vanishes, $\mu^{(1)} = 0$. This generalizes the diagrammatical low-temperature result that included only the leading in-plane fluctuations [12].

The superconducting order parameter has a nonzero one-loop correction, which in the leading order reads

$$\langle\Delta_{0,0}\rangle^{(1)} = -\langle\phi^+_{0,0}\rangle^{(1)} = -\frac{T\Delta}{2}\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right), \tag{21}$$

where we have introduced $T = 1/(\pi\beta J_0|\alpha_0|^2)$ as the reduced temperature. Since $\mu^{(1)} = 0$, no correction of the chemical potential has to be considered in the zero-loop propagators. The momentum integrals which appear in (21) are given by

$$I_d^{(k)}(m) = \frac{1}{2}\int_0^{\Lambda^2} \frac{\mathrm{d}x\; x^{d/2-1}}{(x+m^2)^k}, \tag{22}$$

where Λ is the lattice cutoff of the momentum. The mass m vanishes at half band-filling, with $m^2 = 8\mu^2/\Delta^2$ near the center of the band. $I_d^{(1)}(0)$ exhibits singular behaviour near two dimensions, $I_d^{(1)}(0) \simeq 1/(d-2)$. Generally, one has $I_d^{(k)}(0) \simeq 1/(d-2k)$ near $2k$ dimensions. The expression (21) generalizes the many-body theoretical one-loop result of ref. [12] to include the contribution of out-of-plane fluctuations of the pseudo-spins. It signals a stronger suppression of the superconducting order due to the enhanced fluctuations, and is in accordance with the scaling behaviour of the corresponding nonlinear σ-model, as will be discussed below.

4 Two-loop corrections

At two-loop order, the effective 1-point functions are obtained from the seven diagrams depicted in fig. 2. Three classes of diagrams contribute: (a) - (c), which involve three 3-point vertices; (d) - (f), with one 3-point and one 4-point vertex; and (g), which is derived from the 5-point vertex. In comparison, the calculation of the corresponding one-particle propagators in the fermionic diagram theory would involve 3120 different contractions.

4.1 Chemical potential

Evaluating the two-loop contributions to the pair occupation number, $\langle X_{\pi,0}\rangle^{(2)}$, we find the following results for the different diagrams:

$$\langle X_{\pi,0}\rangle^{(2)}_{(a)} = \langle X_{\pi,0}\rangle^{(2)}_{(d)} = \langle X_{\pi,0}\rangle^{(2)}_{(g)} = 0, \tag{23}$$

which in our classification vanish since they contribute only nonsingular terms. One further obtains

$$\begin{aligned}
\langle X_{\pi,0}\rangle^{(2)}_{(b)} &= - \frac{T^2\mu|\alpha_0|^2}{2}\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right)^2, &(24)\\
\langle X_{\pi,0}\rangle^{(2)}_{(c)} &= - T^2\mu|\alpha_0|^2\left([I_d^{(1)}(0)]^2 + [I_d^{(1)}(m)]^2\right), &(25)\\
\langle X_{\pi,0}\rangle^{(2)}_{(e)} &= + \frac{T^2\mu|\alpha_0|^2}{2}\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right)^2, &(26)
\end{aligned}$$

and

$$\langle X_{\pi,0}\rangle^{(2)}_{(f)} = + T^2\mu|\alpha_0|^2\left([I_d^{(1)}(0)]^2 + [I_d^{(1)}(m)]^2\right). \tag{27}$$

These expressions exactly cancel each other, so that one again finds $\langle X_{\pi,0}\rangle^{(2)} = 0$. The chemical potential is therefore not modified, $\mu^{(2)} = 0$, and retains its saddle-point value (9) up to nonsingular terms also at the two-loop level.

4.2 Order parameters

For the 1-point vertex related to $X_{0,0}$ also at two-loop order the same argument as in the one-loop case applies, so that one immediately deduces

$$\langle X_{0,0}\rangle^{(2)} = 0. \tag{28}$$

Since at half band-filling, where the full $O(3)$ symmetry of the model is restored, one could have chosen a nonzero saddle-point value $\langle X_{0,0}\rangle^{(0)}$, this result (28) is in accordance with the corresponding two-loop expression $\langle \Delta_{0,0}\rangle^{(2)}$ derived below, eq. (36).

For the correction of the superconducting order parameter it is again sufficient to evaluate $\langle \phi^+_{0,0}\rangle^{(2)}$, whereas $\langle \phi^-_{0,0}\rangle^{(2)} = 0$ due to its massless character. We find the explicit contributions of the diagrams:

$$\begin{aligned}
\Delta^{-1}\langle \Delta_{0,0}\rangle^{(2)}_{(a)} &= - 2T^2|\alpha_0|^2\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right)\left(I_d^{(2)}(0) + I_d^{(2)}(m)\right), &(29)\\
\Delta^{-1}\langle \Delta_{0,0}\rangle^{(2)}_{(b)} &= + T^2\left(|\alpha_0|^2 - \frac{1}{4}\right)\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right)^2, &(30)\\
\Delta^{-1}\langle \Delta_{0,0}\rangle^{(2)}_{(c)} &= + 2T^2|\alpha_0|^2\left([I_d^{(1)}(0)]^2 + [I_d^{(1)}(m)]^2\right)\\
&\quad - 4T^2|\alpha_0|^2\left(I_d^{(1)}(0)I_d^{(2)}(0) + I_d^{(1)}(m)I_d^{(2)}(m)\right), &(31)\\
\Delta^{-1}\langle \Delta_{0,0}\rangle^{(2)}_{(d)} &= + 2T^2|\alpha_0|^2\left(3I_d^{(1)}(0)I_d^{(2)}(0) + 3I_d^{(1)}(m)I_d^{(2)}(m)\right.\\
&\quad \left. + I_d^{(1)}(0)I_d^{(2)}(m) + I_d^{(1)}(m)I_d^{(2)}(0)\right), &(32)\\
\Delta^{-1}\langle \Delta_{0,0}\rangle^{(2)}_{(e)} &= + \frac{T^2}{4}\left(-10|\alpha_0|^2 + \frac{1}{2}\right)\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right)^2, &(33)\\
\Delta^{-1}\langle \Delta_{0,0}\rangle^{(2)}_{(f)} &= + \frac{T^2}{2}\left(-10|\alpha_0|^2 + \frac{1}{2}\right)\left([I_d^{(1)}(0)]^2 + [I_d^{(1)}(m)]^2\right), &(34)
\end{aligned}$$

and

$$\Delta^{-1}\langle\Delta_{0,0}\rangle^{(2)}_{(g)} = \; + \; \frac{3}{2}T^2|\alpha_0|^2\left(3[I_d^{(1)}(0)]^2 + 3[I_d^{(1)}(m)]^2 + 2I_d^{(1)}(0)I_d^{(1)}(m)\right). \qquad (35)$$

Adding up these contributions, (29-35), we find that all terms involving integrals of the type $I_d^{(2)}$ exactly cancel, which is expected from the renormalizability of the nonlinear σ-model in two dimensions [17] and the singular behaviour of $I_d^{(2)}(0) \simeq 1/(d-4)$. Again, since also $\mu^{(2)} = 0$, the chemical potential retains its zero-loop value in all diagrams, and no further contributions need to be considered. One finally obtains for the two-loop correction of the Δ-fields

$$\langle\Delta_{0,0}\rangle^{(2)} = +\frac{T^2\Delta}{8}\left(I_d^{(1)}(0) - I_d^{(1)}(m)\right)^2, \qquad (36)$$

which is positive, contrary to the one-loop result. Combining the expressions (21) and (36), the superconducting order parameter of the strong-coupling negative-U Hubbard model at two-loop order then reads

$$|\alpha| = |\alpha_0|\left[1 - \frac{T}{2}\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right) + \frac{T^2}{8}\left(I_d^{(1)}(0) - I_d^{(1)}(m)\right)^2 + \mathcal{O}(T^3)\right]. \qquad (37)$$

This result is in agreement with the scaling behaviour expected from the XY and Heisenberg case, $n = 2$ and $n = 3$, of the $O(n)$ nonlinear σ-model [18], if we interpret the expression (37) as the second-order expansion of a corresponding scaling relation,

$$|\alpha| = |\alpha_0|\exp\left[-\frac{T}{2}\left(I_d^{(1)}(0) + I_d^{(1)}(m)\right) - \frac{T^2}{2}I_d^{(1)}(0)\,I_d^{(1)}(m) + \mathcal{O}(T^3)\right]. \qquad (38)$$

For $m = 0$ and $m \to \infty$, this reproduces the $n = 3$ and $n = 2$ scaling results.

5 Conclusion

We have applied a functional integral representation of the strong-coupling negative-U Hubbard model involving Grassmann fields with modified periodicity conditions in order to derive an effective fluctuation theory for the order parameter pair fields of the model. This allows for a complete description of quantum fluctuations on the lattice, with both singular and nonsingular modes treated on an equal basis. Expanding the effective action up to fifth order in the fluctuations, the contributions to the chemical potential and to the order parameters of superconductivity and charge-ordering have been derived at two-loop order, taking into account the full symmetry of the model, and keeping the contributions which are leading for low temperatures and in the dimensional singularities. The results are in agreement with the scaling behaviour expected from the corresponding limits of the $O(n)$ nonlinear σ-model.

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Figure 1

One-loop contribution to the 1-point functions.

(● denotes the corresponding 1-point vertex.)

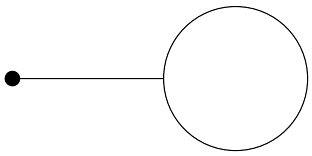

Figure 2

Two-loop contributions to the 1-point functions.