Generation of *d*-wave coupling in the two-dimensional Hubbard model from functional renormalization

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Within the two-dimensional repulsive t-t' Hubbard model, an attractive coupling in the *d*-wave-pairing channel is induced by antiferromagnetic fluctuations. We investigate this coupling using functional renormalization-group equations. The momentum-dependent *d*-wave coupling can be bosonized by the use of scale-dependent field transformations. We propose an effective coarse-grained model for the Hubbard model which is based on the exchange of antiferromagnetic and *d*-wave collective bosons.

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I. INTRODUCTION

The Hubbard model^{1–3} for strongly correlated electrons has been used for a wide variety of phenomena, ranging from high-temperature superconductivity⁴ to the metal-insulator transition or antiferromagnetism. Solving this model is a major theoretical challenge. This is due to the complexity of the effective electron interaction, typically characterized by the competition of different channels, such as the antiferromagnetic or *d*-wave Cooper-pair exchange channels.^{5–13} So far, the development of *d*-wave superconductivity is still a controversial issue. Although several many-body techniques predict the emergence of a *d*-wave instability as leading instability in certain parameter ranges, see, e.g., Ref. 5, numerical studies have difficulties to detect superconductivity^{5,14–20} as a consequence of both finite-size and temperature limitations.

The *d*-wave-pairing interactions are absent in the microscopic Hubbard model. As a plausible mechanism leading to *d*-wave pairing the exchange of effective antiferromagnetic bosonic degrees of freedom has been proposed.^{6–11} This idea was also suggested in Refs. 12 and 13 on the basis of a phenomenological spin-spin susceptibility. The generation of the interaction in the *d*-wave channel has been investigated extensively by the functional renormalization-group study of a momentum-dependent four-electron vertex.²¹⁻³¹ Our investigation employs nonperturbative flow equations based on exact renormalization-group equations for the average action or flowing action.^{32,33} It is complementary to studies of the electron vertex by focusing explicitly on the role of the antiferromagnetic bosons using the technique of partial bosonization during the flow.^{34,35} We investigate the twodimensional Hubbard model with nearest- and next-nearestneighbor hoppings.

The aim of this paper is the derivation of an effective coarse-grained model valid at intermediate length scales k^{-1} larger than the lattice distance *a* but smaller than the scale of macroscopic physics. Our effective model will be based on a description of the electron interactions by the exchange of collective bosons. Near half filling a model with exchange of antiferromagnetic boson has been used^{36,37} for a quantitative computation of effective antiferromagnetic order below the effective critical temperature T_c . It is advocated that in two

dimensions the size of the ordered domains increases exponentially as the temperature decreases toward zero. For $T < T_c$ this size exceeds the size of a typical experimental probe. For all practical purposes the physics is then the same as for an ordered system. This includes the existence of long-range fluctuations associated to Goldstone bosons. For $T_c < T < T_{\rm pc}$ short-range antiferromagnetic order is found with a typical domain size smaller than the experimental probe. Here $T_{\rm pc}$ denotes the pseudocritical temperature below which short-range antiferromagnetic order sets in. In this paper we extend this approach by including the exchange of collective bosons consisting of Cooper pairs in the *d*-wave channel. They are assumed to be a crucial ingredient for the understanding of the Hubbard model away from half filling. Their condensate would lead to superconductivity.

We have investigated earlier the phase transition to superconductivity in an effective *d*-wave exchange model.³⁸ The phase transition is found to be of the Kosterlitz-Thouless type,³⁹ characterized by (modified) essential scaling above T_c , a jump of the superfluid density at T_c , and a gapless excitation with temperature-dependent anomalous dimension below T_c . The present paper constitutes a step for establishing such an effective model as a coarse-grained version of the microscopic Hubbard model. This mapping is not yet complete since we concentrate here only on the generation of the effective electron interaction in the *d*-wave channel and its bosonization, while a more detailed investigation of the propagators and interactions of the *d*-wave bosons is postponed to a subsequent publication.

The partially bosonized model opens the door for a straightforward computation of the flow below the pseudocritical temperature $T_{\rm pc}$, where local order sets in and higher-order boson interactions (e.g., corresponding to eightfermion interactions) play an important role. The lowtemperature region is notoriously difficult for a purely fermionic description since the four-fermion interaction diverges as the pseudocritical temperature $T_{\rm pc}$ is approached from above. Also the important effect of higher fermionic operators can be taken into account most conveniently in a partially bosonized formulation.^{36,37} In the partially bosonized description the divergence of the four-fermion interaction is due to a boson "mass term" or "gap," changing from positive to negative values during the flow. A negative mass term indicates local order, since at a given coarse graining scale k the effective potential has a minimum for a nonzero value of the boson field. If this order persists for k reaching a macroscopic scale, the model exhibits effectively spontaneous symmetry breaking, associated in our model to antiferromagnetism or d-wave superconductivity.

On the other hand, the partially bosonized formulation introduces some bias into the renormalization-group procedure by focusing on one or several boson exchange channels. This can be circumvented in the purely fermionic renormalization-group flow. However, this bias can be systematically reduced by the introduction of further bosonic fields, which yield additional resolution for the description of the interaction between the electrons. The present approach constitutes a first step into this direction and is thus complementary to Refs. 21–31.

II. EFFECTIVE AVERAGE ACTION

We use a functional-integral framework and investigate the effective average action Γ_k ,^{32,33} which includes all quantum and thermal fluctuations with momenta $\mathbf{q}^2 \geq k^2$. This is realized by introducing an infrared cutoff R_k , which suppresses the fluctuations with $\mathbf{q}^2 \leq k^2$. This cutoff will be removed at the end for $k \rightarrow 0$. For k=0 one recovers the usual effective action—the generating functional for the oneparticle irreducible Green functions. For $k \rightarrow \infty$, or $k \rightarrow \Lambda$, with Λ as a suitable ultraviolet scale, the fluctuation effects are negligible and Γ_{Λ} becomes the microscopic or classical action S_{Λ} . Therefore the scale-dependent average action Γ_k interpolates between the microscopic action S_{Λ} and the full quantum effective action Γ ,

$$\lim_{k \to \Lambda} \Gamma_k \simeq S_{\Lambda}, \quad \lim_{k \to 0} \Gamma_k = \Gamma.$$
(1)

The *k*-dependent flow of the average action obeys an exact renormalization-group equation, 32

$$\partial_k \Gamma_k[\chi] = \frac{1}{2} \operatorname{STr}\{[\Gamma_k^{(2)}[\chi] + R_k]^{-1} \partial_k R_k\},\tag{2}$$

where the "supertrace" (STr) runs over field type, momentum, and internal indices and has an additional minus sign for fermionic entries. The functional differential equation (2) involves the full inverse propagator $\Gamma_k^{(2)}[\chi]$ (second functional derivative of Γ_k) regulated by R_k . Approximations to the solution of Eq. (2) proceed by a truncation on the righthand side (rhs) with a suitable ansatz for the form of Γ_k .

On the microscopic level, the Hubbard model is defined as a purely fermionic model for electrons on a lattice. However, it is well known that bosonic degrees of freedom, e.g., Cooper pairs, also play an important role on larger length scales. Hence, the question arises how the optimal description of the relevant degrees of freedom on all scales can be achieved within a functional renormalization-group study. On one hand, we want to accommodate the purely fermionic model at high-momentum scales. On the other hand, we want to study phase transitions and critical behavior for the macroscopic physics. In the vicinity of the critical temperature the long-range fluctuations are dominated by bosonic composite operators. In order to exploit directly the importance of the collective bosonic degrees of freedom, we employ partial bosonization as motivated by a Hubbard-Stratonovich transformation.^{40,41} Spontaneous symmetry breaking can then be described simply by nonzero expectation values of suitable bosonic fields. In a purely fermionic description the four-fermion coupling often diverges for temperatures below a pseudocritical temperature $T_{\rm pc}$. This indicates the onset of local order for $T < T_{\rm pc}$. In the partially bosonized version this simply translates to a vanishing "mass parameter" or gap for the bosons and does not constitute an obstacle for investigations at $T < T_{\rm pc}$.

Antiferromagnetic order for the two-dimensional Hubbard model at half filling has been successfully described in this framework.^{36,37} One investigates a bosonic field **a** which represents an antiferromagnetic fermion bilinear,

$$\widetilde{\mathbf{a}}(X) = \psi^{\dagger}(X)\boldsymbol{\sigma}\psi(X)e^{i\Pi X}.$$
(3)

We use the Matsubara formalism with Euclidean time τ compactified on a torus with circumference $\beta = T^{-1}$. The Matsubara frequencies for the fermions are $\omega = (2n+1)\pi T$, where $n \in \mathbb{Z}$. Bosonic fields obey periodic boundary conditions such that $\omega = 2n\pi T$. We use a compact notation $X = (\tau, \mathbf{x})$, $Q = (\omega, \mathbf{q})$, and

$$\begin{split} \sum_{X} &= \int_{0}^{\beta} d\tau \sum_{\mathbf{x}} , \quad \sum_{Q} = T \sum_{n=-\infty}^{\infty} \int_{-\pi}^{\pi} \frac{d^{2}q}{(2\pi)^{2}}, \\ \delta(X - X') &= \delta(\tau - \tau') \,\delta_{\mathbf{x},\mathbf{x}'}, \\ \delta(Q - Q') &= \beta \,\delta_{n,n'}(2\pi)^{2} \,\delta^{(2)}(\mathbf{q} - \mathbf{q}'). \end{split}$$
(4)

All components of X or Q are measured in units of the lattice distance a or a^{-1} . The discreteness of the lattice is reflected by the 2π periodicity of the momenta **q**. The momentum Π in Eq. (3) is given by

$$\Pi = (0, \pi, \pi). \tag{5}$$

Antiferromagnetic order is indicated by a constant nonzero expectation value $\langle \mathbf{a}(X) \rangle = \mathbf{a}_0$. The simplest description employs a quartic effective potential for \mathbf{a} ,

$$U_{\mathbf{a}}[\mathbf{a}] = \bar{m}_a^2 \alpha + \frac{1}{2} \bar{\lambda}_a \alpha^2, \qquad (6)$$

with $\alpha = \mathbf{a}^2/2$. We will see that a vanishing of \overline{m}_a^2 corresponds to a diverging effective four-fermion coupling, while negative \overline{m}_a^2 leads to a minimum of $U_{\mathbf{a}}$ at $\alpha_0 \neq 0$, and therefore indicates spontaneous symmetry breaking. In the renormalization-group treatment, \overline{m}_a^2 and $\overline{\lambda}_a$ become k-dependent running couplings. A situation with $\overline{m}_a^2(k) < 0$ for $k_{SR} < k < k_{SSB}$, $\overline{m}_a^2(k < k_{SR}) > 0$ describes local order in domains with linear scale between k_{SSB}^{-1} and k_{SR}^{-1} , while no global antiferromagnetism is present. Macroscopic antiferromagnetic order can be observed if the k-dependent location of the potential minimum, $\alpha_0(k)$, stays nonzero as k^{-1} reaches the size of the experimental probe. For $\overline{m}_a^2 < 0$ a crucial ingredient for the determination of α_0 is the quartic bosonic coupling $\overline{\lambda}_a$. In a purely fermionic language this corresponds to an eightWe start with a Yukawa-type ansatz for the effective average action,

$$\Gamma_{k}[\chi] = \Gamma_{F,k}[\chi] + \Gamma_{\mathbf{a},k}[\chi] + \Gamma_{F\mathbf{a},k}[\chi].$$
(7)

It describes fermion fields ψ and the "antiferromagnetic boson field" **a** with $\chi = (\mathbf{a}, \psi, \psi^*)$. The fermionic kinetic term

$$\Gamma_{F,k} = \sum_{Q} \psi^{\dagger}(Q) P_{F}(Q) \psi(Q) \tag{8}$$

involves the inverse fermion propagator

$$P_F(Q) = i\omega + \xi(\mathbf{q}), \tag{9}$$

where

$$\xi(\mathbf{q}) = -\mu - 2t(\cos q_1 + \cos q_2) - 4t' \, \cos q_1 \cos q_2.$$
(10)

This is the classical inverse propagator for the Hubbard model with next-neighbor hopping *t* and diagonal hopping *t'*. The chemical potential is denoted by μ . We have included neither self-energy corrections for the fermionic propagator, whose significance is still under debate,^{42–44} nor possible Pomeranchuk instabilities, see, e.g., Ref. 23. In the present paper we restrict ourselves to a parameter and scale range where the spin correlations are maximal at the commensurate antiferromagnetic wave vector (5), e.g., we use t'=0 or t'/t=0.05.

The purely bosonic term is described by a kinetic term and a local effective potential U_{a} , cf. Eq. (6),

$$\Gamma_{a,k} = \frac{1}{2} \sum_{Q} \mathbf{a}^{T} (-Q) P_{a}(Q) \mathbf{a}(Q) + \sum_{X} U_{a,k}[\mathbf{a}].$$
(11)

The kinetic term P_a involves the *Q*-dependent part of the inverse antiferromagnetic propagator and is discussed in detail in the Appendix. The Yukawa-type interaction term couples the bosonic field to the fermions,

$$\Gamma_{F\mathbf{a},k} = -\bar{h}_a \sum_{Q} \mathbf{a}^T (-Q) \tilde{\mathbf{a}}(Q)$$
$$= -\bar{h}_a \sum_{K,Q,Q'} \delta(K + \Pi - Q + Q') \mathbf{a}(K)$$
$$\times \left[\psi^{\dagger}(Q) \boldsymbol{\sigma} \psi(Q') \right]. \tag{12}$$

This simplest truncation contains five k-dependent couplings, namely, \bar{m}_a^2 , $\bar{\lambda}_a$, \bar{h}_a , as well as the wave-function renormalization A_a , and the shape parameter D which parametrize $P_a(Q)$.

Inserting our truncation into the exact flow, Eq. (2) yields a coupled system of flow equations for \bar{m}_a^2 , $\bar{\lambda}_a$, \bar{h}_a , and P_a . This is solved numerically. We start at the microscopic scale $k=\Lambda$ with initial conditions

$$\bar{m}_a^2|_{\Lambda} = U_m, \quad \bar{h}_a|_{\Lambda} = U_m, \quad \bar{\lambda}_a|_{\Lambda} = 0, \quad P_a(Q)|_{\Lambda} = 0.$$
(13)

Since for this choice the effective action is quadratic in **a**, it is easy to solve for **a** as a functional of ψ , ψ^* . Reinserting

this solution into Γ_{Λ} yields the well-known microscopic action for the Hubbard model with four-fermion coupling U given by $U=3U_m$. Equivalently, we can use $S_{\Lambda}=\Gamma_{\Lambda}$ in the defining functional integral and perform the Gaussian integration over the "auxiliary" field **a**. This shows that our model is equivalent to the fermionic Hubbard model.⁴⁵

The equivalence between the Hubbard model and our description of antiferromagnetic boson exchange is exact, but this particular form of partial bosonization is not unique. Due to the possibility of a Fierz reordering of the local fourfermion interaction, one could also start with a coupling both in the charge and the antiferromagnetic channel on initial scale or include even further channels.⁴⁵ Distributing the local four-fermion action differently into the bosonic channels would alter the relation $U=3U_m$. Since the different possible versions of partial bosonization are all equivalent to the Hubbard model, one may question the reliability of our quantitative results based on $U_m = U/3$. In fact, mean-field theory shows a strong dependence of the phase diagram on the choice of partial bosonization.⁴⁵ However, mean-field theory neglects the effects of bosonic fluctuations and their inclusion substantially reduces the dependence of the results on the choice of bosonization.^{36,46} (Without truncations all exact partial bosonizations should be exactly equivalent such that the dependence on the choice can be used as a check of the validity of approximations.) In this paper, we concentrate on antiferromagnetic and d-wave fluctuations and do not include the charge channel. The inclusion of charge fluctuations within our bosonized language is in principle possible, and a first study³⁶ has indeed revealed that the results depend only weakly on the initial distribution of the four-fermion interaction into the antiferromagnetic and charge-density wave channels.

In this paper we want to understand the physics associated to fermion bilinears whose expectation value describes *d*-wave superconductivity. We therefore have to extend the simplest truncation (7). We introduce in addition a bosonic field *d* associated with the appropriate Cooper pairs \tilde{d} ,

$$\widetilde{d}(X) = \frac{1}{2}\psi^{T}\left(X - \frac{\hat{e}_{1}}{2}\right)\epsilon\psi\left(X + \frac{\hat{e}_{1}}{2}\right) - \frac{1}{2}\psi^{T}\left(X - \frac{\hat{e}_{2}}{2}\right)\epsilon\psi\left(X + \frac{\hat{e}_{2}}{2}\right).$$
(14)

Here, \hat{e}_1 and \hat{e}_2 are the unit vectors in the plane and $\epsilon = i\sigma_2$. [Equation (14) is used here only as a shorthand for the definition of \tilde{d} in momentum space, Eq. (34), since the Grassmann variables are not located at the lattice sites. A definition of \tilde{d} in position space and the appropriate Fourier transformation can be found, e.g., in Ref. 5.]

For the purely bosonic part we add in our truncation solely a mass term of the d boson,

$$\Gamma_{d,k} = \overline{m}_d^2 \sum_Q d^*(Q) d(Q).$$
⁽¹⁵⁾

The *d*-field couples to the fermions by a Yukawa term,



FIG. 1. (Color online) d-wave form factor.

$$\begin{split} \Gamma_{Fd,k} &= -\bar{h}_d \sum_X \left[d^*(X) \tilde{d}(X) + d(X) \tilde{d}^*(X) \right] \\ &= -\bar{h}_d \sum_Q \left[d^*(Q) \tilde{d}(Q) + d(Q) \tilde{d}^*(Q) \right] \\ &= -\frac{\bar{h}_d}{2} \sum_{K,Q,Q'} \delta(K - Q - Q') f_d(\mathbf{q} - \mathbf{q}') \\ &\times \left\{ d^*(K) \left[\psi^T(Q) \epsilon \psi(Q') \right] - d(K) \left[\psi^{\dagger}(Q) \epsilon \psi^*(Q') \right] \right\}, \end{split}$$
(16)

with Yukawa coupling \bar{h}_d . The *d*-wave form factor

$$f_d(\mathbf{q}) \equiv \cos\frac{q_1}{2} - \cos\frac{q_2}{2} \tag{17}$$

is kept fixed and shown in Fig. 1. We note the characteristic change in sign under rotations of 90°. In our approximation, only the momentum-independent coupling \bar{h}_d depends on the scale k. The extended truncation has two further running couplings, \bar{m}_d^2 and \bar{h}_d .

The initial values in the *d*-wave channel are

$$\overline{m}_d^2|_{\Lambda} = 1, \quad \overline{h}_d|_{\Lambda} = 0. \tag{18}$$

At the microscopic scale the *d* boson therefore decouples from the fermions and the **a** boson, such that the microscopic action is not modified. Our model remains exactly equivalent to the Hubbard model. For $k < \Lambda$, however, a nonzero Yukawa coupling \bar{h}_d is generated, as shown in Fig. 2. "Integrating out" the *d* boson by solving the field equations as a functional of ψ , and reinserting into Γ_k , yields an effective four-fermion interaction in the *d*-wave-pairing channel,

$$\Gamma^d_{F,4} = \lambda^d_F \sum_X \tilde{d}^*(X) \tilde{d}(X), \quad \lambda^d_F = -\frac{\bar{h}^2_d}{\bar{m}^2_d}.$$
 (19)

Even though absent microscopically, this interaction is generated during the flow by the coupling to the antiferromagnetic channel, as derived before in a purely fermionic language.^{21–24,26–31} The effective coupling λ_F^d is shown graphically in Fig. 2.



FIG. 2. (Color online) Generation of *d*-wave coupling. The solid line shows the flow of the *d*-wave channel fermionic coupling λ_F^d for T/t=0.13, $\mu/t=-0.1$, and t'=0. The dashed line shows the flow of the Yukawa coupling in the *d*-wave channel \bar{h}_d , as given by rebosonization for the same T, μ , t', and initial conditions (18).

III. FLOW EQUATIONS

In addition to the truncation of the effective average action, the regulator functions have to be defined. Our choice for the fermionic regulator is inspired by the fact that at nonzero temperature, the inverse fermionic propagator $P_F(Q)=2\pi i(n_F+\frac{1}{2})T+\xi_q$ has no zero eigenvalue. The temperature itself acts as a regulator. We put this into use by the regulator function³⁶

$$R_{k}^{F}(Q) = i\omega \left(\frac{T_{k}}{T} - 1\right) = 2\pi i \left(n_{F} + \frac{1}{2}\right)(T_{k} - T), \quad (20)$$

with

$$T_k^4 = T^4 + k^4,$$

$$\partial_k T_k = (k/T_k)^3 \longrightarrow \begin{cases} 1 & \text{if } k \ge T \\ (k/T)^3 & \text{if } k \ll T. \end{cases}$$
(21)

For $k \ge T$ the cutoff R_k^F in the inverse fermion propagator suppresses the contribution of all fluctuations with momenta $|\mathbf{q}-\mathbf{q}_F|^2 < (\pi k)^2$ even for T=0. It becomes ineffective for $k \le T$ where no cutoff is needed anyhow. Basically, the temperature T is replaced by the scale-dependent "temperature" T_k —we cool the fermions down to the temperature of interest during the flow. For $k \to \infty$ the cutoff diverges for all T such that fermion fluctuations are completely suppressed, and we start with the same initial conditions for all T. For $k \to 0$ the cutoff function vanishes for all T and one recovers the quantum effective action. For finite k^{-1} , corresponding to a finite macroscopic size of the probe or a finite experimental wavelength, the temperature dependence of the cutoff is small for $k \ll T$. In principal, different functional forms of $T_k(k)$ can be used for a test of the robustness of our truncation.

For bosons the situation is different. Here, long-range bosonic modes may cause infrared problems which cannot be regularized by the same type of regulator function we use for the fermions. In particular, near a second-order phase transition the bosonic correlation length diverges, which is the same as a vanishing boson mass term. Our regulator R_k^a is devised in order to cut off the long-range bosonic fluctua-

tions. We specify the regularization of the \mathbf{a} bosons in detail in the Appendix. No regularization of the *d* bosons is needed for the investigations in the present paper.

The flow equations for the couplings follow from projection of the flow equation (2) onto the corresponding monomial of fields. For the mass parameter in the effective potential one derives³⁶

$$\partial_k \bar{m}_a^2 = 2\bar{h}_a^2 \sum_Q \tilde{\partial}_k \frac{1}{P_F^k(Q) P_F^k(Q + \Pi)} + \frac{5}{2} \bar{\lambda}_a \sum_Q \tilde{\partial}_k \frac{1}{P_a^k(Q) + \bar{m}_a^2},$$
(22)

where

$$P_{a}^{k}(Q) = P_{a}(Q) + R_{k}^{a}(Q), \quad P_{F}^{k}(Q) = P_{F}(Q) + R_{k}^{F}(Q).$$
(23)

The derivative $\tilde{\partial}_k$ acts only onto the explicit k dependence introduced by the regulator functions and not on the couplings. For the quartic coupling the flow equation reads

$$\partial_k \bar{\lambda}_a = 4 \bar{h}_a^4 \sum_Q \tilde{\partial}_k \frac{1}{\left[P_F^k(Q) P_F^k(Q + \Pi)\right]^2} - \frac{11}{2} \bar{\lambda}_a^2 \sum_Q \tilde{\partial}_k \frac{1}{\left[P_a^k(Q) + \bar{m}_a^2\right]^2}.$$
 (24)

The flow of the kinetic term $P_a(Q)$ is discussed in the Appendix.

The flow equation for the Yukawa coupling consists of a direct contribution $\beta_{\overline{h}_a}^{\underline{d}}$ and a contribution $\beta_{\overline{h}_a}^{\mathrm{rb}}$ which comes from rebosonization of regenerated fermionic couplings,³⁴

$$\partial_k \bar{h}_a = \beta^d_{\bar{h}_a} + \beta^{\rm rb}_{\bar{h}_a}.$$
 (25)

The first contribution reads

$$\beta_{\bar{h}_{a}}^{d} = -\bar{h}_{a}^{3} \sum_{Q} \tilde{\partial}_{k} \frac{1}{P_{F}^{k}(Q) P_{F}^{k}(Q+\Pi) [P_{a}^{k}(Q) + \bar{m}_{a}^{2}]}.$$
 (26)

The second contribution is discussed in Sec. IV together with the flow equation for \bar{h}_d . For the mass parameter \bar{m}_d^2 for the *d* boson we find

$$\partial_k \bar{m}_d^2 = -\bar{h}_d^2 \sum_Q \tilde{\partial}_k \frac{f_d^2(2\mathbf{q})}{P_F^k(-Q)P_F^k(Q)}.$$
(27)

IV. GENERATION OF *d*-WAVE COUPLING

In this section we discuss how a coupling in the *d*-wave channel is generated by the exchange of antiferromagnetic bosons. This mechanism was suggested, e.g., in Refs. 5 and 23. At the microscopic scale Λ we have a local repulsive four-fermion interaction described in our picture by the exchange of **a** bosons. No other channel is present. However, even in the case of purely repulsive forces between the electrons, the system may become unstable against Cooper-pair formation.⁴⁷ On lower momentum scales we indeed observe a generation of an attractive coupling in a Cooper-pair chan-



FIG. 3. One-loop corrections (box diagrams) to the four-fermion interaction. Solid lines represent fermions and wiggly lines represent \mathbf{a} bosons.

nel which turns out to have a *d*-wave symmetry. This may become critical in an appropriate parameter region.

We show in Fig. 3 the box diagrams exchanging **a** bosons. They generate an effective momentum-dependent four-fermion vertex $\Gamma_F^{(4)}$,

$$\Gamma_{4} = \frac{1}{4} \sum_{Q_{1},\dots,Q_{4}} \Gamma_{F,\alpha\beta\gamma\delta}^{(4)}(Q_{1},Q_{2},Q_{3},Q_{4}) \,\delta(Q_{1}-Q_{2}+Q_{3}-Q_{4}) \\ \times \psi_{\alpha}^{*}(Q_{1})\psi_{\beta}(Q_{2})\psi_{\gamma}^{*}(Q_{3})\psi_{\delta}(Q_{4}).$$
(28)

This irreducible vertex has to be added to the effective interaction arising from the exchange of bosons if we account for the total effective action between the electrons. It receives further contributions beyond the box diagrams since it has to include all contributions to the total four-fermion vertex which are not accounted for by the antiferromagnetic boson exchange in a given truncation. In particular, the fluctuations of the antiferromagnetic bosons induce a momentumdependent piece in the effective Yukawa coupling between the electrons and the a bosons. This momentum-dependent part is not reproduced by our truncation where a constant \bar{h}_a is evaluated for a particular choice of external momenta. We have therefore added this piece to Γ_4 . Our computation of the sum of Γ_4 and the antiferromagnetic boson exchange agrees with a purely fermionic computation in one-loop order, such that the results are identical as long as U/t remains small.

The *d*-wave channel interaction is part of $\Gamma^{(4)}(Q_i)$. Since the coupling $\Gamma^{(4)}(Q_i)$ contains contributions from various channels we will next project onto its contributions from the *d*-wave and the antiferromagnetic channels. For spin rotation invariant systems the spin structure of the four-fermion interaction has the general form

$$\Gamma_{F,\alpha\beta\gamma\delta}^{(4)}(Q_1,Q_2,Q_3,Q_4) = \Gamma_{F,s}^{(4)}(Q_1,Q_2,Q_3,Q_4)S_{\alpha\gamma;\beta\delta} + \Gamma_{F,t}^{(4)}(Q_1,Q_2,Q_3,Q_4)T_{\alpha\gamma;\beta\delta},$$
(29)

where $S_{\alpha\gamma,\beta\delta} = \delta_{\alpha\beta}\delta_{\gamma\delta} - \delta_{\gamma\beta}\delta_{\alpha\delta}$ and $T_{\alpha\gamma,\beta\delta} = \delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\gamma\beta}\delta_{\alpha\delta}$ project onto spin singlet and spin triplet states in the fermion pair channels, respectively. Here, we are interested in spin singlet states and we choose $Q_1 = -Q_3 \equiv L = (\pi T, \mathbf{l})$ and $Q_2 = -Q_4 \equiv L' = (\pi T, \mathbf{l}')$. For the projection onto the *d*-wave Cooper-pair channel we use the fact that the *d*-wave coupling changes its sign under rotation of 90°. We therefore define a momentum-dependent *d*-wave channel coupling $\lambda_f^d(\mathbf{l}, \mathbf{l}')$ by



FIG. 4. (Color online) Momentum dependence of *d*-wave coupling. In (a) and (c) we show the normalized momentum dependence of the rhs of the flow equation for the fermionic coupling, $\frac{1}{4}[\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')/\partial_k \lambda_F^d]$. In (b) and (d) we display the residual coupling after the subtraction of the bosonized part, $\frac{1}{4}[\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')/\partial_k \lambda_F^d] - f_d(2\mathbf{l})f_d(2\mathbf{l}')]$ [cf. Eq. (31)]. We use t'=0 in all plots. Notice that these plots are independent of U.

$$\lambda_{F}^{d}(\mathbf{l},\mathbf{l}') = -\frac{1}{2} \{ \Gamma_{F,s}^{(4)}(L,L',-L,-L') - \Gamma_{F,s}^{(4)}[R(L),L',-R(L),-L'] \},$$
(30)

where R(L) denotes a rotation of the spatial components **l** of L by 90°. For definition (30) we have kept L' fixed and subtracted the same contribution after a rotation of 90° of the spacelike components of L. For instance, the antiferromagnetic channel and the *s*-wave channel are subtracted in this way.

We compute $\partial_k \Gamma_F^{(4)}$ and $\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')$ by taking the fourth functional derivative of Eq. (2) with respect to the fermion fields. Within our truncation this corresponds to the box diagrams in Fig. 3. We find that $\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')$ is well approximated by the flow of a simple *d*-wave channel coupling λ_F^d of the form

$$\lambda_F^d(\mathbf{l},\mathbf{l}') = f_d(2\mathbf{l})f_d(2\mathbf{l}')\lambda_F^d. \tag{31}$$

In Figs. 4(a) and 4(c) we show the flow of the left-hand side of Eq. (31) as a function of I for I' = $(0, \pi)$ (for $k = \Lambda$ and with appropriate overall normalization). There is a good qualitative agreement with the *d*-wave form factor displayed in Fig. 1. We determine the flow of λ_F^d by choosing $I = (\pi, 0)$, I' = $(0, \pi)$, i.e., $\partial_k \lambda_F^d = \partial_k \lambda_F^d [(\pi, 0), (0, \pi)]$.

Next, we show how this fermionic quartic coupling can be bosonized on all scales k. This means that we trade the fourfermion coupling λ_F^d in favor of a Yukawa coupling of the d bosons. After this transformation, the d-boson exchange induces the effective interaction in the d-wave-pairing channel. We achieve this reformulation by a variable transformation in the functional flow equation (2). The flow equation (2) describes the scale dependence of Γ_k at fixed fields χ . We will now switch to other *k*-dependent variables χ_k and derive modified flow equations that describe the *k* dependence of Γ_k at fixed χ_k . For a suitable choice of χ_k this will realize the desired bosonization.^{34,35}

More precisely, we choose scale-dependent bosonic fields $\mathbf{B}_k = \mathbf{B}_k[\psi, \psi^*, \mathbf{B}; \mathbf{k}] = (\mathbf{a}_k, d_k, d_k^*)$ and perform the variable transformation in the exact flow equation,

$$\frac{d}{dk}\Gamma_{k}[\psi,\psi^{*},\mathbf{B}_{k}]|_{\mathbf{B}_{k}}$$

$$=\partial_{k}\Gamma_{k}[\psi,\psi^{*},\mathbf{B}]|_{\mathbf{B}=\mathbf{B}_{k}}+\sum_{Q}\left(\frac{\delta}{\delta\mathbf{a}_{k}(Q)}\Gamma_{k}[\psi,\psi^{*},\mathbf{B}_{k}]\right)\partial_{k}\mathbf{a}_{k}(Q)$$

$$+\sum_{Q}\left(\frac{\delta}{\delta d_{k}(Q)}\Gamma_{k}[\psi,\psi^{*},\mathbf{B}_{k}]\right)\partial_{k}d_{k}(Q)$$

$$+\sum_{Q}\left(\frac{\delta}{\delta d_{k}^{*}(Q)}\Gamma_{k}[\psi,\psi^{*},\mathbf{B}_{k}]\right)\partial_{k}d_{k}^{*}(Q).$$
(32)

This equation is our starting point for the construction of the "perfect bosons"³⁴ on all scales. The first term on the rhs is given by Eq. (2).

The scale-dependent boson fields are defined by adding suitable fermion bilinears,

$$\mathbf{a}_{k}(Q) = \mathbf{a}_{\Lambda}(Q) - \alpha_{k}^{a} \widetilde{\mathbf{a}}(Q),$$
$$d_{k}(Q) = d_{\Lambda}(Q) - \alpha_{k}^{d} \widetilde{d}(Q).$$
(33)

Here the fermion bilinears

$$\widetilde{\mathbf{a}}(Q) = \sum_{P} \psi^{\dagger}(P) \,\boldsymbol{\sigma} \psi(P - \Pi + Q),$$
$$\widetilde{d}(Q) = \frac{1}{2} \sum_{P} f_d(2\mathbf{p} - \mathbf{q}) \psi^T(P) \,\boldsymbol{\epsilon} \psi(Q - P), \qquad (34)$$

correspond to the Fourier transforms of Eqs. (3) and (14). In Eq. (33), we denote by \mathbf{a}_{Λ} and d_{Λ} the original microscopic fields appearing in the microscopic action Γ_{Λ} . These are the *k*-independent fields that are kept fixed in Eq. (2) or in the first term on the rhs of Eq. (32). The fermion fields are kept scale independent and we infer

$$\partial_k \mathbf{a}_k(Q) = -\partial_k \alpha_k^a \widetilde{\mathbf{a}}(Q), \quad \partial_k d_k^{(*)}(Q) = -\partial_k \alpha_k^d \widetilde{d}^{(*)}(Q).$$
(35)

The variable transformation in Eq. (32) induces other Yukawa and four-fermion couplings, given in our truncation by

$$\frac{d}{dk}\Gamma_{k}|_{\mathbf{B}_{k}} = \partial_{k}\Gamma_{k}|_{\mathbf{B}=\mathbf{B}_{k}} - \sum_{Q} (\partial_{k}\alpha_{k}^{a})[P_{a}(Q) + \bar{m}_{a}^{2}]\mathbf{a}_{k}(-Q) \cdot \tilde{\mathbf{a}}(Q)
- \sum_{Q} (\partial_{k}\alpha_{k}^{d})\bar{m}_{d}^{2}\{d_{k}^{*}(Q)\tilde{d}(Q) + d_{k}(Q)\tilde{d}^{*}(Q)\}
+ \sum_{Q} (\partial_{k}\alpha_{k}^{a})\bar{h}_{a}\tilde{\mathbf{a}}(Q) \cdot \tilde{\mathbf{a}}(-Q)
+ 2\sum_{Q} (\partial_{k}\alpha_{k}^{d})\bar{h}_{d}\tilde{d}^{*}(Q)\tilde{d}(Q).$$
(36)

Here the couplings \bar{h}_a , \bar{h}_d , etc. correspond to suitable functional derivatives of Γ_k at fixed **B**_k.

For a suitable choice of α_k^d , we can use the four-fermion interaction in the *d*-wave-pairing channel generated by the variable transformation in order to cancel a corresponding piece $\partial_k \lambda_F^d$ generated by the diagrams of Fig. 3 in $\partial_k \Gamma_k |_{\mathbf{B}}$. More precisely, we fix $\partial_k \alpha_k^d$ by the requirement

$$0 = \partial_k \lambda_F^d + 2\bar{h}_d \partial_k \alpha_k^d, \tag{37}$$

where the first term is computed from Eqs. (2) and (28)–(31). The coupling $\lambda_F^d|_{\mathbf{B}_k}(\mathbf{l},\mathbf{l}')$ is defined similar to Eq. (30). However, it is now given by the functional derivative of Γ_k at fixed \mathbf{B}_k . This means that its flow is obtained from the flow of $\lambda_F^d(\mathbf{l},\mathbf{l}')$ (at fixed **B**) by subtracting the "bosonized piece"

$$\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')|_{\mathbf{B}_k} = \partial_k \lambda_F^d(\mathbf{l},\mathbf{l}') - \partial_k \lambda_F^d f_d(2\mathbf{l}) f_d(2\mathbf{l}').$$
(38)

In particular, if we define $\lambda_F^d|_{\mathbf{B}_k}$ in analogy to Eq. (31), one has $\partial_k \lambda_F^d|_{\mathbf{B}_k} = 0$. We show $\partial_k \lambda_F^d(\mathbf{I},\mathbf{I}')|_{\mathbf{B}_k}$ in Figs. 4(b) and 4(d) (in a suitable normalization where $\partial_k \lambda_F^d$ is divided out). Comparison with Figs. 4(a) and 4(c) shows that the major part of $\partial_k \lambda_E^d(\mathbf{l}, \mathbf{l}')$ can indeed be absorbed by the bosonization. The "residual part" $\partial_k \lambda_F^d(\mathbf{l}, \mathbf{l}') |_{\mathbf{B}_k}$ contains higher harmonics—the dominant piece in Figs. 4(b) and 4(d) has a periodicity in momenta with period π instead of the leading piece with periodicity 2π in Figs. 4(a) and 4(c). In principle, this residual interaction can be partially absorbed by a more complex k-dependent field in Eq. (33). We will not do this here and simply neglect in our truncation the residual interaction in $\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')|_{\mathbf{B}_i}$. As can be seen by a comparison of Figs. 4(b) and 4(d), the accuracy of this approximation gets better for larger $|\mu/t|$. After the variable transformation, we can work with a vanishing four-fermion coupling in the d-wavepairing channel.

From Eq. (32) we can now infer the additional contributions to the flow of the Yukawa coupling \bar{h}_d . It accounts for the fact that after the variable change a leading contribution to the four-fermion interaction is mediated by the exchange of bosons and is no longer contained in λ_F . One obtains a modified flow equation for the Yukawa coupling for the *d* boson,

$$\partial_k \bar{h}_d = \partial_k \bar{h}_d |_{\mathbf{B}} + \bar{m}_d^2 \partial_k \alpha_k^d. \tag{39}$$

Thereby inserting $\partial_k \alpha_k^d$ from Eq. (37) yields



FIG. 5. Effective four-fermion interaction in the *d*-wave-pairing channel mediated by *d*-boson exchange.

$$\partial_k \bar{h}_d = \partial_k \bar{h}_d |_{\mathbf{B}} - \frac{\bar{m}_d^2 \partial_k \lambda_F^d}{2\bar{h}_d} \tag{40}$$

for the *d* boson. In our truncation one has $\partial_k \bar{h}_d |_{\mathbf{B}} = 0$. The numerical solution to this flow equation is shown in Fig. 2. We can reconstruct the effective four-fermion interaction in the *d*-wave-pairing channel by computing the tree diagram from the *d*-boson exchange (cf. Fig. 5),

$$\lambda_{F,\text{eff}}^{d}(Q_{1},Q_{2},Q_{3},Q_{4}) = -\frac{\bar{h}_{d}^{2}}{\bar{m}_{d}^{2}}f_{d}(\mathbf{q}_{1}-\mathbf{q}_{3})f_{d}(\mathbf{q}_{2}-\mathbf{q}_{4})\,\delta(Q_{1}-Q_{2}+Q_{3}-Q_{4}).$$
(41)

Similar as the *d* boson, the Yukawa coupling of the **a** boson receives an additional contribution due to the rebosonization of the four-fermion interaction in the antiferromagnetic channel,³⁶

$$\partial_k \bar{h}_a = \partial_k \bar{h}_a |_{\mathbf{B}} + \bar{m}_a^2 \partial_k \alpha_k^a. \tag{42}$$

We define the projection onto the four-fermion interaction in the antiferromagnetic channel by

$$\lambda_F^a = \frac{1}{8} \Gamma_{F,1221}^{(4)}(0,\Pi,0,-\Pi)$$
(43)

and determine $\partial_k \alpha_k^a$ by

$$0 = \partial_k \lambda_F^a + \bar{h}_a \partial_k \alpha_k^a. \tag{44}$$

This yields



FIG. 6. (Color online) Scale dependence of \bar{m}_a^2 , \bar{m}_a^2 , and A_a for temperature above $T_{\rm pc}$ (T/t=0.12, solid lines) and below $T_{\rm pc}$ (T/t=0.09, dashed lines). We use $\mu/t=-0.1$, t'=0, and U/t=3.



FIG. 7. (Color online) $\ln(-\lambda_F^d/t)$ for k=0 is plotted as a function of T/t for $T \ge T_{pc} = 0.1004t$, $\mu/t = -0.1$, and t' = 0.

$$\partial_k \bar{h}_a = \partial_k \bar{h}_a |_{\mathbf{B}} - \frac{\bar{m}_a^2}{\bar{h}_a} \partial_k \lambda_F^a = \beta_{\bar{h}_a}^d + \beta_{\bar{h}_a}^{\rm rb}$$
(45)

for the flow of the Yukawa coupling of the \mathbf{a} boson. The first contribution was given in Eq. (26). The second contribution comes from rebosonization and we find, in agreement with Ref. 36,

$$\beta_{\bar{h}_{a}}^{\text{rb}} = \bar{m}_{a}^{2} \sum_{Q} \bar{h}_{a}^{3} \tilde{\partial}_{k} \frac{1}{\left[P_{a}^{k}(Q) + \bar{m}_{a}^{2}\right] \left[P_{a}^{k}(\Pi - Q) + \bar{m}_{a}^{2}\right]} \\ \times \frac{1}{P_{F}^{k}(-Q)} \left\{\frac{1}{P_{F}^{k}(\Pi - Q)} - \frac{1}{P_{F}^{k}(Q)}\right\}.$$
(46)

We have solved the flow equations for the couplings \bar{h}_a , \bar{h}_d , \bar{m}_a^2 , \bar{m}_d^2 , A_a , and D numerically. In Fig. 6 we show the k dependence of \bar{m}_a^2 , \bar{m}_d^2 , and A_a . For $T > T_{\rm pc}$ both \bar{m}_a^2 and \bar{m}_d^2 remain positive for all k. We show the temperature dependence of the effective four-fermion couplings in the d wave and the antiferromagnetic channel, λ_F^d and λ_F^a , in Figs. 7 and 8. Both couplings are evaluated for k=0.

V. PSEUDOCRITICAL TEMPERATURE

For $T \rightarrow T_{pc}$ the mass term \overline{m}_a^2 reaches zero at a nonzero value of k, and therefore λ_F^a diverges. This feature extends to all $T \leq T_{pc}$ and signals the onset of local antiferromagnetic order in domains of linear size k^{-1} . For smaller k, the flow has to be continued in the "spontaneously broken regime,"^{36,37} where the minimum of the effective potential occurs for nonzero **a**. In the present paper we do not continue the flow beyond the scale where \overline{m}_a^2 vanishes but rather stop



FIG. 8. (Color online) $\ln(-\lambda_F^a/t)$ for k=0 is plotted as a function of T/t for $T \ge T_{pc} = 0.1004t$, $\mu/t = -0.1$, and t' = 0.



FIG. 9. (Color online) Pseudocritical temperature $T_{\rm pc}/t$ as a function of μ/t for U/t=3 and t'=0 (solid line) and t'=-0.05t (dashed line).

once \overline{m}_a^2 reaches zero. The corresponding pseudocritical temperature T_{pc} is shown in Fig. 9 as a function of the chemical potential. We also show the dependence of T_{pc} on the Hubbard coupling U in Fig. 10. For U/t=3 and $\mu=t'=0$ we find for T_{pc} a value that is about 30% smaller than in Ref. 36. This is due to the different ansatz for the propagator of the **a** boson and may be taken as an indication for the size of the error. In the present work we restrict ourselves to Hubbard couplings $U/t \le 3$ and to temperature $T/t \ge 0.02$. In order to extend the lines in Fig. 10 to smaller T one has to improve our simple truncation of the frequency dependence of the propagator of the **a** boson. This issue will be addressed in a forthcoming work.

Another interesting quantity is the relative strength of the effective four-fermion interaction in the d-wave pairing and the antiferromagnetic channel. We plot the ratio

$$R = \frac{\lambda_F^d}{\lambda_F^a} = \frac{2\bar{h}_d^2 \bar{m}_a^2}{\bar{h}_a^2 \bar{m}_d^2} \tag{47}$$

in Fig. 11 for different values of μ . In these plots the ratio *R* first increases due to the generation of a nonvanishing \overline{h}_d and subsequently decreases since \overline{m}_a^2 approaches zero or small values. We see the tendency that the maximum of *R* increases with increasing μ .

Our present truncation does not remain valid for low k if $|\mu/t|$ becomes large. The reason is that A_a or $\overline{\lambda}_a$ reach zero



FIG. 10. (Color online) Pseudocritical temperature T_{pc}/t as a function of U/t for $\mu=0$, t'=0 (solid line), and $\mu/t=-0.12$ and t'/t=-0.05 (dashed line).



FIG. 11. (Color online) Relative strength of *d*-wave and antiferromagnetic coupling. The ratio *R*, defined in Eq. (47) is plotted for four parameter choices: (1) T/t=0.1235, $\mu=0$ (2) T/t=0.115, μ/t = -0.09 (3) T/t=0.08, $\mu/t=-0.15$, and (4) T/t=0.05, $\mu/t=-0.3$. We use U/t=3, t'=0.

before either \overline{m}_a^2 or \overline{m}_d^2 vanishes. This means that our approximation for the momentum dependence in $P_a(Q)$, or for the polynomial approximation for U_a , becomes insufficient. An extended truncation can cure these problems, which will be addressed in a future publication. In our figures the breakdown of the approximations can be seen by the end of the curves in Figs. 9 and 11. The insufficiency of the truncation is the reason why we cannot access the values of $|\mu|$ and k where R becomes large in the present paper.

VI. CONCLUSIONS

We have shown how the renormalization flow turns the microscopic Hubbard model into an effective boson exchange model at intermediate length scales k^{-1} . This "mesoscopic" model is characterized by the exchange of collective electron or electron-hole pairs, which are described by bosonic fields. The most important channels are the exchange of electron-hole pairs of the antiferromagnetic type (the **a** boson) and *d*-wave electron pairs (the *d* boson). The coupling of these bosons to the electrons is described by Yukawa-type couplings \bar{h}_a and \bar{h}_d , which multiply the form factors appropriate for the respective channels. The effective model is characterized by the effective action, cf. Eqs. (7), (15), and (16), $\Gamma = \Gamma_F + \Gamma_a + \Gamma_{Fa} + \Gamma_{Fd} - \Gamma_{Fd}$. Besides the Yukawa couplings, important ingredients are the propagator and the effective potential for the **a** bosons and the *d* bosons.

The effective boson exchange model has several coupling constants, as \bar{h}_a , \bar{n}_d , \bar{m}_a^2 , \bar{m}_d^2 , as well as bosonic self-interactions, and couplings parametrizing the bosonic propagators (cf. Appendix). These couplings depend on the momentum scale k at which the effective model is considered. We may consider the effective boson exchange model as a coarse-grained version of the microscopic Hubbard model with coarse graining length k^{-1} . Its couplings can therefore be related to the couplings t, t', and U of the Hubbard model, and we have done so by the use of the functional renormalization flow. This flow shows how an effective coupling in the d-wave-pairing channel is generated by the fluctuations of the **a** bosons.

One may also consider the effective boson exchange model with arbitrary parameters. This can then be interpreted

as a generalization of the Hubbard model. The particular case $\bar{h}_a=0$, where the **a** bosons play no role, has already been discussed with the help of functional flow equations in Ref. 38. For low temperatures one finds superfluidity. The investigation of Ref. 38 has covered the critical behavior at the phase transition and the low-temperature "ordered phase." The phase transition was found to be in the universality class of the Kosterlitz-Thouless phase transition. Reinterpreted in the context of our investigation of the Hubbard model, the model³⁸ becomes a valid approximation if at some scale k the antiferromagnetic channel coupling $\lambda_F^a = -\bar{h}_a^2/2\bar{m}_a^2$ becomes much smaller than the *d*-wave coupling $\lambda_F^d = -\bar{h}_d^2/\bar{m}_d^2$. The corresponding large values of R are reached, however, only in a region for μ/t where our present approximation for the propagator of the antiferromagnetic bosons becomes insufficient.

As we have mentioned in Sec. V, our present investigation is limited to the range of k where the propagator for the **a** boson is well described by the approximation discussed in the Appendix. In particular, this requires $A_a \ge 0$. We implicitly assume that commensurate antiferromagnetic fluctuations are dominant as compared to the incommensurate antiferromagnetism or ferromagnetism. The latter plays an important role in other parameter ranges of this model.^{27,48–51} Within the present truncation the positivity of A_a is not realized for all μ , t, t', U, and T if k becomes small. Also the simple dependence of P_a on the Matsubara frequency does not remain appropriate for $T \rightarrow 0$. We will discuss a more general form of P_a , as well as a momentum-dependent propagator for the d boson, in a forthcoming work. We are confident that a suitable truncation of the functional renormalization-group equations will give access to the whole phase diagram of the Hubbard model.

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APPENDIX: BOSONIC PROPAGATOR

In order to gain some first information on the general shape of the momentum-dependent piece in the inverse propagator for the antiferromagnetic boson, we compute the contribution from the fermionic loop

$$\Delta G_a^{-1}(Q) = \sum_{P} \frac{\bar{h}_a^2}{P_F(Q + P + \Pi)P_F(P)} + (Q \to -Q).$$
(A1)

The general features of this one-loop contribution will be used in order to motivate a suitable truncation. Performing the Matsubara sum one finds



FIG. 12. (Color online) Mean-field calculation of the frequency dependence of the bosonic propagator at zero spatial momenta, $\bar{m}_{a}^{2}|_{\Lambda} + \Delta G_{a}^{-1}(2\pi mT, \mathbf{q}=0)$ for U/t=3, T/t=0.25, t'=0, and $\mu=0$.

$$\Delta G_a^{-1}(\omega, \mathbf{q}) = -\frac{\overline{h}_a^2}{2} \int_{-\pi}^{\pi} \frac{d^2 p}{(2\pi)^2} \frac{\tanh\left(\frac{\xi_{\mathbf{p}}}{2T}\right) - \tanh\left(\frac{\xi_{\mathbf{q}+\mathbf{p}+\pi}}{2T} + \frac{i\omega}{2T}\right)}{\xi_{\mathbf{p}} - \xi_{\mathbf{q}+\mathbf{p}+\pi} - i\omega} + (Q \to -Q).$$
(A2)

In Fig. 12 we plot the frequency dependence at vanishing spatial momenta while the dependence on spatial momenta at vanishing frequency is plotted in Fig. 13(a).

We approximate the inverse bosonic propagator at zero frequency by

$$P_{a,k}(0,\mathbf{q}) = \Delta G_{a,k}^{-1}(Q) + \bar{m}_a^2|_{\Lambda} - \bar{m}_a^2|_k = A_a \frac{[\mathbf{q}]^2 D^2}{D^2 + [\mathbf{q}]^2},$$
(A3)

where $[\mathbf{q}]^2$ is defined as $[\mathbf{q}]^2 = q_1^2 + q_2^2$ for $q_i \in [-\pi, \pi]$ and continued periodically otherwise. It is convenient to define the gradient coefficient A_q and the shape coefficient D by

$$A_{a} = \frac{1}{2} \frac{\partial^{2}}{\partial l^{2}} P_{a}(0, l, 0) \big|_{l=0}$$
(A4)

and

$$D^{2} = \frac{1}{A_{a}} [P_{a}(0,\pi,\pi) - P_{a}(0,0,0)].$$
(A5)

Comparison between Figs. 13(a) and 13(b) shows that this choice reproduces the mean-field result rather well. [Note that $P_a(0, \pi, \pi)$ computed from Eqs. (A3)–(A5) deviates slightly from the mean-field result for this momentum choice.] The lowest-order perturbative contribution from the fermions reads



FIG. 13. (Color online) The mean-field approximation for the spatial momentum dependence of the bosonic propagator at zero frequency $\bar{m}_a^2|_{\Lambda} + \Delta G_a^{-1}(0, \mathbf{q})$ is shown in (a). We use U/t=3, $\mu=0$, t'=0, and T/t=0.25. In (b) the parametrization in terms of Eq. (A3) is displayed for a renormalization scale k=0.

$$A_a = \sum_Q \bar{h}_a^2 \frac{\partial^2}{\partial l^2} \left. \frac{1}{P_F^k(Q) P_F^k(K + Q + \Pi)} \right|_{l=0}.$$
 (A6)

For frequencies different from zero we set for all **q**,

$$P_a(\omega \neq 0, \mathbf{q}) = \bar{m}_a^2 |_{\Lambda} - \bar{m}_a^2 |_k.$$
(A7)

In practice, this means that we include the fluctuation effects only for the zero Matsubara frequency mode. In the temperature range of interest in this work, this is a well-justified approximation, cf. Fig. 12. On the other hand, truncation (A7) is not suited for very low T and therefore limits the temperature range for our investigation in the present paper.

Within the functional renormalization-group approach, we describe the scale dependence of the inverse bosonic propagator by flow equations for the parameters A_a and D. The flow equation for the gradient coefficient is

$$\partial_k A_a = \sum_Q \left. \overline{h_a^2} \overline{\partial}_k \frac{\partial^2}{\partial l^2} \left. \frac{1}{P_F^k(Q) P_F^k(K + Q + \Pi)} \right|_{l=0}, \quad (A8)$$

where K = (0, l, 0). At the initial scale the gradient coefficient vanishes $A_a|_{\Lambda} = 0$. The boson is not dynamic on this scale and can be regarded as an auxiliary field. The difference $P_a(0, \pi, \pi) - P_a(0, 0, 0)$ in Eq. (A5) is also scale dependent. From this, and Eqs. (A5) and (A8), one infers the flow equation for *D*. Again, *D* vanishes at the initial scale Λ . The result of approximation (A3), as calculated from the flow equation, is displayed in Fig. 13(b). Comparison with the one-loop result in Fig. 13(a) shows satisfactory agreement.

The infrared cutoff R_k^a for the **a** boson is adapted to Eq. (A3). We use an "optimized cutoff,"^{35,52,53}

$$R_{k}^{a}(Q) = A_{a} \left(k^{2} - \frac{[\mathbf{q}]^{2} D^{2}}{D^{2} + [\mathbf{q}]^{2}} \right) \Theta \left(k^{2} - \frac{[\mathbf{q}]^{2} D^{2}}{D^{2} + [\mathbf{q}]^{2}} \right).$$
(A9)

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