Flow equations and the strong-coupling expansion for the Hubbard model

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Abstract

Applying the method of continuous unitary transformations to a class of Hubbard models, the derivation of the t/U-expansion for the strong-coupling case is re-examined. The flow equations for the coupling parameters of the higher-order effective interactions can be solved exactly, resulting in a systematic expansion of the Hamiltonian in powers of t/U, valid for any lattice in arbitrary dimension and for general band-filling. The expansion ensures a correct treatment of the operator products generated by the transformation, and only involves the explicit recursive calculation of numerical coefficients. This scheme provides a unifying framework to study the strong-coupling expansion for the Hubbard model, which clarifies and circumvents several difficulties inherent to earlier approaches. Our results are compared with those of other methods, and it is shown that the freedom in the choice of the unitary transformation that eliminates interactions between different Hubbard bands can affect the effective Hamiltonian only at order t^3/U^2 or higher.

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1 Introduction

The Hubbard model with both repulsive [1] and attractive [2] interaction of local electron pairs has been extensively studied in the context of a variety of physical problems, *e.g.* in the theoretical description of magnetic ordering, the metal-insulator transition, bipolaronic systems, and the high-temperature superconductors. In general, the Hubbard model is the simplest model which combines strong correlations with itinerant behavior. The expansion of the Hubbard Hamiltonian around the limit of strong coupling, *i.e.* in powers of t/U, has a long history, since this limit provides several simplifications which make the model more tractable.

Applying different variants of degenerate perturbation theory, a number of results up to several orders of t/U have been obtained. These include the derivation of the effective spin Hamiltonian [3] in second order, while higher-order calculations, based on the perturbation theory of Kato [4], des Cloizeaux [5], and Primas [6], have been performed only for special cases. Klein and Seitz [7] obtained the sixth-order spin interaction for the linear Hubbard chain, while Bulaevskii [8] and Takahashi [9] derived the fourth-order term for the Hubbard model with half-filled band in more than one dimension. More recently, these perturbative methods have also been applied to Hubbard models with more general interactions [10].

Another approach to study the effective Hamiltonian is based on unitary transformations [11]. Harris and Lange [12] and also Kapustin [13] used such a transformation to derive second-order results and to calculate spectral properties of the Hubbard model. A number of authors [14] subsequently applied unitary transformations in low orders to study several systems described by Hubbard models. A transformation which methodically includes also higher orders in t/U has been proposed by Chao, Spałek, and Oleś [15]. In their expansion, closed expressions for the effective interaction are obtained in any order. However, beyond second order, their results are an uncontrolled approximation, since the transformation of the Hamiltonian involves an approximation for the band energies, and in higher orders does not eliminate interaction terms which mix different Hubbard bands [16]. A systematic transformation scheme to remove unphysical terms, and to derive the t/U-expansion, has been formulated by MacDonald, Girvin, and Yoshioka [17]. In their approach, interaction terms which do not conserve the number of local electron pairs are removed from the Hamiltonian order by order in an iterative treatment, generating new interactions and thus improving the accuracy of the transformation in each step.

In the present work we utilize Wegner's method [18] of continuous unitary transformations to re-examine the derivation of a systematic and exact expansion of the Hubbard Hamiltonian in powers of t/U for the strong-coupling case. The goal of such a transformation is to obtain a classification of all possible interaction terms in t/U, with the strong-coupling constraint that terms which connect different Hubbard bands are eliminated. This corresponds to a block-diagonalization of the Hubbard Hamiltonian. Such a continuous transformation generates all higher interactions at once. The flow equations for the couplings of these effective interactions can be solved exactly, and explicit solutions will be given up to fifth order. We also derive sum rules for the coupling functions, which may serve as a useful check of the calculations. For higher orders, recursion relations for the coefficients of the exact solutions are obtained and closed general expressions for the coupling coefficients are derived for special cases. Therefore, the derivation of a systematic strong-coupling expansion is reduced to a recursive calculation of numerical coefficients, whereas operator properties need not be considered any more. This method thus provides a simplified expansion scheme for the Hubbard model. It also sheds new light on the systematic relation between previous approaches and allows to clarify some of the deficiencies of their results. In particular, the continuous transformation which leads to the results of Chao, Spałek, and Oleś is obtained, and the interaction terms which are neglected in their approximation are identified. Additionally, a systematic improvement of this approximation is proposed, which results in a consistent expansion eliminating linear interaction terms from the original Hubbard model. It is also found that the effective interactions which correspond to the exact solutions of the flow equations are in agreement with the Hamiltonian derived by the transformation scheme of MacDonald, Girvin, and Yoshioka to third order in t/U, while in higher orders certain differences occur. These differences in the coupling coefficients appear to be a consequence of the continuous nature of our transformation and reflect the remaining freedom in the choice of the unitary transformation which eliminates interactions between different Hubbard bands. Finally, it is shown that in general the effective Hamiltonian derived from the Hubbard model is sensitive for such a choice of the transformation only at order t^3/U^2 or higher.

2 Flow equations and solutions

We consider the Hubbard model on a general lattice Λ and in arbitrary spatial dimension,

$$H = tT + UV = \sum_{\mathbf{r}\mathbf{r}'\sigma} t_{\mathbf{r}\mathbf{r}'}\, c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \tag{1}$$

where $c^\dagger_{\mathbf{r}\sigma}$ creates an electron with spin σ at site $\mathbf{r}$, and $t_{\mathbf{r}\mathbf{r}'} = tD_{\mathbf{r}\mathbf{r}'}$, with the hopping matrix $D_{\mathbf{r}\mathbf{r}'} = D^*_{\mathbf{r}'\mathbf{r}}$ which may connect any two of the N sites on the lattice. The local pairing energy U may be taken positive or negative, although we are mainly interested in the strong-coupling regime which requires $|t/U| \ll 1$. The fermionic Hilbert space of the model, $\mathcal{H} = \oplus_{k=0}^N \mathcal{H}_k$, can be decomposed into the subspaces $\mathcal{H}_k$ which are related to the total number k of local electron pairs in the system. The projectors P_k on these subspaces are defined via the generating function

$$\sum_{k=0}^{N} P_k\, x^k = \prod_{\mathbf{r}\in\Lambda} \left(1 - (1-x) n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}\right). \tag{2}$$

The terms appearing in the kinetic energy T can also be classified according to the change of the number of electron pairs which they involve, $T_m = \sum_{k=0}^N P_{k+m} T P_k$, with $m = 0, \pm 1$. Expressed by the electron operators, they are explicitly given by

$$\begin{aligned}
T_0 &= \sum_{\mathbf{r}\mathbf{r}'\sigma} D_{\mathbf{r}\mathbf{r}'} \left(n_{\mathbf{r}-\sigma} c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} n_{\mathbf{r}'-\sigma} + (1-n_{\mathbf{r}-\sigma}) c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} (1-n_{\mathbf{r}'-\sigma}) \right), \\
T_{+1} &= \sum_{\mathbf{r}\mathbf{r}'\sigma} D_{\mathbf{r}\mathbf{r}'}\, n_{\mathbf{r}-\sigma} c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} (1-n_{\mathbf{r}'-\sigma}), \\
T_{-1} &= \sum_{\mathbf{r}\mathbf{r}'\sigma} D_{\mathbf{r}\mathbf{r}'}\, (1-n_{\mathbf{r}-\sigma}) c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} n_{\mathbf{r}'-\sigma}.
\end{aligned} \tag{3}$$

One then has $T = T_0 + T_{+1} + T_{-1}$, and can easily verify that the relation $[V, T_m] = m\, T_m$ holds, reflecting the transition from the Hilbert space sector $\mathcal{H}_k$ to $\mathcal{H}_{k+m}$. To allow for variable band-filling, one may add a chemical potential to the Hamiltonian. This does not change the subsequent discussion, since the T_m conserve the number of particles. To discuss the higher-order interaction terms in which we are eventually interested, it is useful to introduce products of hopping operators, $T^{(k)}(\mathbf{m}) = T_{m_1} T_{m_2} \cdots T_{m_k}$, with the index vectors $\mathbf{m} = (m_1, m_2, \ldots, m_k)$. It is found that the commutator of such an operator product with V involves the total "weight" of the product, $M(\mathbf{m}) = \sum_{i=1}^{k} m_i$, and generally reads

$$[V, T^{(k)}(\mathbf{m})] = M(\mathbf{m}) T^{(k)}(\mathbf{m}). \tag{4}$$

In the strong-coupling case of the Hubbard model, when $|t| \ll |U|$, the energy spectrum splits into well-separated subbands with bandwidth $\sim t^2/|U|$ (or $\sim |t|$, depending on the sign of U and the band-filling), and a gap $\sim |U|$ opens up between them. To study physical properties of such a strong-coupling model at energy and temperature scales which are well below the Hubbard energy $|U|$, it is thus desirable to consider an effective Hamiltonian which does not mix different Hilbert space sectors $\mathcal{H}_k$, *i.e.* which conserves the total number of local electron pairs and is thus block-diagonal.

2.1 The effective interactions

In order to derive such an effective Hamiltonian, we apply a continuous unitary transformation which allows to remove interactions with nonvanishing overlap between different Hilbert space sectors. Of course, this transformation is valid for an arbitrary ratio t/U, although it is especially suitable for the strong-coupling case. The Hamiltonian then depends on a continuous flow parameter l,

$$H(l) = t\Theta(l) + UV, \tag{5}$$

where the generalized "kinetic" energy $\Theta(l)$ also contains all higher-order interactions which are generated by the transformation,

$$\Theta(l) = \sum_{k=1}^{\infty} \frac{t^{k-1}}{U^{k-1}} \sum_{\{\mathbf{m}\}} F^{(k)}(l; \mathbf{m})\, T^{(k)}(\mathbf{m}). \tag{6}$$

The flow equations will be given for the l-dependent coupling functions $F^{(k)}(l; \mathbf{m})$. As is shown below, a unitary transformation which eventually eliminates all terms from the Hamiltonian that do not conserve the number of local pairs, can be constructed with the (antihermitean) generator

$$\eta(l) = \frac{t}{U}[V, \Theta(l)] = \sum_{k=1}^{\infty} \frac{t^k}{U^k} \sum_{\{\mathbf{m}\}} M(\mathbf{m})\, F^{(k)}(l; \mathbf{m})\, T^{(k)}(\mathbf{m}). \tag{7}$$

The flow equations for the coupling functions then follow from the basic transformation of the Hamiltonian [18],

$$\frac{\mathrm{d}H(l)}{\mathrm{d}l} = [\eta(l), H(l)], \tag{8}$$

and the initial conditions determined by the original Hubbard Hamiltonian,

$$F^{(1)}(0;m) = 1 \qquad \text{and} \qquad F^{(k)}(0;\mathbf{m}) = 0 \quad \text{for} \quad k > 1. \tag{9}$$

At this point it may be worth noting that the accuracy of the effective Hamiltonian derived by our continuous transformation (7) only depends on the order of t/U at which one finally wishes to truncate the calculations. Since the flow equations for the coupling functions can be solved exactly, and our approach in contrast to others [*cf.* section 3] does neither involve approximations nor the neglect of any of the newly generated higher-order interactions, error terms can be systematically included, improving the accuracy of the transformed Hamiltonian to any desired order.

Before we obtain and solve the resulting set of coupled differential equations, it is useful to discuss some general symmetry properties of the Hamiltonian, which will result in identities between the coupling functions. Introducing a reversed index vector $\overline{\mathbf{m}} = (m_k, m_{k-1}, \ldots, m_1)$, one notes that $T_m^\dagger = T_{-m}$ and $(T^{(k)}(\mathbf{m}))^\dagger = T^{(k)}(-\overline{\mathbf{m}})$. With these relations, a first symmetry requirement for the coupling functions follows from the hermiteicity of the Hamiltonian (and from the antihermiteicity of the generator η). A second one is obtained from the observation that the global particle-hole transformation $c_{\mathbf{r}\sigma}^\dagger \to c_{\mathbf{r}\sigma}$ reverses the sign of the hopping energy, $t \to -t$, and also results in $T_m \to T_{-m}$. Since the $F^{(k)}$ are real-valued functions, as is seen below [*cf.* Eqs. (22-23)], these considerations lead to the symmetry relations

$$\begin{aligned} F^{(k)}(l;-\overline{\mathbf{m}}) &= F^{(k)}(l;\mathbf{m}) \\ F^{(k)}(l;-\mathbf{m}) &= (-1)^{k+1}\, F^{(k)}(l;\mathbf{m}). \end{aligned} \tag{10}$$

Unfortunately, no further information is obtained from the complete $SO(4)$ symmetry of the Hubbard model [19], since up to the particle-hole transformation each T_m is itself an invariant of this symmetry.

Inserting now our *ansatz* for the effective interaction (6) and for the generator (7) into the flow equation (8) yields

$$\frac{\mathrm{d}}{\mathrm{d}l}\Theta(l) = -[V,[V,\Theta(l)]] + \frac{t}{U}[[V,\Theta(l)],\Theta(l)], \tag{11}$$

resulting in a set of coupled nonlinear differential equations for the coupling functions,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}l}F^{(k)}(l;\mathbf{m}) &= -|M(\mathbf{m})|^2\, F^{(k)}(l;\mathbf{m}) + \\ &+ \sum_{n=1}^{k-1} \sum_{\substack{\{\mathbf{m}_1,\mathbf{m}_2\} \\ \mathbf{m}=(\mathbf{m}_1,\mathbf{m}_2)}} (M(\mathbf{m}_1) - M(\mathbf{m}_2))\; F^{(n)}(l;\mathbf{m}_1) F^{(k-n)}(l;\mathbf{m}_2), \end{aligned} \tag{12}$$

with the obvious condition $\mathbf{m} = (\mathbf{m}_1, \mathbf{m}_2)$ which reflects the generation of higher products $T^{(k)}$ by the transformation. From these equations (12) one can immediately deduce

$$F^{(k)}(l;\mathbf{m}) \equiv 0 \qquad \text{if} \quad |M(\mathbf{m})| > 1, \tag{13}$$

which reduces the number of possible interactions significantly. Thus, the unitary transformation resulting from (7) intermediately generates only such interaction terms which connect identical or adjacent Hubbard bands. A further simplification arises from the symmetry properties (10), which imply

$$F^{(k)}(l;\mathbf{m}) \equiv 0 \qquad \text{if} \quad k \text{ even} \quad \text{and} \quad \overline{\mathbf{m}} = \mathbf{m}. \tag{14}$$

It is also apparent from (12) that terms with $M(\mathbf{m}) \neq 0$ are exponentially damped and in the limit $l \to \infty$ vanish. Extracting such an exponential prefactor from the coupling functions, we may write

$$F^{(k)}(l;\mathbf{m}) = \exp\left(-|M(\mathbf{m})|^2\, l\right) \cdot f^{(k)}(l;\mathbf{m}). \tag{15}$$

Introducing the weight index $\lambda = M(\mathbf{m})$, with the possible values $\lambda = 0, \pm 1$, from Eqs. (12) we obtain the final form of the flow equations,

$$e^{2l} \frac{\mathrm{d}}{\mathrm{d}l} f_0^{(k)}(l;\mathbf{m}) = 2 \sum_{n=1}^{k-1} \sum_{\substack{\{\mathbf{m}_1,\mathbf{m}_2\} \\ \mathbf{m}=(\mathbf{m}_1,\mathbf{m}_2)}} \left(f_{+1}^{(n)}(l;\mathbf{m}_1)\, f_{-1}^{(k-n)}(l;\mathbf{m}_2) - f_{-1}^{(n)}(l;\mathbf{m}_1)\, f_{+1}^{(k-n)}(l;\mathbf{m}_2) \right) \tag{16}$$

for the "physical" interactions with $\lambda = 0$, and

$$\frac{\mathrm{d}}{\mathrm{d}l} f_\lambda^{(k)}(l;\mathbf{m}) = \lambda \sum_{n=1}^{k-1} \sum_{\substack{\{\mathbf{m}_1,\mathbf{m}_2\} \\ \mathbf{m}=(\mathbf{m}_1,\mathbf{m}_2)}} \left(f_\lambda^{(n)}(l;\mathbf{m}_1)\, f_0^{(k-n)}(l;\mathbf{m}_2) - f_0^{(n)}(l;\mathbf{m}_1)\, f_\lambda^{(k-n)}(l;\mathbf{m}_2) \right) \tag{17}$$

for the unphysical terms with $|\lambda| = 1$. Although in the process of the transformation flow these unphysical interactions in the $l \to \infty$ limit will finally be removed from the Hamiltonian, we nevertheless have to determine the corresponding coupling functions, since intermediately they are coupled to the physical ones. Having solved the flow equations (16) and (17), one finds the coupling coefficients for the physical interaction terms, $C^{(k)}(\mathbf{m}) = F_0^{(k)}(\infty;\mathbf{m})$. Explicit results for the coupling functions and coefficients are listed in tables I and II. The typical cases for the behaviour of the functions $F^{(k)}(l;\mathbf{m})$ are shown in figure 1.

2.2 Recursion relations

At a given order k, the maximal possible number $\mathcal{N}_\lambda(k)$ of interactions with $M(\mathbf{m}) = \lambda$ is obtained from the expression

$$\mathcal{N}_\lambda(k) = \sum_{n=1}^{\left[\frac{k+|\lambda|}{2}\right]} \binom{k}{n} \binom{k-n}{n-|\lambda|} \qquad \text{for} \quad k \geq 2. \tag{18}$$

Due to (14), not all of the corresponding coupling coefficients are nonzero, and as a consequence of the symmetry properties (10) many follow trivially from others. The number of nonvanishing interaction terms is further reduced by restrictions of the physical Hilbert space sector due to the band-filling. Depending on the sign of U, in the ground state the maximal or minimal possible number of local electron pairs is present in the system. Therefore, certain conditions apply for the number of pairs which intermediately can be destroyed or generated by the effective interactions. Denoting the number of particles in the system by N_e, one finds that for the nonvanishing interactions $T^{(k)}(\mathbf{m})$ *all* partial weights $M^{(n)}(\mathbf{m}) = \sum_{i=1}^{n} m_i$, with $1 \le n \le k$, must satisfy the inequalities

$$-\frac{1}{2}\min(N_\mathrm{e}, 2N - N_\mathrm{e}) \le \mathrm{sgn}(U)\, M^{(n)}(\mathbf{m}) \le 0. \tag{19}$$

At precisely half filling, $N_\mathrm{e} = N$, and if $U > 0$, or for $U < 0$ and arbitrary filling, if N_e is even, one has strictly $\mathrm{sgn}(U)\, M^{(n)}(\mathbf{m}) < 0$, if $n = 1$ or $M^{(n-1)}(\mathbf{m}) = 0$. These restrictions rule out many terms, however, $\mathcal{N}(k)$ rapidly increases with k, *e.g.*

$$\begin{array}{lllll} \mathcal{N}_0(1) = 1, & \mathcal{N}_0(2) = 2, & \mathcal{N}_0(3) = 6, & \mathcal{N}_0(4) = 18, & \mathcal{N}_0(5) = 50, \\ \mathcal{N}_0(6) = 140, & \mathcal{N}_0(7) = 392, & \mathcal{N}_0(8) = 1106, & \mathcal{N}_0(9) = 3138, & \mathcal{N}_0(10) = 8952, \end{array} \tag{20}$$

and

$$\begin{array}{lllll} \mathcal{N}_1(1) = 1, & \mathcal{N}_1(2) = 2, & \mathcal{N}_1(3) = 6, & \mathcal{N}_1(4) = 16, & \mathcal{N}_1(5) = 45, \\ \mathcal{N}_1(6) = 126, & \mathcal{N}_1(7) = 357, & \mathcal{N}_1(8) = 1016, & \mathcal{N}_1(9) = 2907, & \mathcal{N}_1(10) = 8350. \end{array} \tag{21}$$

Thus, at higher orders the solutions of the flow equations become increasingly complicated, but they are recursively related to the lower-order expressions.

To obtain the recursion relations for the higher-order terms, we note that the solutions of the differential equations (16-17) and the initial conditions (9) can be written in the form

$$f_\lambda^{(k)}(l; \mathbf{m}) = \sum_{\mu=0}^{\Gamma(\mathbf{m})} P_\mu^{(k)}(l; \mathbf{m})\, e^{-2\mu l}, \tag{22}$$

where $\Gamma(\mathbf{m}) = \frac{1}{2}(\sum_{i=1}^{k} |m_i| - |\lambda|)$, and the $P_\mu^{(k)}$ are polynomials in l, at most of degree k,

$$P_\mu^{(k)}(l; \mathbf{m}) = \sum_{\nu=0}^{k} a_{\mu,\nu}^{(k)}(\mathbf{m})\, l^\nu. \tag{23}$$

From (16-17) it then follows, that the coefficients $a_{\mu,\nu}^{(k)}$ obey the nonlinear recursion relations

$$\begin{aligned} a_{\mu,\nu}^{(k)}(\mathbf{m}) &= -\frac{1}{\nu!}\sum_{\kappa=0}^{k-\nu} \frac{(\nu+\kappa)!}{(2\mu)^{\kappa+1}} b_{\mu,\nu+\kappa}^{(k)}(\mathbf{m}) \qquad \text{for} \quad \mu \ge 1, \\ a_{0,\nu}^{(k)}(\mathbf{m}) &= 0 \qquad \text{for} \quad \nu \ge 1, \end{aligned} \tag{24}$$

with

$$\begin{aligned} b_{\mu,\nu}^{(k)}(\mathbf{m}) = \sum_{n=1}^{k-1} \sum_{\substack{\{\mathbf{m}_1,\mathbf{m}_2\} \\ \mathbf{m}=(\mathbf{m}_1,\mathbf{m}_2)}} \sum_{\mu'=0}^{\Gamma(\mathbf{m}_1)} \sum_{r=0}^{\nu} &(M(\mathbf{m}_1) - M(\mathbf{m}_2)) \times \\ &\times a_{\mu',r}^{(n)}(\mathbf{m}_1)\, a_{\mu-\mu'-1+|M(\mathbf{m})|,\nu-r}^{(k-n)}(\mathbf{m}_2). \end{aligned} \tag{25}$$

The physical coupling coefficients can be obtained from these solutions and the corresponding initial conditions,

$$C^{(k)}(\mathbf{m}) = a_{0,0}^{(k)}(\mathbf{m}) = -\sum_{\mu=1}^{\Gamma(\mathbf{m})} a_{\mu,0}^{(k)}(\mathbf{m}). \tag{26}$$

The recursion relations (24-25) are closed equations at any given finite order of t/U, *i.e.* they involve only coefficients of lower order. They provide the explicit conditions which determine the coupling coefficients for the effective interactions of the transformed Hubbard Hamiltonian, and thus define a simplified expansion scheme for the strong-coupling model which facilitates calculations at higher orders.

2.3 Sum rules

Prior to the solution of the flow equations for the coupling functions, from (16-17) a number of sum rules for the $f_\lambda^{(k)}(l;\mathbf{m})$ at a given order k may be derived, which facilitate the calculations and provide a useful check for the corresponding explicit results. Thus, for fixed k the coupling functions and consequently the coefficients $C^{(k)}(\mathbf{m})$ are not all independent from each other. Apart from results which are also obvious by inspection of tables I and II,

$$\begin{aligned} F^{(3)}(l;+1,0,-1) + 2F^{(3)}(l;+1,-1,0) &= 0, \\ F^{(3)}(l;0,+1,0) + 2F^{(3)}(l;+1,0,0) &= 0, \\ F^{(3)}(l;+1,-1,+1) + 2F^{(3)}(l;+1,+1,-1) &= 0, \\ F^{(4)}(l;+1,-1,+1,-1) + 2F^{(4)}(l;+1,+1,-1,-1) &= 0, \end{aligned} \tag{27}$$

the following sum rules can be obtained:

$$\begin{aligned} F^{(4)}(l;+1,0,-1,0) + F^{(4)}(l;0,+1,-1,0) + 2F^{(4)}(l;+1,-1,0,0) &= 0, \\ F^{(4)}(l;+1,-1,+1,0) + F^{(4)}(l;+1,-1,0,+1) + 2F^{(4)}(l;+1,+1,-1,0) &= 0, \end{aligned}$$

and

$$\begin{aligned} F^{(4)}(l;+1,+1,-1,0) + F^{(4)}(l;+1,+1,0,-1) + F^{(4)}(l;+1,0,+1,-1) + \\ +F^{(4)}(l;+1,-1,-1,0) = 0, \end{aligned} \tag{28}$$

for $k = 4$, and

$$\begin{aligned} F^{(5)}(l;+1,-1,+1,-1,0) + F^{(5)}(l;+1,-1,+1,0,-1) + 1/2\, F^{(5)}(l;+1,-1,0,+1,-1) &= 0, \\ F^{(5)}(l;+1,-1,-1,+1,0) + F^{(5)}(l;+1,-1,-1,0,+1) + 1/2\, F^{(5)}(l;+1,-1,0,-1,+1) &= 0, \\ F^{(5)}(l;+1,+1,-1,-1,0) + F^{(5)}(l;+1,+1,-1,0,-1) + 1/2\, F^{(5)}(l;+1,+1,0,-1,-1) &= 0, \end{aligned}$$

and

$$\begin{aligned} F^{(5)}(l;+1,0,0,-1,0) + F^{(5)}(l;+1,0,-1,0,0) + F^{(5)}(l;0,+1,0,-1,0) + \\ +2F^{(5)}(l;0,+1,-1,0,0) = 0, \end{aligned} \tag{29}$$

for $k = 5$. These results can easily be extended for higher orders, although here we restrict ourselves to list only the above relations.

2.4 Construction of general solutions

For special cases closed general expressions for the exact solutions of the flow equations and the corresponding physical coupling coefficients can be derived. For this purpose, let us first consider interaction terms $T^{(k)}(\mathbf{m}(j))$ with only a single nonzero entry of the index vector $\mathbf{m}$ at the j-th position, $\mathbf{m}(j) = (0,\dots,0,m,0,\dots,0)$, with $m = \pm 1$. For the coupling functions $f_m^{(k)}(l;\mathbf{m}(j))$ of these interactions one then finds

$$f_m^{(k)}(l;\mathbf{m}(j)) = \frac{d^{(k)}(j)}{(k-1)!} m^{k-1}\, l^{k-1} \qquad \text{with} \quad k \geq 1, \tag{30}$$

where the flow equation (17) implies the recursion relation

$$d^{(k)}(j) = d^{(k-1)}(j) - d^{(k-1)}(j-1) \quad \text{with} \qquad 1 \leq j \leq k, \tag{31}$$

and the initial condition $d^{(1)}(1) = 1$. This leads to the solution

$$f_m^{(k)}(l;\mathbf{m}(j)) = \frac{m^{k-1}(-1)^{j+1}}{(j-1)!(k-j)!}\, l^{k-1}. \tag{32}$$

With this result one now may evaluate the coupling functions for physical interactions with two nonzero entries of the index vector at positions j_1 and j_2, where $m_{j_1} = -m_{j_2} = m$, so that $\mathbf{m}(j_1,j_2) = (0,\dots,0,m,0,\dots,0,-m,0,\dots,0)$. From (16) one obtains the flow equation

$$\frac{\mathrm{d}}{\mathrm{d}l} f_0^{(k)}(l;\mathbf{m}(j_1,j_2)) = 2me^{-2l} \sum_{\nu=0}^{j_2-j_1-1} f_m^{(j_1+\nu)}(l;\mathbf{m}(j_1))\, f_{-m}^{(k-j_1-\nu)}(l;\mathbf{m}(j_2-j_1-\nu)). \tag{33}$$

Using the results (32) this equation can be solved explicitly, and the corresponding general coupling coefficient is readily derived

$$C^{(k)}(\mathbf{m}(j_1,j_2)) = m^{k+1}(-2)^{j_2-j_1-k+1}\binom{j_2-2}{j_1-1}\binom{k-2}{k-j_2} \quad \text{for} \quad 1 \leq j_1 < j_2 \leq k. \tag{34}$$

Proceeding now to unphysical interactions with $k \geq 3$ and three nonzero entries, we consider the special cases

$$\begin{aligned} \mathbf{m}_{++-} &= (m,m,0,\dots,0,-m), \\ \mathbf{m}_{+-+} &= (m,-m,0,\dots,0,m), \quad \text{and} \\ \mathbf{m}_{+--} &= (m,-m,0,\dots,0,-m). \end{aligned} \tag{35}$$

Applying the results of Eqs. (32-34), for such intermediary interaction terms one derives the following general expressions for the corresponding coupling functions:

$$m^{k+1} f_m^{(k)}(l;\mathbf{m}_{++-}) = l + 1 - k/2 + e^{-2l}\sum_{\nu=0}^{k-3}\frac{2^{\nu-1}(k-2-\nu)}{\nu!}\, l^{\nu}, \tag{36}$$

$$(-1)^k m^{k+1} f_m^{(k)}(l;\mathbf{m}_{+-+}) = l - k/2 + \sum_{\nu=0}^{k-2}\frac{l^{\nu}}{\nu! 2^{k-2-\nu}} + e^{-2l}\sum_{\nu=0}^{k-3}\frac{2^{\nu-1}(k-\nu-2^{\nu-k+3})}{\nu!}\, l^{\nu}, \tag{37}$$

and

$$2^{k-2}(-1)^k m^{k+1} f_{-m}^{(k)}(l;\mathbf{m}_{+--}) = -e^{-2l} + \sum_{\nu=0}^{k-2}\frac{(-2l)^{\nu}}{\nu!}. \tag{38}$$

These general results for the coupling functions encapsulate the explicit expressions listed in table II. They can be used to obtain the solutions for special coupling coefficients with $k \geq 4$ and four nonzero index components:

$$\begin{aligned} C^{(k)}(m,m,0,\ldots,0,-m,-m) &= \frac{m^{k+1}}{2^{k-3}}, \\ C^{(k)}(m,-m,0,\ldots,0,m,-m) &= \frac{(-m)^{k+1}(k-2)}{2^{k-3}}, \\ C^{(k)}(m,-m,0,\ldots,0,-m,m) &= \frac{m^{k+1}}{2^{k-2}}\left((-1)^k - 1\right). \end{aligned} \tag{39}$$

3 Comparison with other approaches

For higher orders of the t/U-expansion it is increasingly inconvenient to carry out the degenerate perturbation theory. Approaches going beyond the leading orders therefore generally utilize a unitary transformation of the original Hubbard Hamiltonian to derive the new effective interactions,

$$H' = e^S H e^{-S} = \sum_{n=0}^{\infty} \frac{1}{n!}\,[S,H]_n, \tag{40}$$

with the n-fold commutator $[S,H]_n = [S,[S,H]_{n-1}]$, and $[S,H]_0 = H$. Depending on the choice for S, different expansion schemes to obtain the higher-order terms have been proposed. While in the approach of Chao, Spałek, and Oleś [15] the transformation is chosen such that the resulting effective Hamiltonian conserves the number of local electron pairs only in *first order* of t/U, a systematic iterative method which eliminates the unphysical interactions order by order in subsequent steps has been formulated by MacDonald, Girvin, and Yoshioka [17]. It is well known that beyond the leading order, *i.e.* $O(t^2/U)$, the Chao-Spałek-Oleś transformation is an uncontrolled approximation [15, 16]. However, the method of continuous unitary transformations, as formulated in the preceding section, allows to clarify the specific assumptions behind this approximation, and to identify the interaction terms which it neglects.

3.1 The Chao-Spałek-Oleś approximation

In this section we show that the results derived in the approximation of Chao, Spałek, and Oleś [15] can be obtained in the framework of the flow equation method, if the generator η of the continuous transformation contains *only* first-order terms, and all higher-order interactions involving at least one T_0 are *neglected.* Chao, Spałek, and Oleś apply a canonical transformation which in our notation can be written

$$S = \frac{t}{U}(T_{+1} - T_{-1}), \tag{41}$$

and by means of (40) directly derive all higher-order interactions, utilizing an approximation for the band energies which neglects the T_0 contribution to the kinetic energy. Thus, we choose a generator

$$\eta(l) = \frac{t}{U} F^{(1)}(l)\,(T_{+1} - T_{-1}). \tag{42}$$

For the effective interactions, we assume that only terms which do not contain T_0 are present,

$$\Theta(l) = \sum_{k=1}^{\infty} \frac{t^{k-1}}{U^{k-1}} \sum_{\{\mathbf{m}\}} F^{(k)}(l;\mathbf{m})\, T^{(k)}(\mathbf{m}) \qquad \text{with} \quad \{\mathbf{m}\} = \{\mathbf{m}|\forall m_i \neq 0\}. \tag{43}$$

The choice (42) for the generator results in the flow equations

$$\frac{\mathrm{d}}{\mathrm{d}l} F^{(1)}(l;m) = -F^{(1)}(l;m) \qquad \text{for} \quad m = \pm 1, \tag{44}$$

while for $k \geq 2$ one finds

$$\frac{\mathrm{d}}{\mathrm{d}l} F^{(k)}(l;\mathbf{m}) = e^{-l} \sum_{\substack{\{\mathbf{m}_1,\mathbf{m}_2\}\\ \mathbf{m}=(\mathbf{m}_1,\mathbf{m}_2)}} \Big(m_1\, F^{(k-1)}(l;\mathbf{m}_2) - m_2\, F^{(k-1)}(l;\mathbf{m}_1) \Big)\,, \tag{45}$$

where terms with $\sum_{i=1}^{k} |m_i| < k$ will be neglected. These equations lead to the solution $F^{(1)}(l;m) = e^{-l}$, and the observation that the coupling functions $F^{(k)}(l;\mathbf{m})$ can be factorized in a coefficient $c^{(k)}(\mathbf{m})$ which depends only on the operator product, and a function $F^{(k)}(l)$ which absorbs the l-dependence,

$$F^{(k)}(l;\mathbf{m}) = c^{(k)}(\mathbf{m})\, F^{(k)}(l). \tag{46}$$

The final form of the flow equations in the Chao-Spałek-Oleś approximation thus reads

$$\frac{\mathrm{d}}{\mathrm{d}l} F^{(k)}(l) = e^{-l}\, F^{(k-1)}(l) \qquad \text{for} \quad k \geq 1, \tag{47}$$

if we define $F^{(0)}(l) = -1$, and the coupling coefficients are given by the recursion relations

$$c^{(k)}(\mathbf{m}) = \sum_{\substack{\{\mathbf{m}_1,\mathbf{m}_2\}\\ \mathbf{m}=(\mathbf{m}_1,\mathbf{m}_2)}} \Big(m_1\, c^{(k-1)}(\mathbf{m}_2) - m_2\, c^{(k-1)}(\mathbf{m}_1) \Big) \qquad \text{for} \quad k \geq 2, \tag{48}$$

with $c^{(1)}(m) = 1$. These relations imply that only terms with $|M(\mathbf{m})| < k$ are nonzero. The solutions of (47) are linear combinations of exponentials,

$$F^{(k)}(l) = \sum_{n=0}^{k} a_n^{(k)}\, e^{-nl}, \tag{49}$$

where the coefficients are determined by the conditions

$$a_n^{(k)} = -\frac{1}{n}\, a_{n-1}^{(k-1)} \quad \text{with} \quad n \geq 1, \qquad \text{and} \quad \sum_{n=0}^{k} a_n^{(k)} = 0 \quad \text{with} \quad k \geq 2. \tag{50}$$

From Eqs. (50) one can derive a relation which involves only the lowest-order coefficients,

$$a_0^{(k)} = \sum_{\kappa=1}^{k} \frac{(-1)^{\kappa+1}}{\kappa!}\, a_0^{(k-\kappa)}, \tag{51}$$

with the initial values $a_0^{(0)} = -1$ and $a_0^{(1)} = 0$. The solutions of the equations (51) are then given by the simple expression

$$a_0^{(k)} = \frac{k-1}{k!}, \tag{52}$$

and more generally

$$a_n^{(k)} = \frac{(-1)^n}{n!} \frac{k-n-1}{(k-n)!}. \tag{53}$$

To solve the flow equations completely, we now have to find the solution for the recursion relations (48). It is straightforward to show by induction that it can be written in the following form:

$$c^{(k)}(\mathbf{m}) = (-1)^k \left(\prod_{i=1}^{k} m_i \right) \sum_{i=1}^{k} \binom{k-1}{i-1} (-1)^i m_i. \tag{54}$$

From (52) and (54) the coupling coefficients $C^{(k)}(\mathbf{m}) = c^{(k)}(\mathbf{m})\, a_0^{(k)}$ are finally obtained, which agree with the results of Chao, Spałek, and Oleś [15]. For $k \leq 6$, the coupling functions and coefficients are listed in table III.

3.2 An improved linear approximation

In the original formulation of the Chao-Spałek-Oleś approximation, all interaction terms which involve T_0 have been disregarded, due to the neglect of the finite width of the Hubbard bands. This appears to be crucial for the development of their formalism, and it is difficult to incorporate a systematic improvement of this deficiency in the original treatment. However, in the framework of the flow equation method such an approximation for the band width is not necessary. To the contrary, the neglect of interaction terms which are generated by the transformation flow seems very unnatural and unmotivated. Within the continuous unitary transformation formulated in the preceding section, one may thus easily find an improvement of the expansion of Chao, Spałek, and Oleś by simply taking into account these neglected terms. Closed expressions can again be derived for the corresponding coupling coefficients. Therefore, we again start with the generator (42), which contains only linear contributions, and in the process of the transformation keep *all* higher-order interactions. Also for these new interaction terms the results (44-51) still apply. Since nothing changes for the interaction terms without a T_0, which we have studied so far, in the following we only consider contributions which involve a T_0 term. One finds that such interactions can contain at most *one* T_0 operator, due to the linear approximation (42) for the flow generator η which does not involve T_0. Therefore, the new interactions are described by an index vector $\mathbf{m}_j = (m_1, \ldots, m_j, 0, m_{j+1}, \ldots, m_k)$, where $m_i = \pm 1$. Since T_0 itself is invariant under the transformation flow, with $F^{(1)}(l) = 1$ one obtains the starting condition $c^{(1)}(0) = 1$, and the initial values $a_0^{(0)} = 0$ and $a_0^{(1)} = 1$. For the new terms the solutions of Eq. (51) then read

$$a_0^{(k)} = \frac{1}{(k-1)!} \qquad \text{and} \quad a_n^{(k)} = \frac{(-1)^n}{n!} \frac{1}{(k-n-1)!}. \tag{55}$$

To complete the solution for general $C^{(k)}(\mathbf{m})$, one again shows by induction that for the new interaction terms the recursive relations (48) are satisfied by the expression

$$c^{(k+1)}(\mathbf{m}_j) = (-1)^{k+j} \binom{k}{j} \left(\prod_{i=1}^{k} m_i \right) \qquad \text{with} \quad 0 \leq j \leq k. \tag{56}$$

The corresponding coupling functions and coefficients are listed in table IV. These results yield a systematic improvement of the expansion of Chao, Spałek, and Oleś, and provide a *consistent linear approximation*. Keeping all effective interactions which are generated by this transformation, terms connecting different Hubbard bands are eliminated to first order from the Hamiltonian.

3.3 The MacDonald-Girvin-Yoshioka scheme

A unitary transformation of the Hubbard model which eventually removes all terms from the Hamiltonian that connect different sectors of the Hilbert space has been proposed by MacDonald, Girvin, and Yoshioka [17]. In their scheme, the transformation S is determined iteratively in such a way, that all interactions which do not conserve the number of local electron pairs are eliminated up to a certain order of t/U. This generates new interaction terms in higher orders, and some of them need to be removed in a next step. Thus, the transformation is constructed order by order, and S can be written in the form

$$S = \sum_{k=1}^{\infty} \frac{t^k}{U^k} S^{(k)}. \tag{57}$$

In first order, all unphysical interaction terms are eliminated if one chooses

$$S^{(1)} = T_{+1} - T_{-1}. \tag{58}$$

This choice for S generates new interactions of order t^2/U, which again couple different Hilbert subspaces and need to be eliminated. This is achieved with

$$S^{(2)} = [T_{+1}, T_0] + [T_{-1}, T_0]. \tag{59}$$

In contrast to the results derived from the flow equations, here in higher orders of t/U the unphysical interactions which are generated intermediately also involve terms with $|M(\mathbf{m})| > 1$, *e.g.*

$$\begin{aligned} S^{(3)} = 1/4\,[[T_{+1}, T_0], T_{+1}] - 1/4\,[[T_{-1}, T_0], T_{-1}] + [[T_{+1}, T_0], T_0] - [[T_{-1}, T_0], T_0] \\ -2/3\,[[T_{+1}, T_{-1}], T_{+1}] - 2/3\,[[T_{+1}, T_{-1}], T_{-1}]. \end{aligned} \tag{60}$$

Repeating this procedure up to the desired order gives the corresponding effective Hamiltonian. To third order in t/U, the coupling coefficients of the resulting effective interactions in the physical Hilbert subspace are in agreement with the $C^{(k)}(\mathbf{m})$ obtained from the solutions of the flow equations as given in table I. In higher orders, however, there are some differing results for the two methods.[1] These differences can be understood, if we consider

[1] The first discrepancy between our results and those explicitly listed in ref. [17] is found for $k = 4$, with $C^{(4)}(0, +1, -1, 0) = 0$ and $C^{(4)}(+1, -1, 0, 0) = 1/2$, in contrast to the values given in table I.

the complete unitary transformation which is obtained after integrating out the continuous transformation flow. The flow equation (8) corresponds to the transformation

$$e^{S(l)} = \mathrm{T}_l \exp\left(\int_0^l \mathrm{d}l'\,\eta(l')\right), \tag{61}$$

where T_l performes l-ordering in the usual manner. One then finds

$$S(l) = \int_0^l \mathrm{d}l'\,\eta(l') + \frac{1}{2}\int_0^l \mathrm{d}l' \int_0^{l'} \mathrm{d}l''\,[\eta(l'),\eta(l'')] + \cdots . \tag{62}$$

If we now insert our flow generator (7) together with the coupling functions of table II into this equation, at order t^3/U^3 the resulting $S(\infty)$ is found to differ from the $S = S_{\mathrm{MGY}}$ obtained by MacDonald, Girvin, and Yoshioka, $S(\infty) = S_{\mathrm{MGY}} + \Delta S$, with

$$\Delta S = \frac{t^3}{4U^3}\left([[T_{-1},T_0],T_{+1}] - [[T_{+1},T_0],T_{-1}]\right) + \cdots . \tag{63}$$

This difference ΔS is due to the continuous adjustment of the unitary transformation to the couplings of the Hamiltonian. It reflects a residual freedom in the choice of the transformation which eliminates interactions between *different* Hubbard bands, since such a transformation is uniquely determined at most up to arbitrary transformations *within* the bands. It is this result (63) for ΔS which precisely accounts for the differences of the coupling coefficients at order $k = 4$. It is also worth noting that the generation of interaction terms with $|M(\mathbf{m})| > 1$ is peculiar for performing the unitary transformation in one step, corresponding to $S(\infty)$ as given by (62), whereas the continuous transformation flow does not involve such terms.

3.4 General unitary transformations

Since the unitary transformation which leads to a t/U-expanded effective Hamiltonian for the Hubbard model is not unique, let us finally consider the possible consequences related to the remaining degree of freedom. The arbitrary transformations ΔS within the Hubbard bands can be written in the general form

$$\Delta S = \sum_{k=1}^{\infty} \frac{t^k}{U^k} \sum_{\substack{\{\mathbf{m}\}\\ M(\mathbf{m})=0}} D^{(k)}(\mathbf{m})\, T^{(k)}(\mathbf{m}), \tag{64}$$

where due to the antihermiteicity of the generator and the particle-hole symmetry of the Hamiltonian one analogously to the symmetry properties (10) finds the relations

$$\begin{aligned} D^{(k)}(-\overline{\mathbf{m}}) &= -\left(D^{(k)}(\mathbf{m})\right)^* \\ D^{(k)}(-\mathbf{m}) &= (-1)^k\, D^{(k)}(\mathbf{m}). \end{aligned} \tag{65}$$

These symmetry requirements imply that $D^{(1)} = 0$, so that ΔS is at least of second order in t/U. Since $[V, \Delta S] = 0$, the lowest-order contribution of ΔS to the effective Hamiltonian may occur only at order t^3/U^2 or higher. Although in general different unitary transformations may thus lead to a different form of the effective Hamiltonian expressed by the T_m operators, for the half-filled Hubbard model the effective spin interactions derived by the flow equation method to fifth order agree with those obtained by degenerate perturbation theory and by the MacDonald-Girvin-Yoshioka approach, as is shown in the next section.

3.5 The spin interactions

To illustrate the result for the effective Hamiltonian for an interesting case and to compare with expressions obtained by other approaches, we consider the Hubbard model with positive U and with a half-filled band. In the subspace with lowest energy, this corresponds to single occupancy of each lattice site, and in this subspace the interactions can be expressed completely by spin operators. Following the arguments given in section 2.2 [*cf.* Eq. (19)], at half band-filling the number of contributing interaction terms at a given order in t/U reduces significantly. Up to fifth order, one obtains the effective Hamiltonian

$$H(\infty) = -\frac{t^2}{U}T_{-1}T_{+1} + \frac{t^4}{U^3}\left(T_{-1}T_{+1}T_{-1}T_{+1} - T_{-1}T_0T_0T_{+1} - \frac{1}{2}T_{-1}T_{-1}T_{+1}T_{+1}\right), \quad (66)$$

where terms with odd powers in t vanish due to the particle-hole symmetry and the resulting invariance of the spectrum under $t \to -t$. This is in accordance with a general theorem shown by Takahashi [9]. Therefore, we find the effective spin Hamiltonian

$$H_{\text{spin}} = \frac{t^2}{U}H_2 + \frac{t^4}{U^3}H_4 + \cdots. \quad (67)$$

In order to calculate the explicit form of the interactions in spin space, we have to reexpress the T_m in terms of fermionic operators according with (3), and then identify the spins, $\mathbf{s_r} = c^\dagger_{\mathbf{r}\sigma}\sigma_{\sigma\sigma'}c_{\mathbf{r}\sigma'}$. In this way one finds in leading order the well-known mapping on the antiferromagnetic Heisenberg model,

$$H_2 = \frac{1}{2}\sum_{\mathbf{r}_1\mathbf{r}_2} D_{\mathbf{r}_1\mathbf{r}_2}(\mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_2} - 1). \quad (68)$$

The next higher-order interactions are given by

$$\begin{aligned}H_4 = &-2\sum_{\mathbf{r}_1\mathbf{r}_2} D_{\mathbf{r}_1\mathbf{r}_2}(\mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_2} - 1) + \frac{1}{2}\sum_{\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3} D_{\mathbf{r}_1\mathbf{r}_2}D_{\mathbf{r}_2\mathbf{r}_3}(\mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_3} - 1)\\ &+\frac{1}{8}\sum_{\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4} D_{\mathbf{r}_1\mathbf{r}_2}D_{\mathbf{r}_2\mathbf{r}_3}D_{\mathbf{r}_3\mathbf{r}_4}D_{\mathbf{r}_4\mathbf{r}_1}\{(1 - \mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_2} - \mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_3} - \mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_4} - \mathbf{s}_{\mathbf{r}_2}\cdot\mathbf{s}_{\mathbf{r}_3}\\ &-\mathbf{s}_{\mathbf{r}_2}\cdot\mathbf{s}_{\mathbf{r}_4} - \mathbf{s}_{\mathbf{r}_3}\cdot\mathbf{s}_{\mathbf{r}_4}) + 5[(\mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_2})(\mathbf{s}_{\mathbf{r}_3}\cdot\mathbf{s}_{\mathbf{r}_4}) + (\mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_4})(\mathbf{s}_{\mathbf{r}_2}\cdot\mathbf{s}_{\mathbf{r}_3}) - (\mathbf{s}_{\mathbf{r}_1}\cdot\mathbf{s}_{\mathbf{r}_3})(\mathbf{s}_{\mathbf{r}_2}\cdot\mathbf{s}_{\mathbf{r}_4})]\},\end{aligned} \quad (69)$$

where the sums are over sets of distinct site labels. This expression is still valid for arbitrary lattice and spatial dimension, since all information about the details of the lattice is contained in the connectivity matrix $D_{\mathbf{rr}'}$. The result (69) is in agreement with earlier calculations for the half-filled positive-U Hubbard model [9, 17]. The agreement with the fourth-order result of MacDonald, Girvin, and Yoshioka is already apparent from (66), since at half band-filling those $T^{(4)}(\mathbf{m})$ which due to (63) carry differing coupling coefficients in the flow equation method give a vanishing contribution.[2]

Also away from half filling the fourth-order results for the spin Hamiltonians derived by the two methods agree. For negative U and an even number of particles in the system, only empty or doubly occupied sites are present in the lowest-energy subspace, so that again the differing terms vanish. In the positive-U case, due to the corresponding first sum rule in Eq. (28) which is obeyed by the results of both approaches, the differing contributions add up to the same spin interaction.

[2] *Cf.* footnote 1 and note that T_0 annihilates all lowest-energy states of a half-filled band for $U > 0$, and all those states at arbitrary filling and even particle number for $U < 0$.

4 Summary and conclusions

In this work the method of continuous unitary transformations has been applied to the Hubbard model. It has been shown that such a transformation can be used to derive a systematic and exact t/U-expansion of the original Hubbard Hamiltonian which eliminates all interaction terms that are nondiagonal in relation to the Hilbert space sectors belonging to a different number of local electron pairs. The resulting flow equations for the effective interactions can be solved exactly, leading to recursive relations which only involve the calculation of numerical coefficients. These recursion relations are closed at any order of t/U, and provide a simplified scheme to perform calculations at higher orders. To third order, the explicit results for the effective Hamiltonian obtained within this framework are equivalent to those derived previously by MacDonald, Girvin, and Yoshioka. Due to the remaining freedom in the choice of the unitary transformation, in higher orders some differences are found. The resulting spin interactions, however, are in agreement. Our approach additionally allows to derive sum rules for the coupling functions and to obtain general expressions for the exact solutions of special cases of the physical coupling coefficients. The flow equation method also clarifies some of the approximations and assumptions which are employed in the perturbative treatment of Chao, Spałek, and Oleś. It is able to identify the interaction terms which are neglected in their derivation, and suggests a systematic improvement of their results which leads to a consistent linear approximation. Finally, it has been shown that different unitary transformations which block-diagonalize the Hubbard Hamiltonian may lead to different forms for the explicit t/U-expansion only at order t^3/U^2 or higher.

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Table I

The solutions of the flow equations for the coupling functions $F^{(k)}(l;\mathbf{m})$, with $M(\mathbf{m}) = 0$ and $k \leq 5$, and the corresponding coupling coefficients $C^{(k)}(\mathbf{m})$. Additional nonzero coupling functions can be obtained from the symmetry relations, Eqs. (10). For a general expression for the $C^{(k)}(\mathbf{m})$, *cf.* Eqs. (34) and (39).

k	$(\mathbf{m})$	$C^{(k)}(\mathbf{m})$	$F^{(k)}(l;\mathbf{m})$
1	(0)	$+1$	1
2	$(+1,-1)$	$+1$	$1-e^{-2l}$
3	$(+1,0,-1)$	$+1$	$1-(2l+1)e^{-2l}$
	$(+1,-1,0)$	$-\frac{1}{2}$	$-\frac{1}{2}(1-(2l+1)e^{-2l})$
4	$(+1,0,0,-1)$	$+1$	$1-(2l^2+2l+1)e^{-2l}$
	$(+1,0,-1,0)$	-1	$-(1-(2l^2+2l+1)e^{-2l})$
	$(0,+1,-1,0)$	$+\frac{1}{2}$	$\frac{1}{2}(1-(2l^2+2l+1)e^{-2l})$
	$(+1,-1,0,0)$	$+\frac{1}{4}$	$\frac{1}{4}(1-(2l^2+2l+1)e^{-2l})$
	$(+1,-1,+1,-1)$	-1	$-(1-4le^{-2l}-e^{-4l})$
	$(+1,+1,-1,-1)$	$+\frac{1}{2}$	$\frac{1}{2}(1-4le^{-2l}-e^{-4l})$
5	$(+1,0,0,0,-1)$	$+1$	$1-(\frac{4}{3}l^3+2l^2+2l+1)e^{-2l}$
	$(0,+1,0,0,-1)$	$-\frac{3}{2}$	$-\frac{3}{2}(1-(\frac{4}{3}l^3+2l^2+2l+1)e^{-2l})$
	$(0,0,+1,0,-1)$	$+\frac{3}{4}$	$\frac{3}{4}(1-(\frac{4}{3}l^3+2l^2+2l+1)e^{-2l})$
	$(0,0,0,+1,-1)$	$-\frac{1}{8}$	$-\frac{1}{8}(1-(\frac{4}{3}l^3+2l^2+2l+1)e^{-2l})$
	$(0,+1,-1,0,0)$	$-\frac{3}{8}$	$-\frac{3}{8}(1-(\frac{4}{3}l^3+2l^2+2l+1)e^{-2l})$
	$(0,+1,0,-1,0)$	$+\frac{3}{2}$	$\frac{3}{2}(1-(\frac{4}{3}l^3+2l^2+2l+1)e^{-2l})$
	$(+1,-1,+1,-1,0)$	$+\frac{9}{8}$	$\frac{9}{8}-(\frac{7}{2}l^2+2l+\frac{3}{4})e^{-2l}-(l+\frac{3}{8})e^{-4l}$
	$(+1,-1,-1,+1,0)$	$-\frac{3}{8}$	$-\frac{3}{8}(1-(4l^2+2)e^{-2l}+e^{-4l})$
	$(+1,-1,+1,0,-1)$	$-\frac{3}{2}$	$-\frac{3}{2}+(4l^2+4l)e^{-2l}+(2l+\frac{3}{2})e^{-4l}$
	$(+1,-1,-1,0,+1)$	$+\frac{1}{2}$	$\frac{1}{2}(1-(4l^2+2)e^{-2l}+e^{-4l})$
	$(+1,-1,0,-1,+1)$	$-\frac{1}{4}$	$-\frac{1}{4}(1-(4l^2+2)e^{-2l}+e^{-4l})$
	$(+1,+1,-1,0,-1)$	$+\frac{1}{2}$	$\frac{1}{2}(1-(4l^2+2)e^{-2l}+e^{-4l})$
	$(+1,+1,0,-1,-1)$	$+\frac{1}{4}$	$\frac{1}{4}-(2l-1)e^{-2l}-(l+\frac{5}{4})e^{-4l}$
	$(+1,-1,0,+1,-1)$	$+\frac{3}{4}$	$\frac{3}{4}-(l^2+4l-\frac{3}{2})e^{-2l}-(2l+\frac{9}{4})e^{-4l}$
	$(+1,+1,-1,-1,0)$	$-\frac{5}{8}$	$-\frac{5}{8}+(2l^2+l+\frac{1}{2})e^{-2l}+(\frac{1}{2}l+\frac{1}{8})e^{-4l}$

Table II

The solutions of the flow equations for the coupling functions $F^{(k)}(l;\mathbf{m})$, with $|M(\mathbf{m})| = 1$ and $k \leq 4$. As in table I, only functions which are not related by symmetry are listed. For general expressions, *cf.* Eqs. (32) and (36-38).

k	$(\mathbf{m})$	$F^{(k)}(l;\mathbf{m})$
1	$(+1)$	e^{-l}
2	$(+1,0)$	le^{-l}
3	$(+1,+1,-1)$	$(l-\frac{1}{2})e^{-l}+\frac{1}{2}e^{-3l}$
	$(+1,-1,+1)$	$-2((l-\frac{1}{2})e^{-l}+\frac{1}{2}e^{-3l})$
	$(+1,0,0)$	$\frac{1}{2}l^2e^{-l}$
	$(0,+1,0)$	$-l^2e^{-l}$
4	$(+1,0,0,0)$	$\frac{1}{6}l^3e^{-l}$
	$(0,+1,0,0)$	$-\frac{1}{2}l^3e^{-l}$
	$(+1,-1,+1,0)$	$(-\frac{3}{2}l^2+\frac{1}{2}l+\frac{1}{4})e^{-l}-(l+\frac{1}{4})e^{-3l}$
	$(+1,+1,-1,0)$	$(\frac{1}{2}l^2-l+\frac{3}{4})e^{-l}-(\frac{1}{2}l+\frac{3}{4})e^{-3l}$
	$(+1,-1,-1,0)$	$(-l^2+\frac{1}{2}l)e^{-l}-\frac{1}{2}le^{-3l}$
	$(+1,0,+1,-1)$	$(\frac{1}{2}l^2-\frac{1}{2}l+\frac{1}{4})e^{-l}-\frac{1}{4}e^{-3l}$
	$(+1,0,-1,+1)$	$(-\frac{1}{2}l^2-\frac{3}{2}l+\frac{7}{4})e^{-l}-(2l+\frac{7}{4})e^{-3l}$
	$(+1,0,-1,-1)$	$(l-1)e^{-l}+(l+1)e^{-3l}$

Table III

The solutions of the flow equations for the coupling functions $F^{(k)}(l;\mathbf{m}) = c^{(k)}(\mathbf{m})\,F^{(k)}(l)$, and the coupling coefficients $C^{(k)}(\mathbf{m})$ for $k \leq 6$, as obtained in the Chao-Spałek-Oleś approximation, Eqs. (42-43). Note that $F^{(k)}(l)$ is given with the normalisation $a_0^{(k)} = 1$.

k	$(\mathbf{m})$	$C^{(k)}(\mathbf{m})$	$F^{(k)}(l)$
1	$(+1)$	0	e^{-l}
2	$(+1,-1)$	$+1$	$1-e^{-2l}$
3	$(+1,+1,-1)$	$+\frac{2}{3}$	$1-\frac{3}{2}e^{-l}+\frac{1}{2}e^{-3l}$
	$(+1,-1,+1)$	$-\frac{4}{3}$	
4	$(+1,+1,-1,-1)$	$+\frac{1}{2}$	$1-\frac{8}{3}e^{-l}+2e^{-2l}-\frac{1}{3}e^{-4l}$
	$(+1,-1,+1,-1)$	-1	
	$(+1,+1,+1,-1)$	$+\frac{1}{4}$	
	$(+1,+1,-1,+1)$	$-\frac{3}{4}$	
5	$(+1,+1,+1,+1,-1)$	$+\frac{1}{15}$	$1-\frac{15}{4}e^{-l}+5e^{-2l}-\frac{5}{2}e^{-3l}+\frac{1}{4}e^{-5l}$
	$(+1,+1,+1,-1,+1)$	$-\frac{4}{15}$	
	$(+1,+1,-1,+1,+1)$	$+\frac{2}{5}$	
	$(+1,+1,+1,-1,-1)$	$+\frac{1}{5}$	
	$(+1,+1,-1,-1,+1)$	$-\frac{2}{15}$	
	$(+1,+1,-1,+1,-1)$	$-\frac{7}{15}$	
	$(+1,-1,+1,+1,-1)$	$+\frac{1}{5}$	
	$(-1,+1,+1,+1,-1)$	$-\frac{2}{15}$	
	$(+1,-1,+1,-1,+1)$	$+\frac{8}{15}$	
6	$(+1,+1,+1,+1,+1,-1)$	$+\frac{1}{72}$	$1-\frac{24}{5}e^{-l}+9e^{-2l}-8e^{-3l}+3e^{-4l}-\frac{1}{5}e^{-6l}$
	$(+1,+1,+1,+1,-1,+1)$	$-\frac{5}{72}$	
	$(+1,+1,+1,-1,+1,+1)$	$+\frac{5}{36}$	
	$(+1,+1,+1,+1,-1,-1)$	$+\frac{1}{18}$	
	$(+1,+1,+1,-1,-1,+1)$	$-\frac{5}{72}$	
	$(+1,+1,+1,-1,+1,-1)$	$-\frac{11}{72}$	
	$(+1,+1,-1,+1,-1,+1)$	$+\frac{5}{24}$	
	$(+1,+1,-1,+1,+1,-1)$	$+\frac{1}{8}$	
	$(+1,-1,+1,+1,+1,-1)$	$-\frac{1}{12}$	
	$(+1,+1,+1,-1,-1,-1)$	$+\frac{1}{12}$	
	$(+1,+1,-1,-1,-1,+1)$	$-\frac{5}{72}$	
	$(+1,+1,-1,+1,-1,-1)$	$-\frac{7}{36}$	
	$(+1,-1,+1,+1,-1,-1)$	$+\frac{1}{72}$	
	$(+1,-1,-1,+1,-1,+1)$	$-\frac{5}{36}$	
	$(+1,-1,+1,-1,+1,-1)$	$+\frac{2}{9}$	
	$(+1,-1,+1,-1,-1,+1)$	$+\frac{5}{36}$	
	$(+1,-1,-1,+1,+1,-1)$	$-\frac{1}{18}$	

Table IV

The solutions of the flow equations for the coupling functions $F^{(k)}(l;\mathbf{m}) = c^{(k)}(\mathbf{m})\,F^{(k)}(l)$, and the coupling coefficients $C^{(k)}(\mathbf{m})$ for $k \leq 6$, resulting from the improved linear approximation, Eqs. (55-56). Other nonzero coefficients differ at most in the sign and are not listed.

k	$(\mathbf{m})$	$C^{(k)}(\mathbf{m})$	$F^{(k)}(l)$
1	(0)	$+1$	1
2	$(+1,0)$	$+1$	$1-e^{-l}$
3	$(+1,+1,0)$	$+\frac{1}{2}$	$1-2e^{-l}+e^{-2l}$
	$(+1,0,+1)$	-1	
4	$(+1,+1,+1,0)$	$+\frac{1}{6}$	$1-3e^{-l}+3e^{-2l}-e^{-3l}$
	$(+1,+1,0,+1)$	$-\frac{1}{2}$	
5	$(+1,+1,+1,+1,0)$	$+\frac{1}{24}$	$1-4e^{-l}+6e^{-2l}-4e^{-3l}+e^{-4l}$
	$(+1,+1,+1,0,+1)$	$-\frac{1}{6}$	
	$(+1,+1,0,+1,+1)$	$+\frac{1}{4}$	
6	$(+1,+1,+1,+1,+1,0)$	$+\frac{1}{120}$	$1-5e^{-l}+10e^{-2l}-10e^{-3l}+5e^{-4l}-e^{-5l}$
	$(+1,+1,+1,+1,0,+1)$	$-\frac{1}{24}$	
	$(+1,+1,+1,0,+1,+1)$	$+\frac{1}{12}$	

Figure 1

The typical transformation flow of the coupling functions $F^{(k)}(l;\mathbf{m})$ versus the flow parameter l, for $F^{(1)}(l;\pm 1)$ (solid line), for $k>1$ and $M(\mathbf{m})=0$ (dashed line), and for $k>1$ and $|M(\mathbf{m})|=1$ (dotted line).