Exact renormalization group for quantum spin systems

Jan Krieg and Peter Kopietz
Institut für Theoretische Physik, Universität Frankfurt,
Max-von-Laue Straße 1, 60438 Frankfurt, Germany
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We show that the diagrammatic approach to quantum spin systems developed in a seminal work by Vaks, Larkin, and Pikin [Sov. Phys. JETP 26, 188 (1968)] can be embedded in the framework of the functional renormalization group. The crucial insight is that the generating functional of the time-ordered connected spin correlation functions of an arbitrary quantum spin system satisfies an exact renormalization group flow equation which resembles the corresponding flow equation of a system of interacting bosons. The SU(2) spin algebra is implemented via a non-trivial initial condition for the renormalization group flow. Our method is rather general and offers a new non-perturbative approach to quantum spin systems.

Introduction. Quantum spin models play a central role in condensed matter physics and statistical mechanics for gaining a microscopic understanding of the magnetic properties of insulators with localized magnetic moments [1][2]. Although theoretical research in this field has a long history starting with the seminal papers by Ising [3] and Bethe [4], the controlled calculation of the physical properties of realistic quantum spin models describing experimentally accessible materials remains a highly relevant problem of general interest. This is especially challenging in reduced dimensions, where the effect of fluctuations can be sufficiently strong to destroy any long-range magnetic order. But also in three dimensions, competing interactions or geometrical frustration can destroy long-range magnetic order and stabilize exotic states characterized by topological order [5][6].

The low-energy excitations of ordered magnets are usually renormalized spin-waves. In this case an expansion in powers of the inverse spin-quantum number $1/S$, formalized with the help of the Holstein-Primakoff [7] or the Dyson-Maleev [8] transformation, has been extremely successful and continues to be one of the most powerful theoretical methods for ordered magnets [9]. However, in the absence of long-range magnetic order the $1/S$-expansion is not applicable. Several alternative methods have been developed to study quantum magnets without magnetic order, such as modifications of spin-wave theory where the vanishing magnetization is externally enforced [10][11]. Schwinger-boson mean-field theory [12][13], and mean-field theories relying on the representation of the spin operators in terms of Abrikosov pseudofermions [13][14] or Majorana fermions [19][18].

Each of the above methods has its own shortcomings. While the Majorana representation of spin operators generates redundancy in Hilbert space [17], the pseudofermion representation as well as the Schwinger-boson approach introduce unphysical states which should be projected out. In practice, this projection can only be implemented approximately. For pseudofermions this can be achieved using a method due to Popov and Fedotov [19], who showed that the contribution from unphysical states cancels if one introduces a certain imaginary chemical potential [20]. Recently Reuther and Wölffe [21] have developed a functional renormalization group (FRG) [22][24] approach for spin-1/2 systems using the pseudofermion representation.

In this work, we shall develop an alternative FRG approach for quantum spin models with arbitrary spin $S$ which does not rely on any auxiliary representation of the spin operators. The main idea is to formulate the FRG directly in terms of the physical spin operators, thus avoiding the introduction of fermionic or bosonic auxiliary operators acting on an extended Hilbert space. In the recent work [25] this strategy has been adopted to study low-dimensional $S = 1/2$ quantum antiferromagnets within a mean-field decoupling. In fact, an approach to quantum spin systems which works directly with the physical spin operators has been developed half a century ago by Vaks, Larkin, and Pikin (VLP) [26], who showed that the spin operators satisfy a generalized Wick theorem, which can be used to develop a systematic diagrammatic expansion in powers of the inverse range of the exchange interaction. A detailed description of the VLP approach can be found in a textbook by Izyumov and Skryabin [27]. Although this method has been further developed [28][29], it has not gained a wide popularity, perhaps because of the rather cumbersome diagrammatic rules implied by the generalized Wick theorem for spin operators. In this work we show that by embedding the VLP idea into the framework of the FRG, we can avoid this technical problem and obtain a powerful analytical approach to quantum spin systems.

Exact flow equations. Although our method can easily be extended to more general spin models, we consider here for simplicity the quantum Heisenberg Hamiltonian

$$\mathcal{H} = \frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h_0 \sum_i S_i^z,$$

where the subscripts $i, j$ label the $N$ sites $r_i$ of a $D$-dimensional lattice, $h_0$ is an external magnetic field in units of energy, and $J_{ij} = J(r_i - r_j)$ are arbitrary exchange couplings. The spin-$S$ operators $\mathbf{S}_i$ are normal-
ized such that $S_i^2 = S(S + 1)$ and satisfy the usual $SU(2)$-algebra $[S_i^a, S_j^b] = i\delta_{ij} \epsilon^{abc} S_j^c$, where the superscripts $\alpha, \beta, \gamma$ refer to the Cartesian components of $S_i$ and $\epsilon^{abc}$ is the totally antisymmetric $\epsilon$-tensor. We now replace the exchange couplings $J_{ij}$ by some continuous deformation $J_{ij}^\Lambda$, which depends on a dimensionless parameter $\Lambda \in [0, 1]$ such that $J_{ij}^\Lambda = 0$ is sufficiently simple to allow for a controlled solution of the initially deformed spin model, and $J_{ij}^\Lambda = 1$ so that for $\Lambda = 1$ we recover our original model. For example, by choosing $J_{ij}^\Lambda = \Lambda J_{ij}$ our initial model at $\Lambda = 0$ reduces to a trivial system of isolated spins in an external magnetic field.

To begin with, we derive an exact evolution equation for the $\Lambda$-dependent generating functional of the connected Euclidean time-ordered spin correlation functions,

$$G_\Lambda[h] = \ln \text{Tr} \left[ e^{-\beta H_0 + \int_0^\beta d\tau (\sum_i h_i(\tau) \cdot S_i(\tau) - V_i(\tau))} \right]. \quad (2)$$

Here $\beta$ is the inverse temperature, $T$ denotes time-ordering in imaginary time, $h_i(\tau)$ are fluctuating source fields, $H_0 = -h_0 \sum_i S_i^2$ is the local part of the spin Hamiltonian, $V_i(\tau) = \frac{1}{2} \sum_{ij} J_{ij} S_i(\tau) \cdot S_j(\tau)$ is the deformed exchange Hamiltonian, and the time dependence of all operators is in the interaction picture with respect to $H_0$. The connected time-ordered spin correlation functions can be obtained by taking derivatives of $G_\Lambda[h]$ with respect to the sources. For example, the local magnetic moment at lattice site $r_i$ is given by $\langle S_i(\tau) \rangle_\Lambda = \delta G_\Lambda[h]/\delta h_i(\tau)_{h=0}$, and the connected time-ordered spin-spin correlation function can be generated as follows,

$$G_\Lambda^{\alpha\beta}(\tau, \tau') = \langle T [S_i^\alpha(\tau) S_i^\beta(\tau')] \rangle_\Lambda - \langle S_i^\alpha(\tau) \rangle_\Lambda \langle S_i^\beta(\tau') \rangle_\Lambda$$

$$= \left. \frac{\delta^2 G_\Lambda[h]}{\delta h_i^\alpha(\tau) \delta h_j^\beta(\tau')} \right|_{h=0}. \quad (3)$$

By simply differentiating Eq. (2) with respect to the deformation parameter $\Lambda$ we obtain the exact flow equation

$$\frac{d}{d\Lambda} G_\Lambda[h] = -\frac{1}{2} \int_0^\beta d\tau \sum_{ij,\alpha} (\partial_\Lambda J_{ij}^\Lambda) \left[ \frac{\delta^2 G_\Lambda[h]}{\delta h_i^\alpha(\tau) \delta h_j^\alpha(\tau')} + \frac{\delta G_\Lambda[h]}{\delta h_i^\alpha(\tau)} \frac{\delta G_\Lambda[h]}{\delta h_j^\alpha(\tau)} \right]. \quad (4)$$

Note that in the derivation of FRG flow equations for interacting field theories, it is usually assumed that the relevant generating functional can be represented in terms of some unconstrained functional integral over real, complex, or Grassmann fields $\{22\, 23\, 30\}$. However, this assumption is really not necessary, as pointed out before by Machado and Dupuis $\{31\}$, see also Ref. $\{32\}$. This insight is crucial for applying FRG techniques to models defined in terms of operators satisfying neither bosonic nor fermionic commutation relations. The exact flow equation (4) is equivalent to an infinite hierarchy of flow equations for the connected time-ordered $n$-spin correlation functions $G_\Lambda^{\alpha_1...\alpha_n}(\tau_1, \ldots, \tau_n)$, which are defined via the derivatives of $G_\Lambda[h]$ with respect to the sources $h_i^\alpha(\tau)$. The hierarchy of flow equations can be written as

$$\frac{d}{d\Lambda} G_\Lambda^{\alpha_1...\alpha_n}(\tau_1, \ldots, \tau_n) = -\frac{1}{2} \int_0^\beta d\tau \sum_{ij,\alpha} (\partial_\Lambda J_{ij}^\Lambda) \left[ G_\Lambda^{\alpha_1...\alpha_n\alpha}(\tau_1, \ldots, \tau_n, \tau, \tau) + \sum_{m=0}^n S_{1, \ldots, m; m+1, \ldots, n} \left( G_\Lambda^{\alpha_1...\alpha_m\alpha}(\tau_1, \ldots, \tau_m, \tau) G_\Lambda^{\alpha_{m+1}...\alpha_n\alpha}(\tau_{m+1}, \ldots, \tau_n, \tau) \right) \right]. \quad (5)$$

where the symmetrization operator $S_{1, \ldots, m; m+1, \ldots, n}$ symmetrizes the expression in the curly braces with respect to the exchange of all labels $\{23\}$. A graphical representation of Eq. (5) is shown in Fig. 1. The exact flow equation (5) can be used to generate a systematic expansion of the connected spin correlation functions in powers of the exchange couplings. Therefore we choose the deformation scheme $J_{ij}^\Lambda = \Lambda J_{ij}$, so that each slashed line in Fig. 1 gives simply an additional power of $J_{ij}$. A straightforward iteration of the system of flow equations then generates the desired expansion. This algorithm seems to be considerably simpler than the method based on the generalized Wick theorem for spin operators $\{22\}$.

Following the usual procedure $\{22\, 24\, 30\}$, we now introduce the generating functional $\Gamma_\Lambda[M]$ of the irreducible spin vertices via a subtracted Legendre transformation of $G_\Lambda[h]$,

$$\Gamma_\Lambda[M] = \int_0^\beta d\tau \sum_i h_i(\tau) \cdot M_i(\tau) - G_\Lambda[h]$$

$$- \frac{1}{2} \int_0^\beta d\tau \sum_{ij} R_{ij}^\Lambda M_i(\tau) \cdot M_j(\tau), \quad (6)$$

where $R_{ij}^\Lambda = J_{ij}^\Lambda - J_{ij}$ plays the role of a regulator function $\{22\, 24\}$. Taking a derivative of $\Gamma_\Lambda[M]$ with respect to $\Lambda$
of the irreducible vertices of quantum spin systems. They satisfy bosonic Kubo-Martin-Schwinger boundary
condition \([30]\). The bosonic nature of time-ordered spin correlation functions and irreducible vertices are
independent of time. For simplicity we choose again the deformed interaction \(J^λ_{ij} = Λ J_{ij}\). The Hamiltonian of the spin-
S Ising model with ferromagnetic nearest-neighbor coupling \(J\) can be obtained by replacing the operator \(V_λ(τ)\) in
Eq. \([2]\) by \(V_λ = −ΛJ \sum_{(ij)} S_i^α S_j^α\), where \((ij)\) denotes all distinct pairs of nearest neighbors on a
\(D\)-dimensional hypercubic lattice. The magnetic field \(h_i\) and the conjugate magnetization \(M_i\) have then only z-
components, which we denote by \(h_z\) and \(M_z\). In momentum space the vertex expansion of \(Γ_λ[M]\) is then

\[
Γ_λ[M] = \sum_{n=0}^{∞} \frac{1}{n!} \sum_{k_1,..,k_n} \delta_{k_1+…+k_n,0} \times Γ_λ^{(n)}(k_1,..,k_n) M_{k_1}…M_{k_n},
\]

where the Fourier coefficients of the magnetization field are defined by \(M_k = \sum_i e^{-i k \cdot r} M_i\). Substituting the expansion \([12]\) into the exact flow equation \([11]\) we obtain an infinite hierarchy of flow equations for the \(n\)-point
vertices. For simplicity, we set \(h_0 = 0\) and assume that there is no spontaneous magnetization. The flow equation for
\(Γ_λ^{(2)}(k) = Γ_λ^{(2)}(-k, k)\) is then

\[
∂_λ Γ_λ^{(2)}(k) = \frac{β}{2N} \sum_q \hat{G}_λ(q) Γ_λ^{(4)}(-k, k, -q, q),
\]

where \(\hat{G}_λ(k) = -G_λ^∗(k) \partial_λ R_λ(k)\) is the so-called single-scale propagator and \(G_λ(k) = [Γ_λ^{(2)}(k) + β R_λ(k)]^{-1}\)
is the regularized propagator. With our deformation scheme, the Fourier transform of the regulator is \(R_λ(k) = (1−Λ) V_k\),
where \(V_k = 2D J_{-k}\) is the Fourier transform of the exchange interaction and \(γ_κ = D^{-1} \sum_{μ=1}^{D} \cos(κ_μ α)\) is
the nearest-neighbor structure factor of a \(D\)-dimensional hypercubic lattice with lattice spacing \(α\).

To derive the initial condition at \(λ = 0\), we note that for vanishing exchange interaction the generating functional of the connected spin correlation functions is \(G_0[h] = \sum B(βh)\), where \(B(y) = \ln[\sinh((S + 1/2) y)/\sinh(y/2)]\) is the primitive integral of the spin-
S Brillouin function \(b(y) = dB(y)/dy\). The initial value of the two-point vertex is therefore \(Γ_0^{(2)}(k) = 1/b′ - β V_k\),
where \(b′ = S(S + 1)/3\) is the derivative of \(b(y)\) at \(y = 0\).
The calculation of the initial functional \( \Gamma_0[M] \) requires the inversion of the Brillouin function which is not possible in closed form \[33\]. However, we can iteratively calculate the first few terms in the vertex expansion. For example, the initial value of the four-point vertex is

\[
\Gamma_0^{(2)}(k_1, k_2, k_3, k_4) = -b''/(b')^4 \equiv u_0 > 0, \tag{14}
\]

where \( b'' = [1 - (2S + 1)^4]/120 \) is the 3rd derivative of \( b(y) \) at \( y = 0 \). In general, the initial values \( \Gamma_0^{(n)} \) of the higher-order vertices can be expressed in terms of derivatives \( b^{(m)} \) of the Brillouin function up to order \( m \leq n - 1 \).

As a first quantitative test of our SFRG approach, let us calculate the critical temperature \( T_c \) of the spin-\( S \) Ising model, which can be identified with the temperature where \( \Gamma_0^{(2)}(0) = 0 \). If we approximate the two-point vertex at vanishing momentum by its initial value \( \Gamma_0^{(2)}(0) = 1/b' - \beta V_0 \), we obtain the mean-field critical temperature \( T_{c0} = 2DJS(S + 1)/3 \). To go beyond mean-field theory, we need a suitable truncation of the infinite hierarchy of FRG flow equations. For simplicity, let us retain only the flowing two-point and four-point vertices with their initial momentum dependence and close the hierarchy by approximating the six-point vertex by its initial value \( \Gamma_0^{(6)} \). Our results for \( T_c \) for \( S = 1/2 \) and different dimensions \( D \) are summarized in Table I. Note that in \( D = 3 \) our SFRG prediction for \( T_c \) agrees with controlled Monte Carlo results \[35\] with an accuracy of about 1%, while for \( D > 3 \) our SFRG result for \( T_c \) is even more accurate. For higher spins \( S > 1/2 \) (not listed in Table I) we obtain \( T_c \) with similar accuracy. It should be mentioned that some time ago Machado and Dupuis \[31\] developed a lattice FRG approach for classical spin models which produces results for \( T_c \) in \( D = 3 \) with comparable accuracy.

Obviously, in two dimensions our truncated SFRG incorrectly predicts \( T_c = 0 \), indicating that in this case our simple truncation is not sufficient. Fortunately, we can formally use \( 1/D \) as a small parameter to develop a more systematic truncation strategy. Using the fact that the Brillouin-zone average of the \( 2n \)-th power \( \gamma_2^n \) of the structure factor is of the order \( 1/D^n \), we can iterate our hierarchy of flow equations to generate a systematic expansion of \( \Gamma_{\Lambda=1}^{(2)}(0) \) in powers of \( 1/D \). By truncating this expansion at order \( 1/D \) and solving the resulting self-consistency equation for \( T_c \) we obtain

\[
\frac{T_c}{T_{c0}} = \frac{1}{2} \left[ 1 + \sqrt{1 - \frac{u_0(b')^2}{D}} \right]. \tag{15}
\]

The values for \( T_c \) obtained from this expression for \( S = 1/2 \) are listed in the third column of Table I. In two dimensions we now obtain a finite \( T_c = T_{c0}/2 \), but for \( D \geq 3 \) the \( T_c \) obtained from our truncated SFRG turns out to be more accurate than Eq. (15). We have also used our SFRG flow equations to generate the expansion of \( \Gamma_{\Lambda=1}^{(2)}(0) \) for arbitrary spin \( S \) up to order \( 1/D^3 \) \[38\]; for \( D \geq 4 \) the resulting estimate for \( T_c \) (not shown in Table I) significantly improves upon both the leading \( 1/D \) results and the truncated SFRG results listed in Table I.

**Application to quantum spin systems.** Let us now come back to the quantum Heisenberg Hamiltonian \[1\]. The exact FRG flow of the generating functional of the irreducible spin vertices is then given by Eq. (11). By expanding both sides in powers of the components of the fluctuating magnetization \( M^\alpha(\tau) \), we obtain the usual hierarchy of coupled FRG flow equations \[23\]. However, the simple deformation scheme \( J_{ij}^\alpha = \Lambda J_{ij} \) where initially the exchange interaction is completely switched off cannot be used in this case, because then the Legendre transform of the initial generating functional \( G_0[\h] \) does not exist due to the lack of dynamics in the longitudinal fluctuations. This problem can be solved in several ways. For example, we may choose the initial \( J_0^{ij} \) such that for \( \Lambda = 0 \) the system decouples into non-interacting dimers \[38\], which is a convenient initial condition for spin systems with valence-bond ground states \[39\]. Alternatively, we can consider the flow of the amputated connected spin correlation functions, which are generated by \[23\].

\[
\mathcal{F}_\Lambda[M] = G_\Lambda \left[ - \sum_j J_{ij}^\alpha M_j \right] - \frac{1}{2} \int_0^\beta d\tau \sum_{ij} J_{ij}^\alpha M_i \cdot M_j. \tag{16}
\]

This functional satisfies the Polchinski equation \[40\],

\[
\partial_\Lambda \mathcal{F}_\Lambda[M] = \frac{1}{2} \int_0^\beta d\tau \sum_{ij,\alpha} \left( \partial_\Lambda J_{ij}^{\alpha,1} \right) \left[ \frac{\delta^2 \mathcal{F}_\Lambda[M]}{\delta M_i^\alpha(\tau) \delta M_j^\alpha(\tau)} + \frac{\delta \mathcal{F}_\Lambda[M]}{\delta M_i^\alpha(\tau)} \frac{\delta \mathcal{F}_\Lambda[M]}{\delta M_j^\alpha(\tau)} \right] + \frac{1}{2} \text{Tr} \left[ J_{ij}^\alpha \partial_\Lambda J_{ij}^{-1} \right]. \tag{17}
\]

where \( J_{ij}^{-1} \) is the matrix inverse of \( J_{ij}^\alpha \). The precise relation between our SFRG approach and the spin diagram technique developed by VLP \[29\] is established by

| \( D \) | \( T_c/T_{c0} \) for \( S = 1/2 \) | relative error in % |
|---|---|---|
| SFRG | \( \mathcal{O}(D^{-1}) \) | benchmark | SFRG | \( \mathcal{O}(D^{-1}) \) |
| 1 | 0 | 0 | 0 | 0 | 0 |
| 2 | 0 | 0.50 | 0.57 | - | 12 |
| 3 | 0.744 | 0.79 | 0.752 | 1 | 5 |
| 4 | 0.839 | 0.85 | 0.835 | 0.5 | 2 |
| 5 | 0.880 | 0.89 | 0.878 | 0.3 | 1 |
| 6 | 0.904 | 0.908 | 0.903 | 0.2 | 0.6 |
| 7 | 0.920 | 0.923 | 0.919 | 0.1 | 0.4 |
the Legendre transform $\Phi_{\Lambda}[h]$ of $F_{\Lambda}[M]$, which satisfies a flow equation similar to Eq. (11) and is well defined even for vanishing exchange interaction $\Lambda$. In fact, in a scheme where $J^0_{ij} = 0$, the initial vertices generated by $\Phi_0[h]$ can be identified with the generalized blocks introduced in Ref. [27]. These have a non-trivial frequency dependence [26, 27] reflecting the commutation relations between the components of $S_i$ at a given site. For finite $\Lambda$, the functional $\Phi_{\Lambda}[h]$ generates the part of the connected spin correlation functions which is irreducible with respect to cutting a single interaction line. For the two-point function this is precisely the irreducible self-energy calculated diagrammatically by VLP [28], see also Ref. [27]. In fact, by appropriately truncating the hierarchy of flow equations for the vertices generated by $\Phi_{\Lambda}[h]$ we can recover, for example, the expansion for the longitudinal spin-spin correlation function given by VLP [29]. Moreover, in contrast to the perturbative approach of VLP, with a suitable truncation [22, 23] our SFRG can also describe the critical regime.

Summary and outlook. The main result of this work is the insight that the generating functional of the connected time-ordered spin correlation functions and the associated generating functional of the irreducible vertices of an arbitrary quantum spin system satisfy exact flow equations, which are formally identical to the corresponding equations of interacting bosons. The $SU(2)$ spin algebra is taken into account via a non-trivial initial condition involving vertices of arbitrary order. At this point the full potential of our method has not been explored, but our preliminary results [38] are rather promising and indicate that the SFRG is a powerful analytical approach to quantum spin systems. Moreover, our method can be easily generalized to any Hamiltonian which can be expressed in terms of local operators satisfying a non-trivial algebra such as Hubbard X operators [11].

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