A Self-Energy Functional Approach for Spin Systems

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Abstract. We set up a new approach to study the physics of spin systems which uses the resolvent method originally proposed by Keiter and Kuramoto. In analogy to the Baym-Kadanoff formalism the latter introduced the partition sum of a system as a functional of the resolvent of the Hamiltonian and its so called generalized self-energy. This functional is the starting point for a variational cluster method which is based on Potthoff’s self-energy functional approach. In a first step we apply our ansatz to a Heisenberg spin chain.

1. Introduction

In many cases, magnetic materials can be well represented by models of localized spins interacting via an exchange interaction [1]. The simplest of such models is the Heisenberg model [1]:

\[ H = \sum_{i,j} \vec{S}_i \cdot \vec{J}_{ij} \cdot \vec{S}_j - \sum_i \vec{B}_i \cdot \vec{S}_i , \]  

(1)

where we allow for an anisotropic exchange interaction \([J]_{\alpha \beta} = J_{\alpha \beta}\) with \(\alpha, \beta \in \{x, yz\}\) and introduce a possibly site dependent magnetic field. The physics is well-known for the one-dimensional case [2] and for dimensions \(D \geq 4\), where a Weiss mean-field theory is applicable [3]. Moreover, for nearest-neighbor exchange and simple lattices one can use highly efficient Monte-Carlo simulations to investigate the static and dynamic properties of the model (1).

The challenging problems are the so-called frustrated systems. The latter are e.g. realized for triangular lattices or longer-ranged exchange interaction. Here, Monte-Carlo is plagued by a severe sign problem and reliable results for low-temperature properties cannot be obtained. Furthermore, it is often desirable, in addition to numerical data, to have access to analytical results that give hints about the physical processes behind a certain behavior. Typically, these are obtained within mean-field and spin-wave calculations, i.e. perturbational approaches [4].

For itinerant fermions a quite different approach has been proposed recently by Potthoff [5], who used the representation of the free energy as the Luttinger-Ward-Baym-Kadanoff functional [6] to set up a scheme where the interaction is treated exactly for a small, manageable cluster while the cluster parameters are chosen such that the free energy of the lattice is minimized. This allows to create well-defined approximations, one of them being the dynamical mean-field theory [5].

The method introduced by Potthoff strongly relies on the possibility to represent the free energy as a functional of the self-energy with the interaction part strictly separated from the non-interacting part. This property in turn is based on the linked-cluster theorem involving Wick’s theorem or equivalently standard commutation relations among the operators constituting the
non-interacting system [7]. Spin operators, however, form another algebra, and so the standard formalism does not work. There do exist approaches to reconcile this deficiency, via a spin diagram technique [8] or via bosonization of the spin operators [9]. However, attempts to find a suitable expression for the free energy as a functional of spin-propagators up to now led to no results due to fundamental mathematical difficulties which are either related to the definitions of the propagators or simply the necessary proper projection onto the physical Hilbert space.

2. Variational cluster approximation for spin systems

Here we want to propose another approach, based on a resolvent technique devised for Hamiltonians involving operators which do not obey the standard boson or fermion algebra. It uses the full resolvent of the Hamiltonian and the partition function instead of the free energy [10].

Following Kuramoto [11], the partition function of a system with Hamiltonian $H$ can be written as the functional

$$Z[R] - Z_0 = -\beta \Phi[R] + \beta \oint \frac{dz}{2\pi i} e^{-\beta z} \text{Tr} [(z - H_0)R - \ln((z - H_0)R)]$$

of the resolvent $R$ of $H$, with $H_0$ denoting some suitably chosen “non-interacting” system. Note that we put the term “non-interacting” in quotation marks as $H_0$ can actually contain interactions. The only sensible requirement is that the problem defined by $H_0$ should be easier to solve than the full Hamiltonian.

We now introduce a functional $F[\Sigma]$ as the Legendre transform of $\Phi[R]$ to write $Z$ as a functional of the generalized self-energy $\Sigma$. The stationary point $\frac{\delta Z[\Sigma]}{\partial \Sigma} = 0$ delivers the exact self-energy. Following Potthoff’s idea we next consider a reference system $H'$ which has the same interaction part as $H$, but a less complex and solvable $H'_0(p')$, with $p'$ being some variational parameters. We can use the universality of $F[\Sigma]$ to eliminate this functional via combination of the partition functions $Z$ of $H$ and $Z'$ of $H'$. As our central approximation we now set the self-energy of the full system to be the self-energy of the reference system. In this way we transform the partition function $Z$ into a functional of $\Sigma'$:

$$Z[\Sigma'] - Z_0 = Z' - Z_0 - \beta \oint \frac{dz}{2\pi i} e^{-\beta z} \left[ \text{Tr} \ln \left( \frac{z - H_0}{z - H'_0 - \Sigma'} \right) + \text{Tr} \ln \left( \frac{z - H'_0}{z - H'_0 - \Sigma'} \right) \right]$$

Besides $H_0$ only quantities of the reference system appear in this new functional (2). The next step in our scheme is to determine a stationary point $\frac{\delta Z[\Sigma']}{\partial \Sigma'} = 0$ to find an approximate $\Sigma'$ that minimizes the free energy. $H'_0$ and $\Sigma'$ are depending on the variational parameters $p'$ so we can parametrize $Z$ with them. The variational principle then leads to the equations $\frac{\partial Z(p')}{\partial p'} = 0$ which are found to be:

$$0 = \oint \frac{dz}{2\pi i} e^{-\beta z} \left[ \text{Tr} \left( \frac{1}{z - H'_0 - \Sigma'} \frac{\partial \Sigma'}{\partial p'} \right) - \text{Tr} \left( \frac{1}{z - H'_0 - \Sigma'} \frac{\partial \Sigma'}{\partial p'} \right) \right]$$

From this we can determine the variational parameters as functions of the original model parameters of $H$. With the resulting $\Sigma'$, which fulfills the variational principle, we find an approximate resolvent and can compute the corresponding approximation to the partition function respectively the free energy.
3. Discussion and summary

The general scheme constructed in the previous section at least in principle allows to generate systematic approximations for arbitrary spin systems. Our first goal is to apply this scheme to a $S = 1/2$ isotropic Heisenberg model, i.e. $\mathbf{J} = J \mathbf{1}$. To this end we first have to specify possible reference systems. Following Potthoff’s suggestion, we split the original spin system into several identical clusters with extra spins (external degrees of freedom) attached to them. By this procedure we of course enlarge the Hilbert space of the reference system, i.e. we need to trace out the states of these external spins. We will come back to the possible clusters further below.

The second decision we have to make is how to break the Hamiltonian (1) into a ‘non-interacting’ part and an interaction. One possibility of course is to treat the full Heisenberg exchange as the interaction and the magnetic field as the non-interacting system. This at first sight rather intuitive idea turns out to be not very reasonable, because it leads to a trivially fullfilled variational principle (3); our approximate system would just be the collection of separated clusters. Alternative choices are to take the Ising part of (1) to be the non-interacting Hamiltonian and the $XY$-terms to be the interaction or vice versa. Apparently, with this more reasonable choice of $H_0$ one ends up in a quite demanding calculation already at this stage, practically limiting the actual size of the system to which we can apply the variational equation (3). A good choice of the clusters can reduce the computational effort, but the general limitation remains.

As simplest case let us apply the scheme to the one-dimensional, isotropic Heisenberg chain with $S = 1/2$ and the Ising part as $H_0$. As this system is extremely well understood, we have a good handle on judging the quality of results obtained. First, we split the chain into suitable clusters. We then have the freedom of adding extra spins which are coupled via a variational parameter $J'_z$ to the cluster spins. Figure 1 shows examples of clusters for a chain.

As a test we examined a reference system consisting of two-spin clusters of type d) (see Fig. 1), were both spins are coupled to one additional spin via the variational parameter $J'_z$. With this cluster the further computations are easier than with other choices. Obviously, equation (3) always has the trivial solution $J'_z = 0$. As long as $\beta J \lesssim 2.04$ this actually remains the only solution, meaning that spin dimers coupled via an Ising interaction represent the best approximation in the chosen subspace of auxiliary models. For $\beta J \gtrsim 2.04$ we in addition find a hyperbola-like branch of solutions with $J'_z \neq 0$.

In Fig. 2 we compare the approximate free energy with the exact free energy of a four-spin-system with open boundary conditions. For the ferromagnetic Heisenberg model ($J < 0$) we only have the solution $J'_z = 0$. Our approximation obviously does not describe the original system very well due to the neglect of long-ranged spin fluctuations [2], which we completely ignore in our approach. In the antiferromagnetic case $J > 0$ the approximation fits quite well for high temperatures or low interaction strength, where again the only solution is $J'_z = 0$. This means that a system of independent dimers represents a reasonable approximation, which to some extent supports attempts to use dimers as a starting point of perturbational approaches for the antiferromagnetic Heisenberg model. Apparently, our approximation starts to deviate considerably for lower temperatures or strong interactions, which again can be understood by

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**Figure 1.** Different cluster models for the spin chain a) with interaction $J$ and variational parameters $J'$. Examples for one-spin clusters are given in b). Part c) and d) show possible two-spin clusters.
the neglect of the long-ranged fluctuations dominant in a one-dimensional system.

To summarize, we have presented a self-energy variational approach for spin systems based on a resolvent technique for the partition function. It turns out that in contrast to similar theories for itinerant fermions, the present approach is not as straightforward concerning a proper choice of a 'non-interacting' part of the Hamiltonian and of the cluster break-up of the system. We discussed first results for the most simple implementations on a four-site chain. There it turns out that single-site clusters are trivial, while two-spin clusters are already very demanding and the results not very convincing so far. Work is in progress to see if one can improve on that with different cluster choices or increasing system sizes.

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