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Relaxation in the $s = \frac{1}{2}$ isotropic Heisenberg chain at $T = \infty$: towards a simple intuitive interpretation

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Abstract

This work reports a significantly improved estimation of the on-site dynamical spin pair correlation function in the $s = \frac{1}{2}$ isotropic Heisenberg chain at $T = \infty$ with respect to an earlier study (Phys. Rev. B 46 (1992) 14617) which has received some attention in the literature. The calculations have been performed using a recently developed technique for estimating unsolvable infinite continued fractions which are relevant for calculating the relaxation functions. This improvement became possible due to an important advance in the machine based computation of quantum mechanical commutators by M. Böhm and H. Leschke (Physica A 199 (1993) 116). The work reported here builds on the results of Böhm and Leschke and provides new predictions on the behavior of the on-site dynamical spin pair correlation function. This work also provides insights into possible ways to qualitatively understand the complex relaxation at high temperatures associated with a hermitian operator $A(t)$ in a system described by a hermitian Hamiltonian $H = H_0 + H_1$, where none of these three operators commutes with one another.

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1. Introduction

The study of the dynamical spin pair correlations and the corresponding spectral functions for the $s = \frac{1}{2}$ Heisenberg chain is an area of fundamental importance in developing theories of magnetic relaxation. These quantities are not known *exactly* at any temperature. The dynamical structure factor, $S(\boldsymbol{k}, \omega)$, where $\boldsymbol{k}$ and ω are the wave vector and the frequency, respectively, for this system at temperature $T = 0$ has been carefully studied theoretically [1,2], simulationally [3] and, very recently, experimentally [4]. It is generally believed that excellent correspondence exists between theory, simulation and experiment at $T = 0$ [4]. At present, the situation is quite different when one considers theoretical analysis at $T > 0$ for which the dynamical correlations and structure factors

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appear not to be known at all with any certainty [5,6]. To acquire an understanding of relaxation processes in this temperature regime we focus upon the dynamical correlations at $T = \infty$ [7,8]. As is well known, all the energy states are equally weighted at $T = \infty$. Hence, the spin dynamics is typically very rich at such high temperatures.

This work is a significant extension of an earlier set of calculations due to Sen and Long [7] on the on-site dynamical spin pair correlations in the Heisenberg chain at $T = \infty$. That work and some related developments have recently stimulated some additional interest in the study of the dynamics of Heisenberg chains which has already seen enormous development since the discovery of high-temperature superconductivity. Given that the Heisenberg chain does not exhibit a phase transition, we assume that the relaxation behavior will possess the same general characteristics at all temperatures. Hence, we expect that our discussion on the details of the relaxation processes at $T = \infty$ will remain largely valid at finite temperatures.

The $s = \frac{1}{2}$ isotropic Heisenberg chain is described by

$$H = -2J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z), \tag{1}$$

where $S_i^\alpha \equiv \frac{1}{2}\hbar\sigma_i^\alpha$, with σ_i^α the Pauli matrices at site i. In all that follows we set $\hbar \equiv 1$ and can safely regard $N \to \infty$. The reader may recall that the first two terms on the right hand side of Eq. (1) describe the isotropic XY part of the interaction while the third term on the right hand side represents the Ising part of the interaction.

The goal of this work is to study the temporal behavior of the fundamental dynamical correlation function of the system described by Eq. (1), namely, $\langle S_j^x(t) S_j^x(0)\rangle / \langle (S_j^x(0))^2\rangle$, where j is a site index denoting *any* bulk spin. We shall discuss a significantly more sophisticated calculation of the dynamical spin pair correlation function compared to the study in Ref. [7]. The results reported here not only extend the work in Ref. [7] but go beyond the predictions in the recent authoritative study by Böhm and Leschke [9,10] using a very different approach to compute the relaxation functions. These discussions will be followed by an attempt to draw connections between the corresponding relaxation function in the $s = \frac{1}{2}$ isotropic XY and Ising chains and the one in the composite Hamiltonian above. We shall close with a discussion on what this rather well studied problem on quantum spin dynamics teaches us that may be relevant for studying related and more complicated Hamiltonians.

To accomplish our objective we shall exploit the Continued Fractions Formalism [11,12,7,13-16] which is described briefly in Section 2 (for more details the reader is referred to Section II of Ref. [7]). Some of the key results of the earlier study in Ref. [7] are sketched in Section 3. This section offers a relevant first step for developing the presentation of the improved calculations and the new interpretation of the results which appear in Section 4. Section 5 summarizes the present work and discusses how this study could be helpful in understanding related dynamical systems.

2. Formalism

The fundamental equation describing the time evolution of some spin operator, say S_j^x, is the Heisenberg equation of motion,

$$\frac{dS_j^x(t)}{dt} = i[H, S_j^x(t)], \tag{2}$$

and the formal solution to Eq. (2) is

$$S_j^x(t) = \exp(iHt) S_j^x(0) \exp(-iHt) = \sum_{n=0}^{d-1} a_n(t) f_n, \tag{3}$$

where $\{f_n\}$ is a complete set of orthogonal basis vectors in a Hilbert space defined by

$$(f_n, f_m) = \left(\langle f_n f_m^\dagger \rangle - \langle f_n \rangle \langle f_m^\dagger \rangle\right) \delta_{nm}, \tag{4}$$

where $\langle \cdot \rangle$ represents the canonical ensemble average. Choosing $f_0 = S_j^x(0)$ and imposing Eq. (4) allows one to generate $\{f_n\}$ via the recurrence relation [11]

$$f_{n+1} = i[H, f_n] + \Delta_n f_{n-1}, \qquad 0 \leq n \leq (d-1), \tag{5}$$

where

$$\Delta_n \equiv (f_n, f_n)/(f_{n-1}, f_{n-1}), \qquad 1 \leq n \leq (d-1), \tag{6}$$

and $f_{-1} \equiv 0$. With $\{f_n\}$ known, Eq. (3) substituted into Eq. (2) yields $\{a_n(t)\}$. The choice $f_0 = S_j^x(0)$ implies $a_0(t) = \langle S_j^x(t) S_j^x(0) \rangle / \langle (S_j^x(0))^2 \rangle$. It is possible to show that the Laplace transform of $a_0(t)$, $a_0(z)$ can be written as [11,12]

$$a_0(z) = 1/z + \Delta_1/[z + \Delta_2/(z + \Delta_3/\{z + ...\})], \tag{7}$$

where typically the right hand side of Eq. (7) has an infinite number of terms [7]. Thus, studying $a_0(t)$ amounts to (i) obtaining as many Δ_n's as possible, and (ii) estimating Eq. (7) as accurately as possible based upon the available information.

3. Summary of earlier work

Previous studies on the dynamics of $s = \frac{1}{2}$ Heisenberg spin chains [5,6] have considered the first few (typically upto 8) moments or Δ_n's. The key difference between these studies and Ref. [7] and the present one lies in (i) the suggestion that the envelope of the relaxation function appears to have an overall exponential-like tail and (ii) the interpretation of the spectral function that has been attempted in Ref. [7] for the first time as far as we are aware of, has been significantly developed here. The work in Ref. [7] considered the first seven exact Δ_n's at $T = \infty$. Based upon that knowledge an extrapolation was constructed for all Δ_n's for $8 \leq n \leq \infty$. Then, using a recently developed and highly successful method of estimating Eq. (7) (described in Ref. [17])

an approximate estimation of $a_0(t)$ was obtained. Regardless of the details of the extrapolation scheme chosen to approximate the higher Δ_n's, the envelope of the function $a_0(t)$ exhibited an overall exponential-like decay in time. The Fourier transform of $a_0(t)$ yields the spectral function $a_0(\omega)$. The spectral function obtained in Ref. [7] lends itself to a simple interpretation described below.

The spectral function calculated in Fig. 5 of Ref. [7] had a central peak and a broadened peak (better thought of as a shoulder to a central peak) centered near $2J$. To understand this result let us note the following. $a_0(t)$ at $T = \infty$ for the isotropic XY chain yields a Gaussian, $\exp(-J^2t^2)$, an exact result [20,21]. Also, $a_0(t)$ at $T = \infty$ for an Ising chain yields $\frac{1}{2}(1+\cos 2Jt)$, where $2J$ is the Ising coupling, also an exact result [22,23]. The isotropic Heisenberg chain Hamiltonian in Eq. (1) has equally important XY and Ising parts. Therefore, it is not unreasonable to expect that in a "zeroth order approximation" the spectral function of the Heisenberg chain at $T = \infty$ will possess a broad Gaussian structure (since the cosine transform of a Gaussian $a_0(t)$ is a Gaussian $a_0(\omega)$ [24]) along with a broadened Ising peak in the neighborhood of $2J$. As mentioned above, this is indeed what was reported in the study in Ref. [7]. It turns out that the results claimed in that study were robust against fine tuning of the details of the extrapolation scheme used to obtain the Δ_n's for $8 \leq n \leq \infty$. As we shall see below in more detail, this simplistic explanation for the spectral function of the Heisenberg chain captures some of the more important aspects of the apparently highly complex anharmonic relaxation processes in this model in the high temperature regime [19].

4. Present work

In spite of the apparent success of the simple-minded explanation above in interpreting the spectral function of the isotropic Heisenberg chain at $T = \infty$, one may wonder why it is that there is no "mixing" between the frequencies arising from the Ising and XY parts of the Hamiltonian in an anharmonic system such as this. Naively one would expect such "mixing" to be present in the spectral function. In what follows we show that indeed such "mixing" enters into the spectral function when a more extensive analysis than the one in Ref. [7] is carried out.

Our present calculations suggest that the effects of such "mixing" become apparent when relaxation at *larger length scales* is accurately probed and included in the calculation of $a_0(t)$. Such calculations are extremely difficult in practice. The difficulties are rooted in ones inevitably limited ability to evaluate deeply nested quantum mechanical commutator brackets involving the Pauli operators in a reasonable length of time. The key limitations arise from the rapidly growing sizes of the expressions for the higher $\{f_n\}$'s and computer memory limitations.

A recent important progress in machine based calculation of deeply nested quantum mechanical commutators by Böhm and Leschke [10,9] has resulted in a calculation of the exact coefficients to order time t^{30} of the short time expansion of $a_0(t)$ at $T = \infty$.

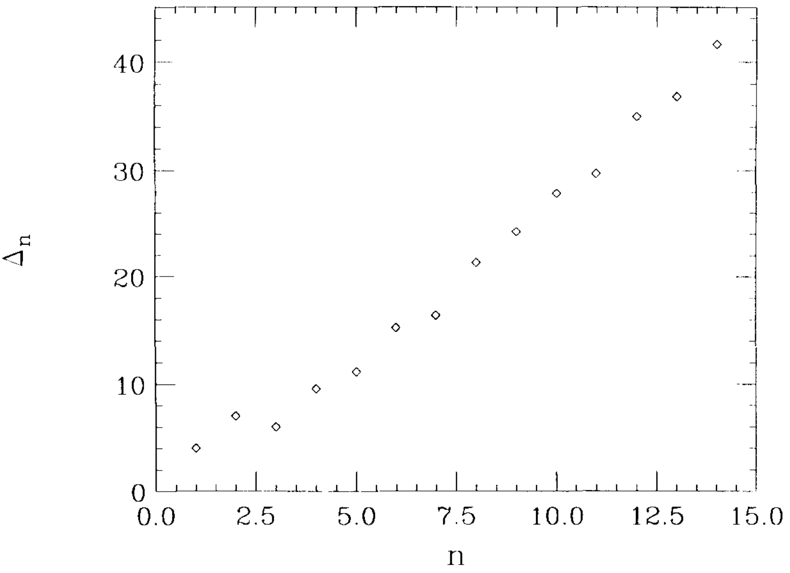

Fig. 1. Plot of Δ_n versus n for the $s = \frac{1}{2}$ isotropic Heisenberg chain at $T = \infty$. The data points for $8 \leq n \leq 15$ have been communicated to the author by Dr. Markus Böhm. The extrapolation scheme used to approximate Δ_{16} through Δ_∞ is $\Delta_n = \frac{10}{3}(n - 15) - 5.83333$. A linear fit is the most reasonable one for the data shown. The behavior of Δ_n versus n is perfectly linear for an isotropic XY chain at $T = \infty$.

This means that it is now possible to obtain, for the first time, the first fifteen exact Δ_n's for the system under study [25]. In what follows we present calculations using the Böhm–Leschke Δ_n's for $1 \leq n \leq 15$ and extrapolated ones for $16 \leq n \leq \infty$ [10,9]. The behavior of these Δ_n versus n and that of Δ_n/n versus $1/n$ and the extrapolation scheme used for the calculation of $a_0(t)$ are presented in Figs. 1 and 2. Comparison with the results in Figs. 1 and 2 of Ref. [7] reveal that the present extrapolation is rather different than the one previously used.

Clearly, we expect that the exact knowledge of the propagation or spreading of an excitation in the Heisenberg chain over larger length scales will reveal more information about the frequencies characterizing the relaxation processes. It turns out that this expectation comes through. Knowledge of Δ_{15} basically means that we have exact information of how spins which are fifteen spins apart from some initial perturbed spin participate in sharing that excitation and in conveying it to the spins which are sixteen spins apart from the initial perturbed spin. For an exact calculation in a quantum spin system discussing this aspect see Ref. [16]. The results for $a_0(t)$ and $a_0(\omega)$ obtained via the direct summation method of estimating the infinite continued fractions (described in Ref. [17]) using the Böhm–Leschke Δ_n's are presented in Figs. 3–5. The dotted lines represent results from the earlier calculations of Ref. [7].

Let us first look into the dynamical spin pair correlation function $a_0(t)$. The plot of $a_0(t)$ versus t in a linear scale (Fig. 3) shows that the present calculations agree with Fig. 1 of Ref. [9] up to $Jt = 3.5$ (which is the maximum time for which the calculations have been reported by Böhm and Leschke). It also demonstrates that

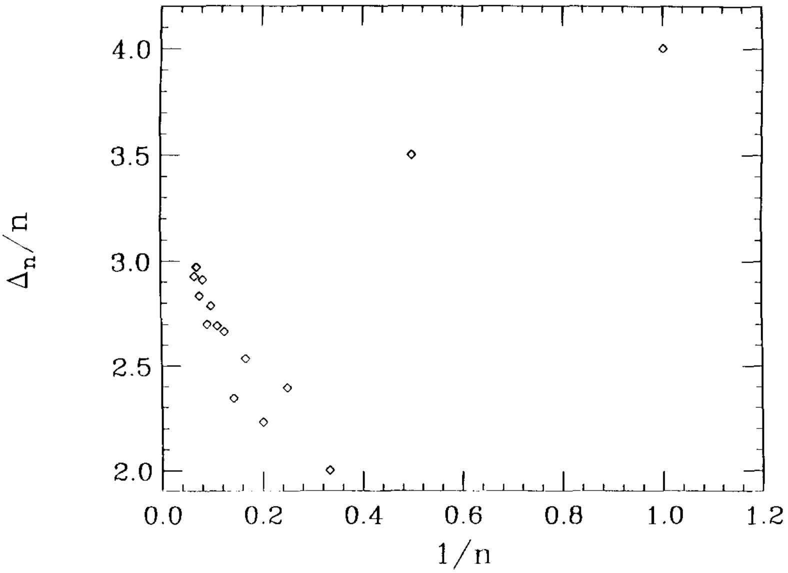

Fig. 2. Plot of Δ_n/n versus $1/n$. This plot provides an easy way of estimating the slope of the extrapolated line.

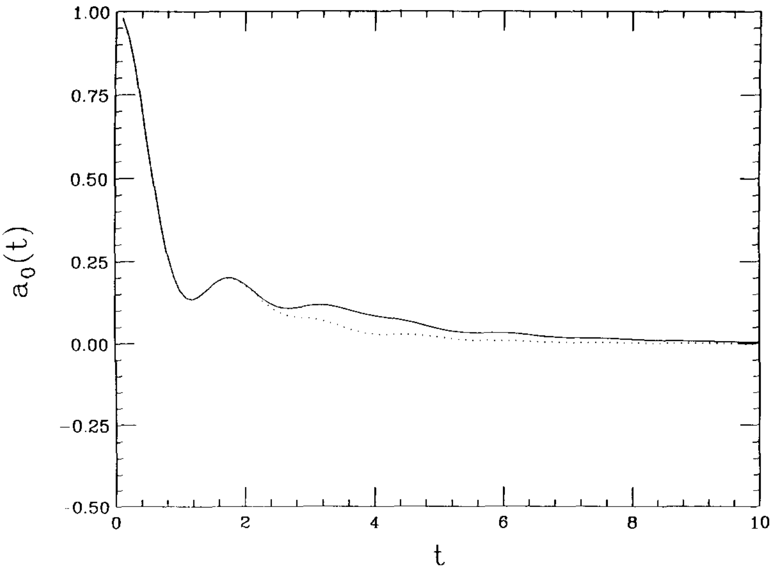

Fig. 3. Plot of $a_0(t)$ versus t. The solid line represents data from present work while the dotted line shows the earlier result of Ref. [7] for comparison.

the direct summation method of approximating continued fractions [17] provides a prediction, based upon the extrapolation scheme used to approximate Δ_n's for $n > 15$ at $Jt > 3.5$ (see Fig. 1 and its caption for details). Our tests using extrapolation schemes with slopes and intercepts differing by a few percent does not lead to any significant

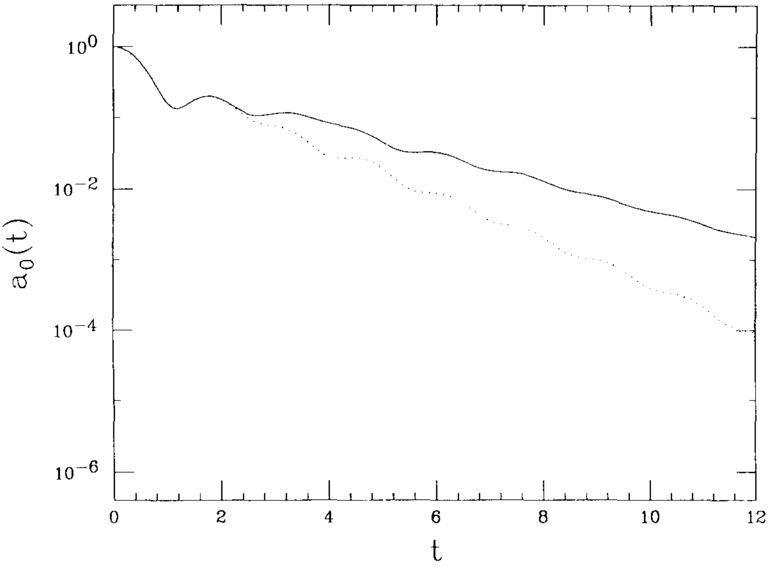

Fig. 4. Plot of $a_0(t)$ on a log scale versus t on a linear scale to demonstrate the negative exponential-like decay of $a_0(t)$.

changes in the magnitude of $a_0(t)$ for $Jt > 3.5$. This indicates that the behavior of $a_0(t)$ predicted here is robust.

Fig. 4 presents a plot of $a_0(t)$ on a semi-log scale with the intention to explore whether the envelope of the relaxation function shows an overall negative exponential-like tail. Our analysis using the data shown in Fig. 4 strongly suggests that the envelope of the relaxation function has a negative exponential-like form with the exponent being 0.47. This figure is significantly different from the earlier prediction in Ref. [7] which was 0.77. The significant correction to this exponent bears testimony to the fact that an enormous amount of information regarding the relaxation process at larger length scales is contained in the present analysis. This statement is consistent with the point that modifications in the upper levels of an infinite continued fraction (or a large but finite continued fraction) as in Eq. (7) affect the relaxation function more significantly than corrections in the deeper levels (see [18]). This is also the reason why changes of a few percent in the slope and the intercept of the linear extrapolation formula typically have little effect on relaxation functions for which the continued fraction representations are quickly convergent (as is the case for all continued fractions of the form of Eq. (7) with linearly growing Δ_n's as a function of n [17]). Further, the new results exhibit a well-defined negative exponential-like behavior that is to be contrasted to the mere suggestion of possible negative exponential-like behavior which emerges from Figs. 3 and 4 in Ref. [7].

In the new result in Fig. 5, instead of a single broadened maximum near the Ising frequency one finds two broadened maxima, one at $\omega \approx 1.5$ and another at $\omega \approx 3.2$ (solid line). Instead of a single broadened maximum at $\omega \approx 2.5$ (dashed line), there

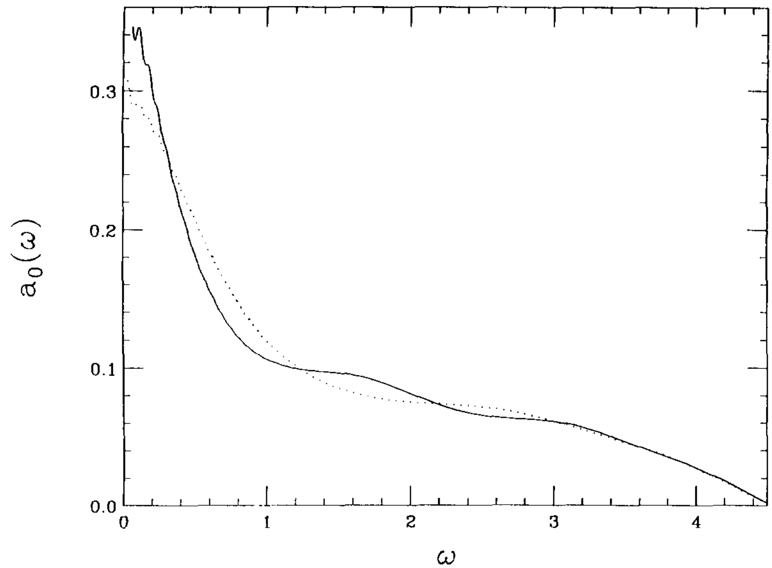

Fig. 5. Plot of $a_0(\omega)$ versus ω. The solid line shows present calculations while the dotted line represents calculations given in Ref. [7]. The irregularities at $\omega \to 0$ enter from limitations in performing a numerical cosine transform of $a_0(t)$ for large times.

now exists a dip in the neighborhood of that frequency. As in most systems involving strongly anharmonic dynamics it is nontrivial to interpret the precise origins of the above mentioned maxima at $\omega \approx 1.5$ and at $\omega \approx 3.2$. However, a simple-minded explanation appears to be consistent with the maxima arising from "mixing effects" between the Ising modes and the *XY* modes. Thus, possibly, the effects of incorporating dynamics at larger length scales is to introduce overdamped "beating effects" between the highest Ising and the zero frequency modes arising from the Ising and *XY* parts of the Hamiltonian in Eq. (1).

5. Significance and summary

It remains to be tested whether or not the simple-minded interpretations of the relaxation processes in systems described by the spin Hamiltonians of the form $H = H_0 + H_1$ offered in Ref. [7] and further elaborated upon in this work are correct and whether such interpretations are also possible at low temperatures and near the critical point for systems exhibiting phase transitions. Also, how possibly do the weights of the contributions from different parts of the Hamiltonian work out for anisotropic systems? It seems very clear that for the simple-minded ideas put forth here to work one must be dealing with systems for which at least one of the parts of the Hamiltonian must exhibit ergodic dynamics [26] and that the dynamical variable should not commute with either H_0 or H_1. To see the former point observe that the Gaussian relaxation of the *XY* chain alluded to above cannot be thought of as arising from the two Ising parts, each of which introduces purely non-ergodic dynamical behavior [22,23,26]. The latter point is meaningful for instance within the context of studying $\langle S_j^z(t) S_j^z(0)\rangle / \langle (S_j^z(0))^2\rangle$ for the strongly anisotropic Ising–Heisenberg chain described by $H = -2J\sum_{i=1}^{N} [S_i^z S_{i+1}^z + \alpha(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)]$, where $\alpha \to 0$. In this system, S_j^z commutes with the Ising part of the Hamiltonian above and the dynamics at short time scales is determined purely by the *XY* part of the Hamiltonian however weak that might be. The relaxation appears to be exponential-like [8] with very low frequency oscillations in this system at intermediate time regimes at $T = \infty$. The precise asymptotic behavior of the relaxation function is unknown for this system at the present time. Clearly, a great deal more needs to be done for similar quantum spin systems and other systems to check whether these ideas hold up. Such work is in progress.

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The reader may note that in estimating infinite continued fractions one usually replaces the infinite

continued fraction by a finite continued fraction with a very large number of levels. The number of levels needed for a good estimate depends upon the behavior of Δ_n versus n in a given continued fraction. Accurate results are obtainable with about 10^4 levels when Δ_n increases approximately linearly with n. Typically, keeping 10^4 levels is adequate for most many body spin Hamiltonian based studies when studied up to relatively long times, where typically long means $Jt \sim 100$. More levels may be needed for some problems. For an especially challenging problem see:
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[26] It appears to be much more complicated to understand the entry of an infinite number of frequencies arising from coupling between two parts of a Hamiltonian where each part yields non-ergodic dynamics, i.e., dynamics characterized by a finite number of frequencies. We do not attempt to provide a simplistic interpretation of the mixing of modes for this class of problems. It is, however, somewhat simpler to probe the dynamical process in which a set of characteristic frequencies mix with some central peak as has been attempted in this work. The deviations from the exact locations of the peaks in the spectral function of the system described by the full Hamiltonian most likely occur due to the strong anharmonicities that characterize the dynamics in these problems (which, of course, have been swept under the rug here for the purposes of attaining a basic understanding of the dynamical problem).