Solving the Liouville Equation for Conservative Systems: Continued Fraction Formalism and a Simple Application

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There are very few formalisms available to solve the Liouville equation for energy conserved systems. The continued fraction formalism, introduced through the works of Zwanzig, Mori, Kubo, Lee, Grigolini and others is described here. A detailed discussion is presented on ways to apply the continued fraction formalism to solve for relaxation functions and for the dynamical variable itself for a simple and exactly solvable quantum spin system.

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I. INTRODUCTION

In solving every dynamical problem one must solve an appropriate equation of motion. Perhaps the most commonly encountered equations of motion are the Newton's equations for describing the dynamics of classical systems and the Heisenberg equation of motion for describing the dynamics of quantum mechanical systems. These two equations are referred to jointly as the Liouville equation [1]. The objective of this article is to present a detailed discussion of how to solve the Liouville equation.

The presentation is geared towards a typical beginning graduate student who has had some background in thermal physics, has seen the Gibbs-Duhem equation (i.e., the combined zeroth, first and second laws of thermodynamics) [2], has been introduced to the canonical ensemble in statistical physics [3] and has had exposure to introductory level quantum mechanics [4] as seen in most undergraduate curricula. The main motivation for this review is to introduce the continued fraction approach as a mathematical and computational tool for dynamical studies of systems that are often of interest in the context of statistical physics, condensed matter physics and materials science. Continued fraction method based approaches have been successfully employed by many authors a cross a period of some forty years in studies of dynamical response of magnetic, semi-conducting, superconducting and lattice systems as well as in liquids [5].

We do not address solving the Liouville equation with a time-dependent Hamiltonian in the system. Driven systems can exhibit far from equilibrium dynamics and hence must often be handled on an individual basis by directly attempting to solve the appropriate dynamical equation. Nor do we address systems in which particles can have relativistic speeds although such an extension of the present discussion may be possible. There are physical systems for which an equilibrium state cannot be guaranteed. Indeed an equilibrium state may not even exist in many systems [6, 8, 9]. Such "non-equilibrium" systems will not be addressed here. However, all other conservative systems, whether they are many body systems, few body systems or one body systems, with interactions that are linear and/or nonlinear, and for which there is an equilibrium state that can be defined, can be studied via the continued fraction formalism. This is precisely what we set out to do below.

Another point to keep in mind is that the continued fraction formalism is typically geared to study dynamical systems in all its detail. The method hence carries all possible dynamical information. Such details may not always be necessary when studying some problems, e.g., when studying the dynamics of particles in a fluid, where the time scale of motion of the fluid particles could be significantly faster than that of motion of the particles. To deal with systems with disparate time scales, one may wish to pursue a Langévin equation [7] approach instead of solving the complete Liouville equation. In the Langévin equation, one would replace the fluid with it's fast time scale dynamics effectively as a viscous medium that offers appropriate frictional effects. Alternately, the Hamiltonian may be suitably modified and the continued fraction formalism for solving the Liouville equation may be used to study the dynamical problem if one desires to carry some of the details of interactions between the fluid and the particles in our example.

The time evolution of some operator $A(t)$ (e.g., the spin at a site in a spin system or the velocity of a particle in a solid or liquid) in a system described by some time-independent Hamiltonian H is described via the Liouville equation as follows:

$$\frac{dA(t)}{dt} = iLA(t), \tag{1}$$

where L is the Liouville operator that carries information about the Hamiltonian of the system. The algebra of the operators used to describe the dynamics of the system also enter into the dynamical calculations. For classical systems, one writes

$$LA \equiv \{H, A\}_{PB} \equiv \sum_{i=1}^{N} \{ \frac{\partial A}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial H}{\partial q_i} \}, \tag{2}$$

where "PB" refers to Poisson's bracket and q_i and p_i refer to position and momentum of particle i in a system of N particles. For quantum systems on the other hand,

$$LA \equiv \frac{1}{\hbar}[H, A], \tag{3}$$

where the square bracket denotes a commutator bracket and $\hbar \equiv \frac{h}{2\pi}$ where h is the Planck's constant. The objective of this article is to describe a way to find $A(t)$. We will assume that the canonical ensemble partition function

$$Z = \sum_{E_n} \exp(-\beta E_n) = Tr\exp(-\beta H), \tag{4}$$

where E_n are the energy eigenvalues of H, $\beta = \frac{1}{kT}$, where k is the Boltzmann constant, T is the temperature of the system and Tr implies a Trace operation, which is the same as summing over the eigenvlues of the system. We will not place any other conditions on our approach.

Once $A(t)$ is known, the relevant dynamical quantities for the system can be obtained. The results can be checked by comparing with results obtained using a different method or perhaps via comparison with experiments, if such a comparison can be justified.

This article is organized as follows. In Sec. II, we outline the continued fraction formalism that allows one to construct a formal solution to $A(t)$. In Sec. III we explicitly work out a problem in which $A(t)$ is constructed and relaxation functions and even certain equilibrium quantities that can be obtained using the continued fraction formalism are worked out. Sec IV closes with a discussion on applications to other systems.

II. THE CONTINUED FRACTION FORMALISM

The formal solution to the Liouville equation can be written for quantum dynamical systems as follows:

$$\begin{aligned} A(t) &= \exp(iLt)A(t=0) \\ &= \exp(iHt)A(t=0)\exp(-iHt). \end{aligned} \tag{5}$$

However, explicitly writing out Equation (5) as function of time, as stated, amounts to performing a Taylor expansion in time. Such expansions tend to get algebraically very complicated and is often of limited value. Hence a Taylor expansion is often not a good way to address a dynamical problem across extended time scales. Particle dynamics based simulations, such as Molecular Dynamics simulations [10], are essentially Taylor expansion based approaches to iteratively evolve a system in time. We are interested in a way to get the behavior of $A(t)$, which is not necessarily expansion based.

We start off by picturing $A(t)$ as a vector in a d dimensional vector space (or as we shall later see, a Hilbert space), as below,

$$A(t) = \sum_{\nu=0}^{(d-1)} a_\nu(t) f_\nu, \tag{6}$$

where the right hand side (RHS) of Equation (6) states that, in general, $A(t)$ can be written in terms of some orthogonal basis vectors f_νs (i.e., completely independent of each other) and time-dependent scalar coefficients, $a_\nu(t)$s [11–13]. The dimensionality d of the vector space is dependent on H. We will talk about how d depends on H below. The picture to keep in mind is very similar to that of describing a vector in terms of unit vectors and associated scalar coefficients in a space of such vectors. The key difference here is that we have not assumed f_νs to be unit vectors. To define orthogonal vectors, it would now be necessary to impose a way to orthogonalize the f_νs.

Constructing orthogonal vectors is a routine problem in mathematical physics. Orthogonal vectors are usually constructed via the Gram-Schmidt process [14] that can be stated as follows. Suppose one has a complete set of vectors denoted by $\{g_1, g_2, \cdots, g_N\}$. Then a complete set of *orthogonal* vectors $\{h_1, h_2, \cdots, h_N\}$ is given by

$$h_n = g_n - \frac{(g_n, h_1)h_1}{(h_1, h_1)} - \frac{(g_n, h_2)h_2}{(h_2, h_2)} - \cdots, \tag{7}$$

where (,) denotes a scalar product. Thus, the scalar product of two vectors in any problem must be defined to generate an orthogonal set of vectors. But how does one choose a scalar product? It turns out that there is no unique choice. Depending upon the system under study, one would typically wish to choose scalar products that render the construction of an orthogonal set of $\{f_\nu\}$s as easy as possible. Thus, the choice of scalar product is an important step and directly affects ones ability to solve a problem.

Since most physical systems are not entirely isolated but are placed in an environment such that the system temperature T typically matters and since often one is interested in the temperature dependent behavior of a system, it is typically convenient to design a scalar product that somehow brings temperature into the problem. The basic thinking may be to rewrite Eq. (6) as follows,

$$A(t) = \sum_{\nu=0}^{(d-1)} a_\nu(t, \beta) f_\nu(\beta), \tag{8}$$

where β dependence can be brought in via the scalar product but $A(t)$ remains temperature independent. Mori and several workers adopted the susceptibility formula [15], which is basically a generalized fluctuation formula, as the scalar product. This quantity is often referred to in the literature as the Kubo scalar product.

One can define the Kubo scalar product of two vectors X and Y as follows,

$$(X,Y) \equiv \frac{1}{\beta}\int_0^\beta d\lambda \langle X(\lambda)Y^\dagger\rangle - \langle X\rangle\langle Y^\dagger\rangle. \quad (9)$$

where the canonical ensemble average of any operator $\mathcal{O}$ can be written as $\langle \mathcal{O}\rangle \equiv \frac{Tr\mathcal{O}\exp(-\beta H)}{Tr\exp(-\beta H)}$, and $X(\lambda) \equiv \exp(-\lambda H)X(\exp(\lambda H)$. Observe that $X(\lambda)$ looks similar to $A(t)$ as written in Equation (5). A simple way to connect the two is by assuming that time $t = -i\beta$ (which is often referred to as the "imaginary time transformation"). We will revisit this intriguing connection between t and β later. For the moment let us just note that the Boltzmann factor $\exp(-\beta H)$ and the time evolution behavior described in Equation (5) appear to have interesting similarities. It is instructive to note that in the limit $\beta \to 0$, i.e., as $T \to \infty$, Equation (9) reduces to the fluctuation formula, $(X,Y)|_{\beta\to 0} = \langle XY^\dagger\rangle - \langle X\rangle\langle Y^\dagger\rangle$. Thus, when working out many problems, it may be more convenient to use the fluctuation formula instead of the Kubo scalar product (or susceptibility formula) [16].

To construct a space of orthogonal vectors we must fix the first vector. This step is analogous to fixing the direction of the $x-$axis when drawing a right handed coordinate system with $x-$, $y-$ and $z-$ axes. At this point, one can make a connection between the work at hand, i.e., solving the Liouville equation and what one calls Linear Response Theory. In Linear Response Theory one imagines that the system has been given a small perturbation. The perturbation is so small that the energy of the system remains unaffected by the energy of the perturbation. We choose $f_0 = A(t=0) \equiv A$ in Equation (6). This choice allows one to describe the dynamics of $A(t)$ in a manner that directly connects with the evolution of operator $A(t)$ that evolves in time due to a perturbation. Further, $A(0) = A = (a_0(0)f_0 + a_1(0)f_1 + \cdots)$ implies that $a_0(0) = 1$ and $a_\nu(0) = 0$ for $\nu > 0$ and that for an orthogonal set of f_νs, $a_0(t) = \frac{(A(t),A)}{(A,A)}$ [17].

Once f_0 has been chosen, the Gram-Schmidt method can be used to orthogonalize the f_νs, for all $\nu > 0$. The scalar product to be used can be the Kubo scalar product defined by Equation (9) above. The Kubo scalar product satisfies the following properties: (i) $(X,Y) = (Y,X)$ and (ii) $(LX,Y) = -(X,LY)$. The derivation of these properties are shown in Appendix A. Properties (i) and (ii) above jointly imply that $(LX,X) = 0$ or $(\dot{X},X) = 0$, i.e., $\dot{X}$ is orthogonal to X. However, using properties (i) and (ii) it is a simple exercise to show that $\{X, LX, L^2X, \cdots, L^NX\}$ do not form a complete and mutually orthogonal set.

Gram-Schmidt orthogonality process tells us that if $f_0 = A$, then $f_1 = iLf_0$. Also, since as stated above, $(Lf_0, f_0) = 0$, f_1 is orthogonal to f_0. We must now find f_2. Let us first assume that $f_2 = iLf_1$. Since $(f_2, f_0) = 0$ and $(f_2, f_1) = 0$, it follows that for the choice of f_2 made, $(f_2, f_0) \neq 0$. To satisfy both of the orthogonality conditions we need to respect, we let $f_2 = iLf_1 + \psi$. The orthogonality conditions imposed on the new f_2 then require that $((iL)^2f_0, f_0) = -(\psi, f_0)$, $(\psi, iLf_0) = 0$ and $(\psi, f_0) = 0$. There are two non-trivial choices that satisfy the above conditions. These choices are: (i) $\psi = cA$ where c is some constant to be determined and (ii) $\psi = c'(iL)^2A$, where c' is some constant. Choice (ii) yields, $((iL)^2f_0, f_0) = -(\psi, f_0) = -c'((iL)^2f_0, f_0)$ or $c' = -1$, which also implies $f_2 = 0$. The choice $\psi = c'(iL)^2A$ violates the completeness requirement of the chosen Hilbert space by forcing the description of all physics into two dimensions (since $d = 2$). Thus, the only admissible choice is $\psi = cA$. For this choice, $((iL)^2f_0, f_0) = -(\psi, f_0)$, or $(\ddot{A}, A) = -(X, A)$, i.e., $c = -\frac{(\ddot{A},A)}{(A,A)} = \frac{(\dot{A},\dot{A})}{(A,A)} = \frac{(f_1,f_1)}{f_0,f_0)} \equiv \Delta_1$. If we now construct $f_3 = (iL)f_2 + \Delta_2 f_1$ where $\Delta_2 = \frac{(f_2,f_2)}{(f_1,f_1)}$, then it can be shown that $(f_3, f_0) = 0$, $(f_3, f_1) = 0$ and $(f_3, f_2) = 0$. The Gram-Schmidt orthogonalization process thus yields,

$$f_1 = iLf_0,$$
$$f_{\nu+1}(\beta) = iLf_\nu(\beta) + \Delta_\nu(\beta)f_{\nu-1}(\beta), \quad \nu \geq 1, \quad (10)$$

where $\Delta_\nu(\beta) \equiv \frac{(f_\nu(\beta), f_\nu(\beta))}{(f_{\nu-1}(\beta), f_{\nu-1}(\beta))}$. The quantities (f_ν, f_ν) (where the β dependence is no longer explicitly mentioned for purposes of brevity) represent the equivalent of the squared length of the basis vector f_ν in the Hilbert space that we have constructed via Equations (8) and (9). Hence, the Δ_νs represent the ratios of the length squared of successive basis vectors and in turn carry information about the "shape" of our Hilbert space (i.e., whether it is some high or even infinite dimensional "hypersphere" or something else). It will become evident in Section III that the Δ_νs carry information about equilibrium correlations in the system. Equation (10) is often referred to in the literature as Recurrence Relation I (RR I). As we shall see, RR I allows us to construct all the f_νs that are allowed by the system Hamiltonian H. These f_νs are, in general, temperature dependent. As we shall see below, when $d < \infty$, there are only a finite number of f_νs that are allowed in the system.

We are still far from having solved the Liouville equation. We must now construct a way to determine the $a_\nu(t, \beta)$. Once $\{f_\nu\}$ and $\{a_\nu\}$ are known, $A(t)$ can be formally obtained. It may be noted that since $A(t)$ is β independent, one may choose to carry out the study of RR I at any specific value of β that may be convenient for calculations, such as at $\beta \to 0$ or $T \to \infty$ or at $\beta \to \infty$ or $T \to 0$.

To obtain the $\{a_\nu(t)\}$, one must substitute Equation (8) into Equation (5) and insure that the f_νs are described by Equation (10) as follows,

$$\dot{A}(t) = \sum_{\nu=0}^{(d-1)} \dot{a}_\nu f_\nu = \sum_{\nu=0}^{(d-1)} a_\nu iLf_\nu$$

$$= \sum_{\nu=0}^{(d-1)} a_\nu f_{\nu+1} - \sum_{\nu=1}^{(d-1)} a_\nu \Delta_\nu f_{\nu-1}$$

$$= \sum_{\nu=1}^{(d-1)} a_{\nu-1} f_\nu - \sum_{\nu=0}^{(d-1)} \Delta_{\nu+1} a_{\nu+1} f_\nu$$

$$= \sum_{\nu=0}^{(d-1)} (a_{\nu-1} f_\nu - \Delta_{\nu+1} a_{\nu+1} f_\nu), \quad a_{-1} \equiv 0,$$

$$\sum_{\nu=0}^{(d-1)} \dot{a}_\nu(t) f_\nu = \sum_{\nu=0}^{(d-1)} (a_{\nu-1} f_\nu - \Delta_{\nu+1} a_{\nu+1} f_\nu). \quad (11)$$

or

$$\Delta_{\nu+1} a_{\nu+1} = -\dot{a}_\nu(t) + a_{\nu-1}, \quad (12)$$

which is referred to in the literature as Recurrence Relation II (RR II). Solving RR I and RR II allows one to completely solve the Liouville equation and construct a solution to A(t) in Equation (5). Observe that since $a_\nu(t = 0) = 0$ for $\nu > 0$ (see discussions between Equations (9) and (10) above) and since $a_{-1} \equiv 0$ (see Equation (11)), Equation (12) implies that $\dot{a}_0(0) = 1$, which is a result with an important consequence, namely that relaxation processes cannot be purely exponential in nature.

A close look at Equation (12) shows that by knowing $a_0(t)$, all $a_\nu(t)$ for $\nu > 0$ can be found. But Equation (12) does not readily reveal much about how to find $a_0(t)$. Recall that $a_0(t) = \frac{(A(t),A)}{(A,A)}$, is a physically meaningful quantity that describes how $A(t)$ "relaxes" to an equilibrium state at time t after the initial perturbation (that led to the time evolution process) was effected. When studying a non-equilibrium relaxation process against some equilibrium state, the relaxation function, $a_0(t)$, turns out to be a quantity of central importance (perhaps just about as important as the partition function itself in equilibrium statistical physics). Studying time evolution processes in interacting many body systems is a formidable task and indeed a handful of exact solutions are known. Thus, construction of a complete solution to the Liouville equation and hence complete knowledge of $A(t)$ is seldom possible [18–24, 27–30]. Yet, for all practical purposes, significant knowledge of relaxation processes in a system can be gained by constructing $a_0(t)$ alone. The primary goal of the continued fraction formalism is to construct $A(t)$. However, when such a goal seems mathematically insurmountable, constructing $a_0(t)$ only turns out to be the next best option. Fourier transform of $a_0(t)$ relates to experimentally accessible quantities of many body systems such as the dynamical structure factor or the dynamical susceptibility [31].

One way to recast Equation (12), i.e., RR II, in a way such that one may be able to find $a_0(t)$, is to take the Laplace transform of both sides. This step amounts to looking at frequency behavior in the problem instead of the time dependent behavior. However, there is no harmonic mode analysis involved in the process of taking the Laplace transform. The Laplace transform of $a_\nu(t)$ is written as

$$a_\nu(z) = \mathcal{T} a_0(t) = \int_0^\infty dt \exp(zt) a_\nu(t), \quad (13)$$

whereas the inverse Laplace transform is written as

$$a_\nu(t) = \mathcal{T}^{-1} a_\nu(z) = \frac{1}{2\pi i} \int_C dt \exp(zt) a_\nu(z). \quad (14)$$

The contour integral in Equation (14) runs to the right of the imaginary axis (the iy-axis) from $-i\infty$ to $i\infty$ and completes a semi-circle at infinity on the negative side of the real axis [32]. Laplace transform of RR II yields the two following equations

$$1 = z a_0(z) + \Delta_1 a_1(z), \quad \nu = 0 \quad (15)$$

$$a_{\nu-1}(z) = z a_\nu(z) + \Delta_{\nu+1} a_{\nu+1}(z), \quad \nu \geq 1, \quad (16)$$

Equation (15) can be written as

$$\frac{1}{a_0(z)} = z + \Delta_1 \frac{a_1(z)}{a_0(z)}, \quad \nu = 0 \quad (17)$$

whereas Equation (16) can be used to write,

$$\frac{a_0}{a_1} = \frac{1}{z} + \Delta_2 \frac{a_2(z)}{a_1(z)}, \quad (18)$$

or, carrying on as in Equation (18),

$$a_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cfrac{\Delta_3}{z + \; to \; (d-1)}}}}. \quad (19)$$

Solving the continued fraction in Equation (19) above solves the problem of determining $a_0(z)$. Once $a_0(z)$ is known, the inverse Laplace transform expressed in Equation (14) may in principle be used to obtain $a_0(t)$. RR II can then be used to find the entire set $\{a_\nu\}$ and combined with the knowledge of $\{f_\nu\}$ it becomes possible to construct $A(t)$.

As can be seen, $a_0(z)$ depends on the behavior of the Δ_νs. The temperature dependent Δ_νs in turn depend on equilibrium properties of the system. These equilibrium properties are typically assumed to be expressed in canonical or grand canonical ensembles.

One can see that $d < \infty$ and $d \to \infty$ are the two possible scenarios that one might encounter in constructing $\{f_\nu\}$. If it turns out that $f_d = 0$, then the series in Equation (6) closes and the Hilbert space becomes d dimensional with $d < \infty$. For $d < \infty$, $a_0(z)$ in the continued fraction in Equation (19) will have d levels and hence d poles. If d is odd, there is always a pole at $z = 0$. If d is even, then the pole at $z = 0$ will be absent. In all cases when $d < \infty$, Inverse Laplace Transform of $a_0(z)$ yields a solution with a finite number of terms, each with oscillatory time dependence. Since most interacting many body systems disperse the energy imparted in a perturbation, it is common to find $d \to \infty$ in most systems. We shall return to these remarks in the discussion following Equation (49) in Sec. III below.

When $d \to \infty$, as is the case for most systems, the continued fraction becomes an infinite continued fraction, i.e., one that does not terminate. Since continued fractions must be evaluated from the lowest level upwards, infinite continued fractions turn out to often be a challenge to handle, especially if the Δ_νs turn out to have some non-tractable pattern [32–36].

In most physical systems where $d \to \infty$, Δ_νs either tend to remain approximately constant or grow as ν increases [37–40]. These equilibrium quantities carry information about how the components (particles or spins or whatever are the objects that are used to describe the energetics of the system) of the system interact across all length scales. There is no bound on Δ_νs as constructed. So, the issue of how to calculate $a_0(z)$ boils down to the issue of how Δ_νs grow as function of ν. Studies show that there are broadly speaking two categories of behavior of Δ_ν versus ν, namely, $\Delta_\nu \sim \nu^\phi$ where (i) $0 \leq \phi < 2$ and (ii) where $\phi \geq 2$. For case (i) above, the infinite number of poles in Equation (19) can be accurately estimated by finite continued fractions with many levels (such as 10^3 or 10^4 levels) across desired time windows through which $a_0(t)$ is being sought. We can call these convergent continued fractions. However, for case (ii) above, the infinite continued fractions cannot be estimated via finite continued fractions through any meaningful time window of interest in the study of $a_0(t)$. We will call these non-convergent continued fractions [32]. By non-convergent what we mean is that one must take into account all the infinite levels in the continued fraction for constructing $a_0(t)$.

There may be connections between Hamiltonians that lead to non-convergent continued fractions and properties of systems that exhibit phase transitions, in particular, properties addressed by the so-called Yang-Lee theorem [41], which states that the phase transition properties of a system cannot be inferred by incomplete knowledge of the temperature dependence of the partition function, i.e., by estimating non-convergent partition functions via Taylor expansions [40].

Before we consider an example in which we can start with the Hamiltonian and end up constructing the formal solution to the Liouville equation using the continued fraction formalism, it is important to see that the Liouville equation can be written in a certain parametrized form, a form that is often seen in the literature and is known as the Generalized Langévin Equation (GLE). We start this discussion by first rewriting RR II (Equation (12)) as follows,

$$1 = za_0 + \Delta_1 a_1 = za_0 + \Phi a_0, \tag{20}$$

where

$$\Phi \equiv \Delta_1 b_1, \quad b_\nu \equiv \frac{a_\nu}{a_0}, \tag{21}$$

The inverse Laplace transform of Equation (20) yields the following,

$$\dot{a}_0(t) + \int_0^t dt' \Phi(t-t') a_0(t') = 0. \tag{22}$$

Since,

$$a_0^{-1} = (z + \Phi), \quad a_0^{-1} = \frac{b_\nu}{a_\nu}, \tag{23}$$

hence

$$b_\nu(z) = (z + \Phi) a_\nu(z), \quad \nu \geq 1. \tag{24}$$

The inverse Laplace transform of Equation (24) yields,

$$\dot{a}_\nu(t) + \int_0^t dt' \Phi(t-t') a_\nu(t') = b_\nu(t). \tag{25}$$

Multiplying Equation (22) by f_0 and Equation (25) by f_ν and summing over from $\nu = 0$ to $\nu = (d-1)$ yields the GLE,

$$\dot{A}(t) + \int_0^t dt' \Phi(t-t') A(t') = F(t),$$
$$\Phi(t) = \Delta_1 b_1(t) = \Delta_1 \frac{a_1}{a_0}. \tag{26}$$

The form of the GLE resembles that of Newton's equation. The term $F(t)$ on the right hand side is called the Generalized Random force, although, as is evident from the derivation of Equation (26), $F(t)$ is not a random quantity but a deterministic quantity. All the terms except $\dot{A}(t)$ are temperature dependent. The quantity $\Phi(t)$ is called the Memory function [42] and can be thought of as a force-force dynamical correlation function. Thus, $\Phi(t)$ is a term that carries the memory of interactions that enter into the evolution of the dynamical variable under study. If we assume $A(t)$ is velocity $p(t)$ and $\Phi(t-t') = -\gamma\delta(t-t')$, then Equation (26) becomes

$$\dot{p}(t) - \gamma p(t) = F(t), \tag{27}$$

which is often seen in the literature and called the Langévin equation [7]. The above special case, $\Phi(t-t') = -\gamma\delta(t-t')$, refers to systems in which memory of interactions is lost instantaneously; such a special case is defined to be the "stochastic limit." In systems with disparate time scales, such as a scenario where many fast moving particles weakly influence some large and slow moving particle, description via the stochastic limit may be a reasonable approximation. The quantity γ is a friction or drag coefficient.

III. APPLICATION: TRANSVERSE DYNAMICS OF ISING MODEL

To illustrate the application of the continued fraction formalism to a non-trivial, yet solvable problem, we consider the so-called "transverse dynamics" of spins in the Ising model [43] in one dimension. The model is described by the following Hamiltonian,

$$H = -J \sum_{i=1}^{N} S_i^z S_{i+1}^z, \tag{28}$$

where the $z-$components of the spins at each site interact with nearest neighbors via some coupling $-J$. Thus, the lowest energy state would be realized when all the spins are parallel to each other, meaning all are "up" or all are "down." If J in Equation (28) is negative, the ground state is the state where every adjacent spin is anti-aligned or anti-parallel. At finite temperatures, the system looks disordered with spins oriented randomly. The equilibrium behavior of the Ising model is well described in many texts (see for example Refs. [3, 44, 45]) and we encourage the reader to read this review with easy access to at least one of these texts. We will consider the Ising model with nearest neighbor interactions in one dimension here. Higher dimensional extensions of this study is mathematically more challenging but does not have a great deal of additional physics to offer. Higher dimensional studies (such as that of transverse dynamics in two and three spatial dimensions) has been sketched elsewhere [19, 25].

The Ising model is well known as one of the simplest models for magnetism [45]. In addition, the model is widely used for a wide array of applications to describe the physics of systems that involve characterizing each site via two possibilities (such as a set of empty sites and a corresponding set of occupied sites as in so-called *Lattice-Gas* models [44]).

We assume that there are N spins in the system. The system may be a ring, where there is periodic boundary condition, i.e., $S_{N+1}^z = S_1^z$. Other boundary conditions such as free ends or fixed ends may also be considered. For our purposes, the dynamics will turn out to have localized excitations. Hence, the details of the boundary conditions will affect the equilibrium averages but will not affect the dynamical behavior of the system. Each site has a spin and each site has two nearest neighbors, i.e., the coordination number $q = 2$. In this system we assume that the sites have quantum mechanical spins $S = \frac{1}{2}$. Thus, the number of spin states is $2S+1$, or two (i.e., one being up and one being down).

The spin operator $S_i^\alpha \equiv \frac{\hbar}{2}\sigma_i^\alpha$, where σ_i^α is the α component of the Pauli spin matrix at site i, α being x, y or z [45] and $\sigma_\alpha^2 = 1$ and hence $(S_i^\alpha)^2 = \frac{\hbar^2}{4}$. The commutation relations of these matrices lead to: $[S_i^x, S_i^y] = i\hbar S_i^z$, $[S_i^y, S_i^z] = i\hbar S_i^x$ and $[S_i^z, S_i^x] = i\hbar S_i^y$, and changing the order of the operators on the left hand side switches the sign on the right hand side in each case. Operators from different sites always commute. We henceforth set $\hbar = 1$ and proceed to use the continued fraction formalism to solve for the relatively simple dynamical problem at hand.

If one picks S_k^z as the dynamical variable and recalls that the dynamics of the operator S_k^z is dictated by the commutation relation between H and S_k^z, one can study the dynamics of S_k^z. It turns out that $[H, S_k^z] = 0$. So, S_k^z for any k is a *constant of motion*, i.e., the S_k^z operator has no dynamics. However, since $[H, S_k^\alpha] \neq 0$, for $\alpha = (x, y)$, S_k^x or S_k^y would be appropriate dynamical variables. To initiate dynamics of the S_k^α spin above in the Hamiltonian in Equation (28), one may introduce a perpendicular magnetic field $h_{perp} \neq 0$ for $t < 0$ but $h_{perp} = 0$ for $t > 0$. This field can be designed to couple with the x or the y components of the spins. Once h_{perp} is switched off, the system Hamiltonian is given by Equation (28) and it becomes possible to study the time evolution of the operator $S_k^\alpha(t)$.

We choose our dynamical variable to be $\sum_{k=1}^N S_k^x(t)$. Thus,

$$\begin{aligned} f_0 &\equiv \sum_{k=1}^{N} S_k^x, \\ (f_0, f_0) &= \sum_{k,l=1}^{N} (S_k^x, S_l^x) \\ &= \sum_{k=1}^{N} (S_k^x, S_k^x) \equiv \chi_{perp}. \end{aligned} \tag{29}$$

It is now possible to use Equation (10) and obtain

$$\begin{aligned} f_1 = \dot{f}_0 = i[H, f_0] &= -i[J \sum_{i=1}^{N} S_i^z S_{i+1}^z, \sum_{k=1}^{N} S_k^x] \\ &= -iJ \sum_{i,k=1}^{N} \{S_i^z [S_{i+1}^z, S_k^x] + [S_i^z, S_k^x] S_{i+1}^z\} \\ &= -iJ \sum_{i,k=1}^{N} \{iS_{k-1}^z S_k^y + iS_k^y S_{k+1}^z\} \\ &= J \sum_{k=1}^{N} \{S_{k-1}^z S_k^y + S_k^y S_{k+1}^z\}. \end{aligned} \tag{30}$$

The corresponding Kubo scalar product is

$$\begin{aligned} &(f_1, f_1) = \\ &J^2 \sum_{k,l=1}^{N} (\{S_{k-1}^z S_k^y + S_k^y S_{k+1}^z\}, \{S_{l-1}^z S_l^y + S_l^y S_{l+1}^z\}) \\ &= J^2 \sum_{k,l}^{N} \{(S_{k-1}^z S_k^y, S_{l-1}^z S_l^y) + (S_{k-1}^z S_k^y, S_l^y S_{l+1}^z) + \end{aligned}$$

$$(S_k^y S_{k+1}^z, S_{l-1}^z S_l^y) + (S_k^y S_{k+1}^z, S_l^y S_{l+1}^z)\}. \tag{31}$$

It can be shown (see Appendix B) that only the $k = l$ terms give non-vanishing contributions. Thus,

$$(f_1, f_1) = 2J^2 \sum_{l=1}^{N} \{\frac{1}{4}(S_l^y, S_l^y) + (S_l^y, S_{l-1}^z S_{l+1}^z S_l^y)\}. \tag{32}$$

The quantity Δ_1 defined below Equation (10) then becomes,

$$\Delta_1 = \frac{(f_1, f_1)}{(f_0, f_0)} = \frac{J^2}{2}[1 + 4\frac{\sum_l (S_l^y, S_{l-1}^z S_{l+1}^z S_l^y)}{\sum_l (S_l^x, S_l^x)}] = \frac{J^2}{2}(1 + 4\chi^*),$$
$$\chi^* \equiv \frac{\sum_l (S_l^y, S_{l-1}^z S_{l+1}^z S_l^y)}{\chi_{perp}}. \tag{33}$$

Proceeding as shown above,

$$f_2 = \dot{f}_1 + \Delta_1 f_0, \tag{34}$$

where

$$\dot{f}_1 = -iJ^2 \sum_{i,k=1}^{N} \{[S_i^z S_{i+1}^z, S_{k-1}^z S_k^y + S_k^y S_{k+1}^z]\}. \tag{35}$$

Using $[AB, CD] = AC[B, D] + A[B, C]D + C[A, D]B + [A, C]DB$, and $[S_k^\alpha]^2 = \frac{1}{4}$, we find,

$$\dot{f}_1 = -2J^2 \sum_{k=1}^{N} \{\frac{1}{4}S_k^x + S_{k-1}^z S_k^x S_{k+1}^z\}$$
$$f_2 = -2J^2 \sum_{k=1}^{N} \{\frac{1}{4}S_k^x + S_{k-1}^z S_k^x S_{k+1}^z\} + \frac{J^2}{2}(1 + 4\chi^*) \sum_{k=1}^{N} S_k^x$$
$$\Rightarrow f_2 = 2J^2 \sum_{k=1}^{N} (\chi^* S_k^x - S_{k-1}^z S_k^x S_{k+1}^z). \tag{36}$$

The scalar product (see Appendix B) then becomes

$$(f_2, f_2) = 4J^4 \chi((\frac{1}{4})^2 - \chi^{*2}), \tag{37}$$

and hence

$$\Delta_2 = \frac{J^2}{2}(1 - 4\chi^*). \tag{38}$$

The next step would be to calculate f_3, which is shown below,

$$f_3 = i[H, f_2] + \Delta_2 f_1,$$
$$\dot{f}_2 = i[H, f_2]$$
$$= -i2J^3 \sum_{i,k=1}^{N} ([S_i^z S_{i+1}^z, \chi^* S_k^x - S_{k-1}^z S_k^x S_{k+1}^z]), \tag{39}$$

We use these commutation rules that can be worked out for any number of operators to the right of the comma inside the bracket, $[AB, C] = A[B, C] + [A, C]B$ and $[AB, CDE] = ACD[B, E] + AC[B, D]E + A[B, C]DE + CD[A, E]B + C[A, D]EB + [A, C]DEB$ to find

$$\dot{f}_2 = 2J^3 \sum_{k=1}^{N} \{(\chi^* - \frac{1}{4})(S_{k-1}^z S_k^y + S_k^y S_{k+1}^z)\}$$
$$\Delta_2 f_1 = \frac{J^3}{2}(1 - 4\chi^*) \sum_{k=1}^{N} (S_{k-1}^z S_k^y + S_k^y S_{k+1}^z),$$
$$\Rightarrow f_3 = \dot{f}_2 + \Delta_2 f_1 = 0. \tag{40}$$

From a physical point of view, the vanishing of f_3 and hence of subsequent f_ν with $\nu > 3$ implies that it is no longer possible to construct orthogonal basis vectors for the given Hamiltonian. As one might expect, if the transverse field is kept alive in the Hamiltonian in Equation (28), then $f_3 \neq 0$. An infinite number of f_νs would then be generated. This problem can be solved at $T = 0$ [18] and at $T \to \infty$ [23].

Given $f_3 = 0$, $(f_3, f_3) = 0$ and hence $\Delta_3 = 0$. All the higher f_νs vanish from here onwards in *this* problem. Thus, the Hamiltonian and f_0 given by Equations (28) and (29), respectively, dictate that $d = 3$ in this problem (see d in Equation (6)). Thus, d, which is an important quantity in the dynamical calculations, is dictated by the nature of the Hamiltonian and the dynamical variable.

For finite d, the continued fraction in Equation (19) is finite and can be written as

$$a_0(z) = \frac{z^2 + \Delta_2}{z^3 + \Delta z}, \quad \Delta \equiv \Delta_1 + \Delta_2 = J^2. \tag{41}$$

and hence

$$a_0(t) = \frac{1}{2\pi i} \int_C dz \exp(zt) \frac{z^2 + \Delta_2}{z^3 + \Delta z}. \tag{42}$$

The integration in Equation (42) and those commonly encountered in analytic studies of this nature can be evaluated by the method of residues, as follows,

$$\lim_{z \to 0} z \frac{\exp(zt)(z^2 + \Delta_2)}{z(z^2 + \Delta)} = \frac{\Delta_2}{\Delta},$$
$$\lim_{z \to i\sqrt{\Delta}} (z - i\sqrt{\Delta}) \frac{\exp(zt)(z^2 + \Delta_2}{z(z - i\sqrt{\Delta})(z + i\sqrt{\Delta})} = \frac{\exp(i\sqrt{\Delta}t)(\Delta_2 - \Delta)}{-2\Delta},$$
$$\lim_{z \to -i\sqrt{\Delta}} (z + i\sqrt{\Delta}) \frac{\exp(zt)(z^2 + \Delta_2}{z(z - i\sqrt{\Delta})(z + i\sqrt{\Delta})} = \frac{\exp(-i\sqrt{\Delta}t)(\Delta_2 - \Delta)}{-2\Delta}. \tag{43}$$

Thus, one finds

$$a_0(t) = \frac{\Delta_2}{\Delta} + \frac{\Delta_2 - \Delta}{-2\Delta}(\exp(i\sqrt{\Delta}t) + \exp(-i\sqrt{\Delta}t)$$

$$= \frac{\Delta_2}{\Delta} + \frac{\Delta_1}{\Delta}\cos(\sqrt{\Delta}t). \quad (44)$$

Using RR II (Equation (12)), one can obtain $a_1(t)$ and $a_2(t)$. The results are:

$$a_1(t) = \frac{1}{\sqrt{\Delta}}\sin(\sqrt{\Delta}t), \quad (45)$$

and

$$a_2(t) = \frac{1}{\Delta}(1-\cos(\sqrt{\Delta}t)). \quad (46)$$

Equations (29), (30), (36), (40) and (44-46) completely solve for $\sum_{k=1}^{N} S_k^x(t)$. Observe that our results are unaffected by the upper limit of $\sum_{k=1}^{N}$ that goes with $S_k^x(t)$.

The calculations presented above reveal that for $d < \infty$, $a_0(t)$ will always be made up of a finite number of frequencies and hence will always be an oscillatory function. When $d \to \infty$, the number of poles diverges and $a_0(t) \to 0$ as $t \to \infty$. This problem is discussed for the transverse dynamics problem in the infinite lattice dimensional limit in Ref. [25].

Physically, when one or more *transverse* spins are "activated" by a perpendicular field in an Ising model, these spins are unable to transfer their energies to other sites. Thus, because of the simple nature of the Ising model, the localized energy at the perturbed sites causes the system to respond at two distinct frequencies. One of these frequencies is that resulting from the two Ising spins that border the perturbed region to the left and right being both "up" or both "down." This frequency equals $\sqrt{\Delta} = J^2$ and is basically the frequency unit in the problem. The other frequency corresponds to one of the bordering spins being "up" and the other being "down." This corresponds to the zero frequency mode that manifests itself as a constant term in the expressions for $a_0(t)$ and $a_2(t)$. If instead of an Ising model, one considers an XY model where the Hamiltonian $H = -J\sum_{i=1}^{N}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$, and sets $f_0 = S_k^z$, the perturbation energy no longer remains localized and spreads all over the chain. Thus for $N \to \infty$, one will be able to generate an infinite set of f_νs for such a system [46].

Most non-trivial physical systems exhibit $d \to \infty$. Further, even a one particle system placed in a heat bath (i.e., studied in the canonical ensemble), such as a simple classical oscillator in a nonlinear potential such as $V(x) = ax^4$, where a is some constant, generates $d \to \infty$. It is important to keep in mind that N does not have any simple relationship with d (see Sen *et al.* in [5]).

We now return to our Ising model problem and make a simple observation. The Boltzmann factor $\exp(-\beta E)$, which describes the contribution of some state with energy E when the system is at some temperature T, where $\beta = 1/kT$ and the solution to the Liouville equation given by Equation (5) have some mathematical similarities. If one makes the mapping $t \to -i\lambda$, where λ is the dummy variable for temperature, the result is

$$A(-i\lambda) = \sum_{k=1}^{N} S_k^x(-i\lambda) = a_0(\lambda)f_0 + a_1(\lambda)f_1 + a_2(\lambda)f_2. \quad (47)$$

But, $\chi_{perp.}$ given by Equation (9) can be written as,

$$\chi_{perp.} = \langle f_0.f_0\rangle\beta^{-1}\int_0^\beta d\lambda a_0(\lambda)$$
$$+\langle f_1.f_0\rangle\beta^{-1}\int_0^\beta d\lambda a_1(\lambda) + \langle f_2.f_0\rangle\beta^{-1}\int_0^\beta d\lambda a_2(\lambda), (48)$$

and hence

$$\chi_{perp.} = \langle f_0.f_0\rangle A_0 + \langle f_1.f_0\rangle A_1 + \langle f_2.f_0\rangle A_2, \quad (49)$$

where we find

$$A_0 = \beta^{-1}\int_0^\beta d\lambda[\frac{\Delta_2}{\Delta} + \frac{\Delta_1}{\Delta}\cosh\sqrt{\Delta}\lambda]$$
$$= \frac{\Delta_2}{\Delta} + \frac{\Delta_1}{\Delta}\frac{\sinh\sqrt{\Delta}\beta}{\sqrt{\Delta}\beta}, \quad (50)$$

$$A_1 = \frac{-i}{\beta\Delta}[\cosh\sqrt{\Delta}\beta - 1], \quad (51)$$

$$A_2 = \frac{1}{\Delta}[1 - \frac{\sinh\sqrt{\Delta}\beta}{\sqrt{\Delta}\beta}]. \quad (52)$$

The equilibrium ensemble averages $\langle f_0.f_0\rangle$, $\langle f_1.f_0\rangle$ and $\langle f_2.f_0\rangle$ can now be obtained. The results are found to be

$$\langle f_0.f_0\rangle = \sum_{k,l=1}^{N}\langle S_k^x S_l^x\rangle = \frac{N}{4}, \quad (53)$$

and

$$\langle f_1.f_0\rangle = J\sum_{k,l=1}^{N}(\langle S_{k-1}^z S_k^y S_l^x\rangle + \langle S_k^y S_{k+1}^z S_l^x\rangle)$$
$$= (-i)\frac{J}{2^3}\sum_{k,l+1}^{N}(\langle\sigma_{k-1}^z\sigma_k^z\rangle + \langle\sigma_k^z\sigma_{k+1}^z\rangle)$$
$$= (-i)\frac{J}{4}N\tanh(\frac{\beta\sqrt{\Delta}}{4}), \quad (54)$$

and

$$\langle f_2.f_0\rangle = 2J^2\sum_{k,l=1}^{N}(\chi^*\langle S_k^x S_l^x\rangle -$$
$$\langle S_{k-1}^z S_k^x S_{k+1}^z S_l^x\rangle)$$
$$= 2J^2\sum_{k=1}^{N}(\chi^*(\frac{1}{4})\langle\sigma_k^x\sigma_k^x\rangle -$$
$$(\frac{1}{16})\langle\sigma_{k-1}^z\sigma_{k+1}^z\sigma_k^x\sigma_k^x\rangle)$$
$$= 2J^2[\frac{N\chi^*}{4} - \frac{N}{16}\tanh^2\frac{\beta\sqrt{\Delta}}{4}], \quad (55)$$

where we have used the well-known formula for near neighbor correlations in an Ising chain, $\langle \sigma_k^z \sigma_{k+r}^z \rangle = \tanh^r(\beta J)$ [47]. Further, since the correlations depend only upon the distance between the neighbors, we have replaced the site index k by 0 to simplify notation. Combining Equations (48-55) and after some algebra we get [48, 49],

$$\chi_{perp.} = \frac{N}{4}[(\frac{\Delta_2}{\Delta} + \frac{\Delta_1}{\Delta}\frac{\sinh y}{y})\langle \sigma_0^x \sigma_0^x \rangle - \frac{\cosh y - 1}{y}\langle \sigma_0^z \sigma_1^z \rangle + (1 - \frac{\sinh y}{y})(\frac{\Delta_1 - \Delta_2}{2\Delta} - \frac{1}{2}\langle \sigma_0^z \sigma_2^z \rangle)]. \quad (56)$$

In deriving Equation (56), we note that $2J^2\chi^* = \frac{\Delta_1 - \Delta_2}{2}$. The final expression for $\chi_{perp.}$ works out to be

$$\chi_{perp.} = \frac{N}{8}[(\cosh K)^{-2} + \frac{\tanh K}{K}], \quad K = \frac{y}{4} = \frac{\beta J}{4}. \quad (57)$$

It is also possible to find χ^*. To do so, we consider two vectors X and Y and observe that

$$\begin{aligned} (X, \dot{Y}) &= i\beta^{-1} \int_0^\beta d\lambda \langle X(\lambda)[H, Y] \rangle \\ &= i\beta^{-1} \int_0^\beta d\lambda \langle \exp(\lambda H) X H \exp(-\lambda H) Y \\ &\quad - \exp(\lambda H) H X \exp(-\lambda H) Y \rangle \\ &= -i\beta^{-1} \int_0^\beta d\lambda \langle \exp(\lambda H)[H, X] \exp(-\lambda H) Y \rangle \\ &= -i\beta^{-1} \int_0^\beta d\lambda \langle [H, X(\lambda)] Y \rangle \\ &= -i\beta^{-1} \int_0^\beta d\lambda \frac{\partial}{\partial \lambda} \langle X(\lambda) Y \rangle \\ &= -i\beta^{-1}(\langle X(\beta) Y \rangle - \langle X(0) Y \rangle) \\ &= i\beta^{-1}(\langle [X, Y] \rangle). \end{aligned} \quad (58)$$

Using $X = f_1$, $Y = f_0$ in Equation (58), a few simple commutation relations reveal that

$$\begin{aligned} \chi^* &= \frac{J^2 N}{16\Delta_1}(1 + 4\chi^*)((\sinh K)^{-2} + \frac{\tanh K}{K}) \\ &= \frac{1}{4}[\frac{1 - 2K(\sinh 2K)^{-1}}{1 + 2K(\sinh 2K)^{-1}}], \quad K = \beta J. \end{aligned} \quad (59)$$

The results obtained for the one dimensional chain here can be extended to Ising models in arbitrary lattice dimensions, although the analysis becomes algebraically challenging. The dimensionality d turns out to be related to the number of nearest neighbors to a given site in the system. For lattices with three nearest neighbors, namely the honeycomb lattice, $q = 3$ and $d = 4$. For the square lattice with four nearest neighbors, i.e., $q = 4$, one finds $d = 5$ and for the triangular lattice with $q = 6$ one finds $d = 7$. The relationship between q and d holds for three dimensional systems also. For simple cubic lattices, $q = 6$ and $d = 7$, etc. In general, on the basis of existing studies, one would infer that $d = q + 1$ [19, 25, 26]. The presence of a parallel magnetic field to the Hamiltonian, i.e., a term $h \sum_{i=1}^N S_i^z$, splits up each frequency (except the zero frequency mode, if any) into two. The relationship between d and q is thus changed to $d = 2q + 1$ in the presence of a parallel field [26].

It turns out that as the number of nearest neighbors $q \to \infty$, the Hilbert space dimension $d \to \infty$. The equilibrium properties of this limit were first studied by Kittel and Shore for a detailed discussion see Ref. [25]). The dynamical properties were studied by Lee and Dekeyser (see Lee and Dekeyser in [46]) and by Sen [25]. The $q \to \infty$ problem case exhibits a phase transition with associated dynamics, which although somewhat artificial is instructive to the learner.

IV. SUMMARY

In this article, the continued fraction formalism for solving the Liouville equation for conservative systems is described. The objective of this review is to illustrate how to solve for the dynamical variable itself. In the event that solving for the dynamical variable is too much of a challenge, one can focus on the simpler problem of obtaining the dynamical correlation function. The procedure for obtaining the dynamical correlation function is outlined above. The connection between the Liouville equation and the Generalized Langévin equation is shown and the derivation of the Langévin equation is sketched.

It is possible to completely solve the dynamical problem for very few systems. We show one such case, that of transverse dynamics of the ising model in one dimension. The references to higher dimensional studies of the Ising model and to lower dimensional studies of other spin models (such as XY and Heisenberg models) are cited in the references. References are also made to studies of harmonic chains and nonlinear systems. The challenges associated with obtaining continued fraction descriptions for systems in the vicinity of a phase transition are mentioned.

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APPENDIX A: PROPERTIES OF SCALAR PRODUCTS

(i) Proof of $(X,Y) = (Y,X)$

$$(X,Y) = \frac{1}{\beta}\int_0^\beta d\lambda \langle \exp(\lambda H) X \exp(-\lambda H) Y^\dagger \rangle - \langle X \rangle \langle Y^\dagger \rangle = (Y,X) \quad (60)$$

provided we do the transformation $\lambda \to -\lambda' + \beta$ and use the cyclic commutation property of the Trace operator, i.e., $TrABCD = TrCDAB$, etc.

(ii) Proof of $(LX,Y) = -(X,LY)$

$$(X,LY) = \frac{1}{\beta}\int_0^\beta d\lambda \langle \exp(\lambda H) X \exp(-\lambda H)(HY^\dagger - Y^\dagger H)\rangle - \langle X \rangle \langle (HY^\dagger - Y^\dagger H)\rangle = -(LX,Y) \quad (61)$$

where we have used the property of H to be transported through the $\exp(-\lambda H)$.

APPENDIX B: DEVELOPMENT OF EQUATION (32)

We first observe that S_k^z from the left side of the comma in the scalar product can be moved to the right side of the scalar product because such an operator commutes with H. The solution for $S_{l+1}^y(\lambda)$ can be easily obtained from Equation (47) and shows that $\langle S_{l+1}^y(\lambda) S_l^x S_{l-1}^z \rangle = 0$. Using similar arguments it can be shown that $\langle S_{l-1}^y(\lambda) S_{l-2}^z S_{l-1}^z S_l^y \rangle = 0$, and all terms with $k = l \pm 1$ do not contribute to (f_1, f_1). However, $k = l$ terms give finite contributions and are computed in Equation (32).

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