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Real-space dynamic renormalization group. I. General formalism

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A general scheme is presented for applying real-space renormalization-group methods to dynamic critical phenomena. The method is based on mapping the time evolution operator for the initial variables onto a new operator acting on the block variables. The general formalism is discussed in the context of the kinetic Ising model. It is shown that all non-Markovian effects in the new operator can be eliminated if the renormalization-group transformation is taken to be the solution of a generalized eigenvalue equation. We show how to solve this equation perturbatively. The resulting transformation is such that the dynamics of the block spins is given by the slowest dynamic modes of the initial spins within a block.

I. INTRODUCTION

We present in this paper a general scheme for applying real-space renormalization-group (RSRG) methods to time-dependent problems.

The renormalization group[1–3] (RG) has previously been applied to both static and dynamic critical phenomena. It has been formulated in two different contexts: in momentum[4] and in position space.[5] As is well known, ϵ-expansion methods[1–3,6] can be combined with the momentum-space RG to give very good results for static critical properties. The momentum-space or continuum approach has also been successfully combined with the mode coupling theory due to Fixman,[7(a)] Kawasaki,[7(b)] and others[8] to obtain a dynamic renormalization-group theory that works quite well in explaining dynamic critical phenomena in a variety of systems. These theories are discussed in a recent review by Hohenberg and Halperin.[9]

While the continuum approach has been very successful in certain circumstances the limitations can be severe. Since one ignores local details from the very beginning, the theory is only useful for determining asymptotic properties. Thus, while one can obtain the critical exponents, it will not yield the value of the transition temperature or how one approaches an asymptotic state. Similarly, the continuum formulation essentially assumes there is a second-order phase transition and only works near such a transition. It is not useful for looking at global properties over the entire thermodynamic plane and cannot easily be used to systematically investigate first-order phase transitions.

Practically speaking, we only know how to treat the model field theories studied in the continuum theories within the framework of perturbation theory where fluctuations are treated as small. Clearly these techniques are not the most appropriate for treating, say, two-dimensional Ising-like systems displaying strong critical fluctuations.

The RSRG method, while not as controlled a method for determining universal quantities as the momentum-space method, has several advantages. One is that it can, at least theoretically, be used in any dimension. The second advantage is that it can be used to determine nonuniversal properties[10] unlike the momentum-space method. There are by now a number[11] of sophisticated methods for applying the RSRG approach to static problems.

It seems natural to extend RSRG methods to the dynamic case. However, no consistent scheme for studying the behavior of the full dynamics of the system under the action of the RG transformation, in real space, has been proposed until the present.[12] The difficulty can be explained in intuitive terms as follows: in real space the variables are initially on a lattice, and, by the RG transformation, new variables, in a larger lattice, are defined. The time propagation in the system (its dynamics) is driven by an operator, the Liouville operator (or, in the Ising case, by a pseudo-Liouville or spin-flip operator). It is necessary to find how this dynamical operator behaves under the action of the RG transformation.

In terms of the Kadanoff block-spin picture[13] the problem is to find the dynamical operator for the new, coarse-grained, block variables, in terms of the initial variables and dynamics. Notice that, since dissipation must be involved, one cannot say that the dynamics is simply given by the effective Hamiltonian of the coarse-grained variables. The problem is more complicated.

The main point of this paper is to introduce a formalism which allows one to conveniently construct the dynamical operator generating the dynamics for the block spins. The RSRG formulation for dynamics that we develop is quite general. In the present work, however, we restrict ourselves, for simplicity, to kinetic Ising (KI) models[14] which we discuss in Sec. II. In Sec. III we show how to obtain unambiguously the spin-flip operator (SFO) acting on the new spin variables, once the initial SFO and RSRG transformations are given.

A very important point, which we elucidate in Sec. IV of the present work, is the presence of non-Markovian memory effects in the renormalized SFO. These effects, which we show would produce an interaction of long range in time, must be eliminated. This elimination is accomplished by an appropriate choice of the RG transformation. This choice, which turns out to have a transparent physical interpretation in terms of elimination of fast modes, is determined by the condition that the transformation function be an eigenfunction of the initial dynamical operator. This eigenvalue method, therefore, solves both the mathematical and physical difficulties which have up to now precluded the implementation of the RSRG for the dynamics. It constitutes the fundamental core of our work.

Some other schemes have been[15] proposed for applying the RSRG to the dynamics of critical phenomena. However, these other methods do not address themselves to the fundamental question of the renormalization of the full dynamical operator and the question of non-Markovian effects.

II. GENERALIZED GLAUBER MODELS

A. Microscopic and macroscopic dynamical systems

In a fully microscopic treatment of dynamical problems in statistical mechanics the statistics are governed by a Boltzmann probability distribution in terms of the Hamiltonian H, describing the system, and the dynamics is generated by the Liouville operator, L, constructed from H. There are however many situations where a fully microscopic analysis of the dynamics of a system seems inappropriate. Important examples are the continuum dynamical theories designed to be compatible with the Ginzburg-Landau-Wilson field theoretic treatment of static critical phenomena. The formal structure of these theories is discussed in some detail in Ma and Mazenko.[16] The basic physics is that if one is near the critical point the details of the underlying microscopics are not important and the statics and dynamics should be described by an appropriate "coarse-grained" Hamiltonian and Liouville operator. In this field theoretic description (depending, say, on a field ϕ) the Hamiltonian is replaced by an "effective" free energy $F[\phi]$ and the Liouville operator is replaced by a generalized Fokker-Planck operator, $\tilde{D}_\phi$.

B. Lattice dynamical models

In this paper we are interested in the dynamics of fixed length spins on a lattice. In the case of x-y or Heisenberg models we simply have to write down the Hamiltonian describing the system and define the appropriate commutation relations or Poisson bracket relations in order to specify the problem in the completely microscopic sense discussed in Sec. II A. We are, of course, interested in these problems, but we also realize that the equilibrium behavior of these systems is considerably more complicated than that of Ising models. This is manifested, for example, in the complicated coexistence curve behavior in three-dimensional Heisenberg magnets due to the Nambu-Goldstone modes. As a further complication the critical behavior in a two-dimensional x-y model involves the Kosterlitz-Thouless vortex unbinding mechanism. For simplicity therefore we restrict ourselves to Ising models.

In discussing Ising models we are forced to an intermediate position between a microscopic and a macroscopic description. The static behavior is given by an Ising Hamiltonian but we must introduce a stochastic time evolution operator. It is conventional in motivating the dynamic evolution of a set of Ising spins to picture the system as being in contact with a heat reservoir. The interactions with the heat reservoir provide the dynamics. Specifically, let us consider a system of N Ising spins (in any dimensions) interacting with a heat bath, let i be an index which numbers the spins and let σ stand for a given spin configuration $\sigma \equiv \{\sigma_1, \sigma_2, \ldots \sigma_N\}$. The equilibrium probability distribution is given by

$$P[\sigma] = e^{H[\sigma]}/Z \ , \tag{2.1}$$

where Z is the partition function and $H[\sigma]$ is the Ising Hamiltonian multiplied by $-\beta$ and is given by

$$H[\sigma] = \tfrac{1}{2} K \sum_{i=1}^{N} \sum_{\delta} \sigma_i \sigma_{i+\delta} \ , \tag{2.2}$$

where K is the coupling constant ($K = +\beta J$ where J is the exchange interaction), and the sum over δ is

over basis vectors connecting a spin i with its nearest neighbors.

The equilibrium spin-spin time correlation functions can be defined in this case

$$C_{ij}(t)=\sum_{\sigma}P[\sigma]\sigma_j e^{\tilde{D}_{\sigma'}t}\sigma_i \ , \tag{2.3}$$

and we must define the pseudo-Liouville operator $\tilde{D}_\sigma$. An operator in this case is a matrix which rotates one spin configuration σ' into another spin configuration σ:

$$\tilde{D}_\sigma A[\sigma]\equiv\sum_{\sigma'}\tilde{D}[\sigma|\sigma']A[\sigma'] \ . \tag{2.4}$$

The adjoint operator D_σ is defined by

$$D[\sigma|\sigma']\equiv\tilde{D}[\sigma'|\sigma] \ . \tag{2.5}$$

We will want to demand that $\tilde{D}_\sigma$ or equivalently D_σ satisfy two basic properties. First we demand that:

$$e^{D_{\sigma'}t}P[\sigma]=P[\sigma] \ , \tag{2.6}$$

or

$$\sum_{\sigma'}D[\sigma|\sigma']P[\sigma']=0 \ , \tag{2.7}$$

which ensures the stationary quality of the equilibrium probability distribution. A second condition follows if we remember that in a fully microscopic theory one has the symmetry relation

$$C_{AB}(t)=C_{BA}(-t) \ . \tag{2.8}$$

If the system is time-reversal invariant and A and B have the same signature under time reversal then:

$$C_{AB}(t)=C_{BA}(t) \ . \tag{2.9}$$

We would like our stochastic dynamical model to also satisfy this symmetry. It is easy to see that this will be satisfied if the operator D_σ satisfies the symmetry or detailed-balance condition

$$D[\sigma|\sigma']P[\sigma']=D[\sigma'|\sigma]P[\sigma] \ . \tag{2.10}$$

Note that Eqs. (2.5) and (2.10) give us the useful identity for any f:

$$\sum_{\sigma'}D[\sigma|\sigma']f[\sigma']P[\sigma'] =P[\sigma]\sum_{\sigma'}\tilde{D}[\sigma|\sigma']f[\sigma'] \ . \tag{2.11}$$

The conditions (2.7) and (2.10) constrain the possible operators D_σ significantly. There is, however, still a great deal of latitude in choosing the appropriate operators and operationally one is guided by arguments of locality and simplicity. In this paper we will focus on a particular class of operators satisfying Eqs. (2.7) and (2.10). This class of operators we will call "spin-flip operators" and have the property that they are of the form

$$\sum_{i_1}\sum_{i_2}\cdots\sum_{i_n}\Lambda_{\sigma,\sigma'}^{(i_1,i_2,\cdots i_n)}F[\sigma|\sigma'] \ ,$$

where

$$\Lambda_{\sigma,\sigma'}^{(i_1,i_2,\cdots i_n)}=\prod_{l\neq(i_1,i_2,\cdots i_n)}\delta_{\sigma_l,\sigma_l'} \tag{2.12}$$

is the operator that sets $\sigma=\sigma'$ on all lattice sites except $i_1, i_2, \ldots, i_n$. Thus D_σ will "operate" on only a restricted set of spins. D_σ is diagonal as far as the other $N-n$ sites are concerned. There are other models one could consider which do not have this property.

The simplest spin-flip operator involves operating on one spin and is of the form

$$\tilde{D}[\sigma|\sigma']=-\tfrac{1}{2}\alpha\sum_i\Lambda_{\sigma,\sigma'}^{(i)}W_i[\sigma]\sigma_i\sigma_i' \ . \tag{2.13}$$

where α^{-1} is a characteristic spin-flip time, and $W_i[\sigma]$ is a dimensionless quantity yet to be specified. Then, if we define

$$F[\sigma,t]=e^{\tilde{D}_{\sigma'}t}F[\sigma] \ , \tag{2.14}$$

we have, using the identity for Ising spins

$$\sigma_i\sigma_i'=\delta_{\sigma_i,\sigma_i'}-\delta_{\sigma_i,-\sigma_i'} \tag{2.15}$$

the "equation of motion"[14]:

$$\frac{dF[\sigma,t]}{dt}=-\tfrac{1}{2}\alpha\sum_i\{W_i[\sigma_1\cdots\sigma_i\cdots\sigma_N]F[\sigma,t] -W_i[\sigma_1\cdots-\sigma_i\cdots\sigma_N] \times F[\sigma_1\cdots-\sigma_i\cdots\sigma_N,t]\} \ . \tag{2.16}$$

The function

$$\alpha W_i[\sigma]\equiv\alpha W_i[\sigma_1\cdots\sigma_i\cdots\sigma_N]$$

has a simple physical interpretation: it is the probability per unit time that the ith spin will flip from σ_i to $-\sigma_i$. We have yet to fully specify $W_i[\sigma]$. Both Eqs. (2.7) and (2.10) are satisfied as long as $W_i[\sigma]P[\sigma]$ is independent of the spin at site i. The simplest choice for $W_i[\sigma]$ is

$$W_i[\sigma]=e^{-\sigma_i E_i[\sigma]} \ , \tag{2.17}$$

where

$$E_i[\sigma]=K\sum_\delta\sigma_{i+\delta} \ . \tag{2.18}$$

More generally we can satisfy Eqs. (2.13) and (2.16)

by choosing

$$W_i[\sigma] = A_i[\sigma] e^{-\sigma_i E_i[\sigma]} , \tag{2.19}$$

where $A_i[\sigma]$ is any function of σ that does not depend on the spin at site i. Typically, however, we expect that $W_i[\sigma]$ is a local function depending only on the spins near site i. $A_i = 1$ is often a convenient choice. In the one dimensional case, the choice

$$A_i[\sigma] = (\cosh E_i[\sigma])^{-1} \tag{2.20}$$

is easily seen to correspond to Glauber's[14] function:

$$W_i[\sigma] = [1 - \tfrac{1}{2}\tanh(2K)\sigma_i(\sigma_{i+1} + \sigma_{i-1})] . \tag{2.21}$$

We will be interested in expressions for $D[\sigma|\sigma']$ more general than Eq. (2.13). The reason for this can be understood by remembering well-known facts about the static RG: if one starts with, say, an Ising Hamiltonian with nearest-neighbor interactions only, the renormalization-group process usually generates new interactions (e.g., 2nd-, 3rd-nearest neighbor). Analogously, we will see that if we start with an operator as given by Eq. (2.13) the renormalization-group operation will generate new terms. In order to gain closure and obtain recursion relations, the initial operator must be taken to be of the general form

$$\begin{aligned} D[\sigma|\sigma'] = {} & \tfrac{1}{2}\sum_i \Lambda^{(i)}_{\sigma,\sigma'} W_i[\sigma'] V_1^{[i]}[\sigma'] \sigma_i \sigma_i' \\ & + \tfrac{1}{4}\sum_{ij} \Lambda^{(i,j)}_{\sigma,\sigma'} W_{ij}[\sigma'](\sigma_i\sigma_j' V_2^{[i,j]}[\sigma'] + \sigma_i\sigma_i'\sigma_j\sigma_j' V_3^{[i,j]}[\sigma']) \\ & + \tfrac{1}{8}\sum_{ijk} \Lambda^{(i,j,k)}_{\sigma,\sigma'} W_{ijk}[\sigma'](\sigma_i\sigma_i'\sigma_j\sigma_k' V_4^{[i,j,k]}[\sigma'] + \sigma_i\sigma_i'\sigma_j\sigma_j'\sigma_k\sigma_k' V_5^{[i,j,k]}[\sigma']) + \cdots , \end{aligned} \tag{2.22}$$

where we have explicitly included up to three spin terms. The W_{ij} are defined as follows: Let $H^{ijk\cdots}$ be the sum of all terms in the Hamiltonian which involve $\sigma_i\sigma_j\sigma_k\cdots$, for example,

$$H^i = \sigma_i E_i[\sigma] , \tag{2.23}$$

or if σ_i, σ_j are neighboring spins

$$H^{ij} = \sigma_i E_i[\sigma] + \sigma_j E_j[\sigma] - K\sigma_i\sigma_j \tag{2.24}$$

(the last term avoids double counting). Then we define

$$W_{i,j,\ldots}[\sigma] = e^{-H^{i,j,\ldots}} . \tag{2.25}$$

It is easy to show that Eq. (2.22) satisfies Eqs. (2.7) and (2.10). The key point is that $V_m^{[i,j,\ldots]} W_{i,j,\ldots} P$ does not depend on the spins $\sigma_i, \sigma_j, \ldots$. It is easy to develop a systematic method for extracting the coefficients $V_1^{[i]}[\sigma]$, $V_2^{[i,j]}[\sigma]$, $\ldots$, $V_m^{[i,j,\ldots]}[\sigma]$, $\ldots$ from a given operator $D[\sigma|\sigma']$. In examples which we will discuss in a companion paper[17] we will never go beyond three spin terms, and we will confine ourselves to very simple choices for the W functions. The general form, however, must be kept in mind when examining the terms obtained in any calculation.

III. RSRG FORMALISM

In this section we will develop our scheme for implementing the RG for dynamics in real space. First, we need to recall some well-known properties of the RSRG.[18]

A. Review of basics in the static RSRG

Let us consider a set of Ising spin variables $\sigma \equiv \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ on a lattice. The renormalization-group transformation function $T[\mu|\sigma]$ maps the set σ onto a new set $\mu \equiv \{\mu_1, \mu_2, \ldots\}$ of spins located on a lattice geometrically similar to the initial one but having a larger lattice constant. If the initial Hamiltonian is designated by $H[\sigma]$, one defines the Hamiltonian $H[\mu]$ on the new μ lattice by the relation

$$e^{H[\mu]} = \sum_\sigma e^{H[\sigma]} T[\mu|\sigma] . \tag{3.1}$$

The demand that the partition function be invariant under this transformation requires that the transformation function satisfy the normalization condition

$$\sum_\mu T[\mu|\sigma] = 1 . \tag{3.2}$$

With the exception of this normalization condition there is no restriction on the choice of $T[\mu|\sigma]$. Physical intuition as to the form of the desired transformation and ease of calculation are the main criteria[19] used in the selection of $T[\mu|\sigma]$.

As a nontrivial example let us consider a system of Ising spins on a two-dimensional triangular lattice. The system is discussed extensively in Ref. 5 and will be the system we concentrate on in this paper. Let us divide the lattice into triangular cells, drawn so as to preserve the symmetry of the lattice (Fig. 1). Each cell will correspond to a new spin, μ_i. We will use an index i to designate each cell (and hence each μ_i). The three σ spins in cell i are designated σ_{i,a_1}, σ_{i,a_2}, σ_{i,a_3}, where the vectors a_1, a_2, a_3 are defined

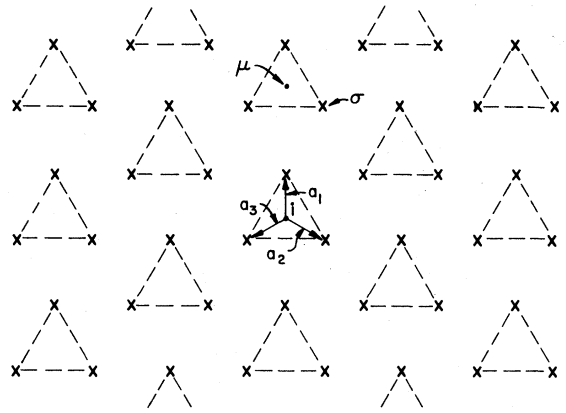

FIG. 1. Two-dimensional triangular lattice divided into three spin cells (labeled by a cell index i in the text) and the set of basis vectors a_1, a_2, a_3.

in Fig. 1. Following Niemeijer and van Leeuwen[5] (NvL) we will consider all intracell interactions to be of zeroth order and all nearest-neighbor intercell couplings to be of first order in λ (λ to be set equal to one at the end of the calculation).

A widely studied class of RG transformation functions corresponds to assuming that T can be written as a product over cells, i.e.,

$$T_0[\mu|\sigma]=\prod_i T^i[\mu|\sigma] \ . \tag{3.3}$$

The subscript 0 signifies that T does not include any intercell couplings. The transformation function for the ith cell, $T^i[\mu|\sigma]$, satisfies

$$\sum_{\mu_i} T^i[\mu|\sigma]=1 \ , \tag{3.4}$$

and can be written in the general form

$$T^i[\mu|\sigma]=\tfrac{1}{2}[1+\mu_i\phi_i(\sigma)] \ , \tag{3.5}$$

where $\phi_i(\sigma)$ depends only on the three σ spins in the ith cell.

It is convenient to choose $T[\mu|\sigma]$ to be invariant under the flip of all μ and σ spins. Consequently we require $\phi_i(\sigma)$ to be an odd function of the σ spins in the ith cell. If we further demand that ϕ_i be a symmetric function under interchange of the three spins in the cell then it can be written in the form

$$\phi_i(\sigma)=N(\sigma_i^T-f\sigma_i^c) \ , \tag{3.6}$$

where N and f are arbitrary constants, σ_i^T is the total spin for the ith cell

$$\sigma_i^T=\sigma_{i,a_2}+\sigma_{i,a_2}+\sigma_{i,a_3} \ , \tag{3.7}$$

and σ_i^c is the product of the three spins in the ith cell

$$\sigma_i^c=\sigma_{i,a_1}\sigma_{i,a_2}\sigma_{i,a_3} \ . \tag{3.8}$$

With this choice for T_0 one can calculate $H[\mu]$ as a cumulant expansion in powers of the intercell coupling λ. The following results are obtained: starting with nearest-neighbor interactions only, to first order in λ only nearest-neighbor interactions are generated. The new coupling constant K' is given in terms of the initial K, by the first term on the right-hand side of Eq. (3.9a) below.

To second order, couplings between second- and third-nearest neighbors are generated. These couplings must be included in the initial Hamiltonian. If we call these couplings L and M, respectively, the recursion relations are given by:

$$K'=2\nu^2K+4\nu^2K^2(1+r-2\nu^2)+3L\nu^2+2M\nu^2 \ , \tag{3.9a}$$

$$\begin{aligned} L'&=\nu^2K^2(1+7r-8\nu^2)+\nu^2M \ , \\ M'&=4K^2\nu^2(r-\nu^2) \ . \end{aligned} \tag{3.9b}$$

Here we have defined the quantities:

$$r=\langle\sigma_{i,a}\sigma_{i,a'}\rangle_0, \quad a\neq a' \ , \tag{3.10}$$

$$\nu=\langle\sigma_{i,a}\phi_i(\sigma)\rangle_0 \ , \tag{3.11}$$

where the average is defined by

$$\langle f(\sigma)\rangle_0\equiv\sum_\sigma P_0[\sigma]f(\sigma) \ , \tag{3.12}$$

where $P_0[\sigma]$ is the probability distribution governing the uncoupled cells. Since we assume $\phi_i(\sigma)$ is symmetric in the three spins in cell i, ν will not depend on the value of the basis vector a.

One appealing choice for $\phi_i(\sigma)$ is given by the "majority rule" due to NvL where

$$\phi_i(\sigma)=\operatorname{sgn}\sigma_i^T=\tfrac{1}{2}(\sigma_i^T-\sigma_i^c) \ , \tag{3.13}$$

and corresponds to $N=\frac{1}{2}$ and $f=1$ in Eq. (3.6). It is easy to show that the recursion relations given by Eq. (3.9) are equivalent to those given by NvL in the particular case where $\phi_i(\sigma)$ is given by Eq. (3.13).

B. Basic RSRG transformation for the time-evolution operator

In the dynamical problems of interest to us the system is specified by the Hamiltonian $H[\sigma]$ and the SFO $D[\sigma|\sigma']$. If we want to apply RG ideas to this problem we want to design transformations which map the old $H[\sigma]$ and $D[\sigma|\sigma']$ onto their counterparts $H[\mu]$ and $D[\mu|\mu']$ defined on the μ lattice. We understand the mapping $H[\sigma]\to H[\mu]$. The problem is with the mapping $D_\sigma\to D_\mu$. The difficulty is that we now have to map one operator onto another operator.

It is useful, in developing the appropriate transfor-

mation, to introduce the time-evolution matrix:

$$G_t[\sigma|\sigma'] = e^{D_{\sigma'}t}\delta_{\sigma,\sigma'}P[\sigma'] \ , \tag{3.14}$$

where $\delta_{\sigma,\sigma'}$ is the matrix setting $\sigma=\sigma'$ of all lattice sites. From this quantity we construct any time correlation function of the form

$$\langle \sigma_i\sigma_j \cdots \sigma_k e^{\tilde{D}_{\sigma'}t}\sigma_m \cdots \sigma_n\rangle \ .$$

We see, for example, that the spin-spin correlation function is given by

$$C_{ij}(t) = \sum_{\sigma}\sum_{\sigma'}\sigma_j G_t[\sigma|\sigma']\sigma_i' = \langle \sigma_i e^{\tilde{D}_{\sigma'}t}\sigma_i\rangle \ , \tag{3.15}$$

where $\langle A_\sigma\rangle \equiv \sum_\sigma P[\sigma]A_\sigma$ is the usual equilibrium average. Remembering the RG transformation (3.1) for the probability distribution and noticing that $G_t[\sigma|\sigma']$ is a matrix depending on two sets of spins it is natural to assume that the new time-evolution matrix for the μ lattice be defined by

$$G_t[\mu|\mu'] = \sum_{\sigma}\sum_{\sigma'} T[\mu|\sigma]G_t[\sigma|\sigma']T[\mu'|\sigma'] \ . \tag{3.16}$$

In this case there are two constraints on the mapping functions T. The first constraint is the same as in the static case, that is Eq. (3.2). The second constraint follows from requiring that the zero-time form of $G_t[\sigma|\sigma']$,

$$G_{t=0}[\sigma|\sigma'] = \delta_{\sigma,\sigma'}P[\sigma] \ , \tag{3.17}$$

be preserved by the transformation

$$\begin{aligned} G_{t=0}[\mu|\mu'] &= \delta_{\mu,\mu'}P[\mu] \equiv \tilde{G}[\mu|\mu'] \\ &= \langle T[\mu|\sigma]T[\mu'|\sigma]\rangle \ . \end{aligned} \tag{3.18}$$

This definition of $G_t[\mu|\mu']$ is a physically sensible dynamical generalization of the static RSRG procedure. To see this, consider the spin-spin correlation function generated by $G_t[\mu|\mu']$:

$$\begin{aligned} C_{ij}'(t) &= \sum_{\mu}\sum_{\mu'}\mu_i G_t[\mu|\mu']\mu_j' \\ &= \sum_{\mu}\sum_{\mu'}\mu_i\sum_{\sigma}\sum_{\sigma'}T[\mu|\sigma]G_t[\sigma|\sigma'] \\ &\quad \times T[\mu'|\sigma']\mu_j' \ . \end{aligned} \tag{3.19}$$

If the mapping function T is of the product form given by Eq. (3.3) then

$$\sum_{\mu}\mu_i T_0[\mu|\sigma] = \phi_i(\sigma) \ , \tag{3.20}$$

and

$$C_{ij}'(t) = \langle \phi_j(\sigma)e^{\tilde{D}_{\sigma'}t}\phi_i(\sigma)\rangle \ , \tag{3.21}$$

which is, as desired, the time correlation for a set of coarse-grained spin variables. This means that we must choose $\phi_i(\sigma)$ to represent the effective spin for a cell. Physically it makes sense to identify $\phi_i(\sigma)$ as the dynamically slowest varying odd spin variable in a cell. We will return to this point later.

Before going further we should comment on the constraint on $T[\mu|\sigma]$ given by Eq. (3.18). In the case of the majority rule choice for $\phi_i(\sigma)$ given by Eq. (3.13) one has that

$$T^i[\mu|\sigma]T^{i'}[\mu'|\sigma] = \delta_{\mu_i,\mu_i'}T^i[\mu|\sigma] \ , \tag{3.22}$$

and Eq. (3.18) is satisfied directly. For other choices for $\phi_i(\sigma)$ the quantity $\langle T_0[\mu|\sigma]T_0[\mu'|\sigma]\rangle$ is not, in general, diagonal in μ and μ'. We will discuss this point further in Sec. IV.

At the beginning of this section we indicate that we are interested in finding the SFO $D[\mu|\mu']$ appropriate to the μ lattice. At present we have only an expression for the time-evolution operator $G_t[\mu|\mu']$. We must now indicate how one can extract D_μ from $G_t[\mu|\mu']$. This identification of D_μ requires some formal development. Rather than working directly with $G_t[\mu|\mu']$ it is more convenient to introduce the Laplace transform

$$G_z[\sigma|\sigma'] = -i\int_0^\infty dt e^{izt}G_t[\sigma|\sigma'] \ . \tag{3.23}$$

Using the definition of G_t given by Eq. (3.14) we can easily carry out the time integration to obtain

$$G_z[\sigma|\sigma'] = R_\sigma(z)\delta_{\sigma,\sigma'}P[\sigma] \ , \tag{3.24}$$

where $R_\sigma(z)$ is the resolvent operator

$$R_\sigma(z) = (z - iD_\sigma)^{-1} \ . \tag{3.25}$$

Using the operator identity

$$zR_\sigma(z) = 1 + iR_\sigma D_\sigma \tag{3.26}$$

we can write

$$(z\delta_{\sigma,\bar{\sigma}} - iD[\sigma|\bar{\sigma}])G_z[\bar{\sigma}|\sigma'] = \delta_{\sigma,\sigma'}P[\sigma] \ . \tag{3.27}$$

Here, and in what follows, summation over all configurations for barred spin indices is implied.

It is then natural, using Eq. (3.18), to define the operator $D[\mu|\mu']$ by the relation

$$(z\delta_{\mu,\bar{\mu}} - iD[\mu|\bar{\mu};z])G_z[\bar{\mu}|\mu'] = \delta_{\mu,\mu'}P[\mu] \ , \tag{3.28}$$

where we have taken into account the fact that $D[\mu|\mu']$ may depend on z. We are now left with the task of deriving an expression for $D[\mu|\mu']$ in terms of $D[\sigma|\sigma']$ and $T[\mu|\sigma]$. The derivation that follows parallels methods used in the memory function formalism for fluids.[20,21] Starting with the Laplace transform of Eq. (3.16),

$$G_z[\mu|\mu'] = \langle T[\mu'|\sigma]\tilde{R}_\sigma(z)T[\mu|\sigma]\rangle \ , \tag{3.29}$$

where $\tilde{R}_\sigma(z)$ is the same as $R_\sigma(z)$ but with the D_σ replaced by $\tilde{D}_\sigma$, one can easily show, using the methods developed in Ref. 21, that $D[\mu|\mu';z]$, defined in Eq. (3.28), is given by

$$D[\mu|\mu';z]=D^s[\mu|\mu']+D^c[\mu|\mu';z] \ , \tag{3.30}$$

where we have specified that all the z dependence (i.e., the non-Markovian part) of D_μ is contained in D^c_μ. D^s_μ is given by

$$D^s[\mu|\mu']P[\mu']=\langle T[\mu'|\sigma]\tilde{D}_\sigma T[\mu|\sigma]\rangle \ , \tag{3.31}$$

while

$$\begin{aligned}D^c[\mu|\mu';z]P[\mu']=&\,i\langle(\tilde{D}_\sigma T[\mu'|\sigma])\tilde{R}_\sigma(z)(\tilde{D}_\sigma T[\mu|\sigma])\rangle\\&-i\langle(\tilde{D}_\sigma T[\mu|\sigma])\tilde{R}_\sigma(z)T[\bar{\mu}|\sigma]\rangle G_z^{-1}[\bar{\mu}|\bar{\mu}']\langle T[\bar{\mu}'|\sigma']\tilde{R}_{\sigma'}(z)(\tilde{D}_{\sigma'}T[\mu'|\sigma'])\rangle \ .\end{aligned} \tag{3.32}$$

Equations (3.30)–(3.32) give us well-defined statistical mechanical expressions for the new SFO on the μ lattice.

To conclude this section, we note that the fundamental constraints imposed originally on $D[\sigma|\sigma']$ are satisfied by $D[\mu|\mu']$. First, the symmetry condition Eq. (2.10) is satisfied separately by $D^s[\mu|\mu']P[\mu']$ and $D^c[\mu|\mu']P[\mu']$. This is readily seen from Eqs. (3.31) and (3.32), taking into account that D_σ satisfies Eqs. (2.10) and (2.11). Secondly, it also follows from the result

$$\sum_{\mu'} D_\sigma T[\mu'|\sigma]P[\sigma]=D_\sigma P[\sigma]=0 \ , \tag{3.33}$$

that

$$\sum_{\mu'} D[\mu|\mu']P[\mu']=0 \ , \tag{3.34}$$

ensuring that the new equilibrium probability distribution is invariant under time translations generated by D_μ.

IV. EIGENVALUE APPROACH TO THE RSRG

A. Dynamic RSRG to zeroth order in the cell coupling

In the previous section, we have developed a formal structure for carrying out dynamical RSRG transformations. We have seen how the new generator of correlation functions, $G_z[\mu|\mu']$ and the new spin-flip operator $D[\mu|\mu']$ are defined in terms of $D[\sigma|\sigma']$ and the RG transformation function $T[\mu|\sigma]$. In a practical implementation of this formalism we realize from the very beginning that we cannot evaluate the sums in the mapping transformations for $H[\mu]$ [Eq. (3.1)] and $D[\mu|\mu']$ [Eqs. (3.30)–(3.32)] exactly. In essentially all cases of physical interest we must resort to some approximate method of evaluation of these averages. Let us assume that $H[\sigma]$ and $\tilde{D}_\sigma$ can be written as a power series in λ,

$$H[\sigma]=\sum_{n=0}^{\infty}\lambda^n H^{(n)}[\sigma] \ , \tag{4.1}$$

$$\tilde{D}[\sigma|\sigma']=\sum_{n=0}^{\infty}\lambda^n\tilde{D}^{(n)}[\sigma|\sigma'] \ , \tag{4.2}$$

where λ is an ordering parameter. We assume that the $n=0$ terms govern the behavior of uncoupled cells and the higher order terms couple cells. The appropriate decompositions to be used in practice in Eqs. (4.1) and (4.2) will be discussed in Ref. 17 and elsewhere. For now we assume that a theory treating the interaction between cells as a small parameter will be useful.

Let us consider first the zeroth-order calculation of $G_t[\mu|\mu']$ involving uncoupled cells. In this case the SFO D^0 involves only intracell coupling and is of the form

$$\tilde{D}^0[\sigma|\sigma']=\sum_i \Lambda^{(i)}_{\sigma,\sigma'}\tilde{D}^{i,0}[\sigma|\sigma'] \ , \tag{4.3}$$

where $\tilde{D}^{i,0}_\sigma$ operates on the cell i only. The static properties of this system are governed by the Hamiltonian

$$H_0[\sigma]=\sum_i H_0^i[\sigma] \ . \tag{4.4}$$

The associated probability distribution is a product of contributions from each cell

$$P_0[\sigma]=\prod_i P_0^i[\sigma]=\prod_i e^{H_0^i[\sigma]}\Big/\sum_\sigma{}^i e^{H_0^i[\sigma]} \ , \tag{4.5}$$

and $\sum^i_\sigma$ means we sum over the degrees of freedom of the spins in the cell i. The RSRG transformation for the statics is relatively trivial in this case

$$P_0[\mu]=\sum_\sigma P_0[\sigma]T_0[\mu|\sigma]=\prod_i \tfrac{1}{2}=2^{-N/n} \ , \tag{4.6}$$

where n is the number of spins per cell and $P_0[\mu]$ is independent of μ.

If matters are arranged properly then $\tilde{D}^{i,0}_\sigma$ and $H_0^i[\sigma]$ are compatible in that the constraints given by Eqs. (2.7) and (2.10) are satisfied cell by cell. For a cell with three spins the operator $D^{i,0}$ is a $2^3\times 2^3$ matrix. In practice it is relatively easy to diagonalize this matrix[22] in order to obtain the eigenfunctions and eigenvalues defined by

$$\tilde{D}_0^{i,0}\psi_i^n(\sigma)=-\lambda_n\psi_i^n(\sigma) \ . \tag{4.7}$$

It is easy to see that the ψ_i's can be chosen to form a

complete and orthonormal set for a given cell with respect to the weight function $P_0^i[\sigma]$. Using these results it is easy to calculate:

$$G_t^0[\mu|\mu'] = \langle T_0[\mu'|\sigma] e^{\tilde{D}_\sigma^0 t} T_0[\mu|\sigma]\rangle_0 = \left\langle T_0[\mu'|\sigma] \prod_i e^{\tilde{D}_\sigma^{i,0} t} T^i[\mu|\sigma]\right\rangle_0 . \quad (4.8)$$

Using the completeness of the cell eigenfunctions we can write

$$T^i[\mu|\sigma] = \frac{1}{2}\left[1 + \mu_i \sum_n c^n \psi_i^n(\sigma)\right] , \quad (4.9a)$$

where

$$c^n = \langle \phi_i(\sigma)\psi_i^n(\sigma)\rangle_0 . \quad (4.9b)$$

Using the eigenvalue Eq. (4.7), the orthogonality for different n of $\psi_i^n(\sigma)$, and noting, since $\phi_i(r)$ is odd under spin flips, that $\langle \psi_i(\sigma)\rangle_0 = 0$, we can explicitly average over the σ variables in Eq. (4.8) to obtain

$$G_t^0[\mu|\mu'] = \prod_i \frac{1}{2}\left[1 + \mu_i\mu_i' \sum_n e^{-\lambda_n t}(c^n)^2\right] P_0[\mu'] , \quad (4.10)$$

where we have used Eq. (4.6). Note that at $t = 0$, using the completeness of the ψ_i^n's we have

$$G_{t=0}^0[\mu|\mu'] = \prod_i \frac{1}{2}(1 + \mu_i\mu_i'\langle\phi_i^2(\sigma)\rangle_0) P_0[\mu'] . \quad (4.11)$$

Looking back to Eq. (3.18) we see that we desire that

$$G_{t=0}^0[\mu|\mu'] = \delta_{\mu,\mu'} P_0[\mu'] . \quad (4.12)$$

We see that this condition can be satisfied if we demand that $\phi_i(\sigma)$ be normalized to unity

$$\langle \phi_i^2(\sigma)\rangle_0 = 1 . \quad (4.13)$$

Using this result in Eq. (4.10) we can, after some rearrangements, rewrite it in the form

$$G_t^0[\mu|\mu'] = e^{D_\mu^0 t} P_0[\mu]\delta_{\mu,\mu'} , \quad (4.14)$$

where the operator D_μ^0 has the matrix elements

$$D^0[\mu|\mu'] = -\sum_i \frac{1}{2}[\alpha'(t)]\mu_i\mu_i'\Lambda^{(i)}_{\mu,\mu'} , \quad (4.15)$$

and the new inverse spin-flip time is given by

$$\alpha'(t) = -\frac{1}{t}\ln \sum_n e^{-\lambda_n t}(c^n)^2 . \quad (4.16)$$

Notice that $D^0[\mu|\mu']$ is of precisely the same form as $D[\sigma|\sigma']$ given by Eq. (2.13) with the interaction between spins set to zero. The new operator has a time-dependent inverse spin-flip time. Looking at Eq. (4.16) we see that for short times

$$\alpha'(t) = \sum_n \lambda_n (c^n)^2 , \quad (4.17)$$

while for long times the smallest λ_n, (λ_1) will dominate the sum over n and

$$\alpha'(t) = \lambda_1 - \frac{1}{t}\ln(c^1)^2 - \frac{1}{t}\left[1 + \sum_{n>1} e^{-(\lambda_n - \lambda_1)t}(c^n/c^1)^2\right] . \quad (4.18)$$

For long times $\alpha'(t) = \lambda_1$ (the eigenvalue for the slowest mode). However it is very worrisome that the long time decay to this constant goes as $1/t$ which indicates a long range in time interaction not included in the original problem. It has been a more standard procedure, in carrying out coarse graining in time-dependent problems, to work in frequency space and, as part of the coarse graining, to keep only the small frequency contributions. If we work in the frequency representation, we find that we can compute directly the matrix elements of the operator $D_\mu(z)$ and they are local in time in the sense that the small z limit is well behaved. This procedure is not dissimilar to the analysis that is carried out in momentum space in treating the generalized Langevin equations. In that case one works with the equation of motion for a single field and investigates the way it behaves under renormalization. This is not as general as looking at the change of the complete pseudo-Liouville operator under the RG. Indeed even though the individual matrix elements are well behaved, there are an infinite number of them which correspond to new couplings which build up in time. These new couplings are highly nonlocal in space and very undesirable from a RG point of view. The time representation and frequency representations are complementary since $D_\mu(t)$ is a local operator in space but nonlocal in time, while $D_\mu(z)$ is local in time, but nonlocal in space. Either way we look at the problem we see that we are in trouble without further constraints in our RG procedure.

Summarizing these results we see that for a given operator D^0 and a given mapping function $T[\mu|\sigma]$ our RSRG procedure leads to complicated and physically unsatisfying results to zeroth order in the coupling between cells. As we shall see the problem is that we cannot choose the mapping function $T[\mu|\sigma]$ arbitrarily once we are considering dynamical problems.

These technical problems in zeroth order, however difficult they may appear, are actually easily remedied: we simply choose the function $\phi_i(\sigma)$ in T^i to be one of the odd eigenfunctions of $\tilde{D}_0^{i,0}$. If we choose $\phi_i(\sigma) = \psi_i^m(\sigma)$ then $c^n = \delta_{m,n}$ and then Eq.

(4.17) reduces to

$$\alpha' = \lambda_m \tag{4.19}$$

and our long-range interaction problems are eliminated.

Physically we want to choose $m=1$ where ψ_i^1 is the odd eigenfunction whose eigenvalue λ_1 is the smallest in magnitude. In general the trivial $\psi_i^0=1$ even eigenfunction corresponds to the lowest ($\lambda_0=0$) eigenvalue, and the next eigenvalue, that is, the lowest nontrivial eigenvalue, corresponds to an odd mode. It is then natural to consider the cell transformation:

$$T'[\mu|\sigma] = \tfrac{1}{2}[1+\mu_i\psi_i^1(\sigma)] \ . \tag{4.20}$$

In this case the effective "block spin" $\psi_i^1(\sigma)$ corresponds to the most slowly decaying odd function of the spins in a cell satisfying the normalization condition (4.13). It is reassuring that this coarse graining in time prescription for specifying the "average" spin leads to a form for $\phi_i(\sigma)$ in agreement with Eq. (3.6) with the constants N and f now determined by the form of $\tilde{D}_\sigma^0$.

It is convenient, in order to appreciate the utility of Eq. (4.20) to look at the effect of applying $\tilde{D}_\sigma^0$ to $T_0[\mu|\sigma]$:

$$\tilde{D}_\sigma^0 T_0[\mu|\sigma] = -\tfrac{1}{2}\sum_i T^{(i)}[\mu|\sigma]\lambda_1\psi_i^1(\sigma)\mu_i \ , \tag{4.21}$$

$$T^{(i)}[\mu|\sigma] = \sum_{k\neq i} T^k[\mu|\sigma] \ . \tag{4.22}$$

The above expression can be rewritten as

$$\tilde{D}_0^0 T[\mu|\sigma] = -\tfrac{1}{2}\lambda_1 \sum_i \sum_{\mu'} T_0[\mu'|\sigma]\mu_i\mu_i' \Lambda^{(i)}_{\mu,\mu'} \ , \tag{4.23}$$

where we have made use of Eq. (3.20). Notice then that Eq. (4.23) can be written in the form

$$\tilde{D}_\sigma^0 T_0[\mu|\sigma] = D_\mu^0 T_0[\mu|\sigma] \ , \tag{4.24}$$

where

$$D^0[\mu|\mu'] = -\sum_i \tfrac{1}{2}(\lambda_1)\Lambda^{(i)}_{\mu,\mu'}\mu_i\mu_i' \ . \tag{4.25}$$

Equation (4.24) is in the form of an eigenvalue problem in σ space where the eigenvalues are operators in μ space. This equation is extremely useful. If we return to Eq. (4.8) with T_0 given by Eqs. (3.3) and (4.20) we see, on repeated use of Eq. (4.24), that

$$\begin{aligned} G_t^0[\mu|\mu'] &= e^{D_\mu^0 t}\langle T_0[\mu'|\sigma]T_0[\mu|\sigma]\rangle_0 \\ &= e^{D_\mu^0 t}\delta_{\mu,\mu'}P_0[\mu] \end{aligned} \tag{4.26}$$

in agreement with our previous analysis. Similarly, if we return to the frequency representation for $D(z)$, discussed in Sec. III we find first, using Eq. (4.24) in Eq. (3.31) that for uncoupled cells

$$D_0^\delta[\mu|\mu']P_0[\mu'] = D^0[\mu|\mu']P_0[\mu'] \ . \tag{4.27}$$

Turning to the calculation of $D_0^\delta[\mu|\mu']$ we see that the last term on the right in Eq. (3.32) is readily shown, by using Eqs. (4.24) and (3.29) to cancel exactly the first term. Hence D_0^δ vanishes. We see, therefore, in this case that the renormalized operator $D^0[\mu|\mu']$ is given by Eq. (4.25) using both the time and frequency representations.

We have seen, therefore, how in this particular example it is possible to choose a transformation $T[\mu|\sigma]$ which, is clearly appropriate from both a physical point of view and also from a calculational point of view. It is extremely convenient since all non-Markovian terms [i.e., $D^c(z)$] are automatically eliminated.

As soon as the choice of the $\phi_i(\sigma)$ in $T_0[\mu|\sigma]$ becomes tied to the dynamical operator $\tilde{D}_\sigma^0$ the recursion relations for static and dynamic parameters may be coupled. This coupling is not surprising from a general RSRG point of view. If we return to the recursion relations (3.9) we note that they depend on the choice of $\phi_i(\sigma)$ through the quantity ν defined by Eq. (3.11). Then, with $\phi_i(\sigma)$ given by Eq. (3.6), we see that the static recursion relations depend on the arbitrary parameters N and f. The majority rule rather arbitrarily sets $N=\frac{1}{2}$ and $f=1$. Other choices are certainly admissible. In the dynamical case N and f are fixed by the choice of $\tilde{D}_\sigma^0$. We will show elsewhere that this apparent coupling between the statics and dynamics can be eliminated through the proper choice for $\tilde{D}_\sigma^0$.

B. General eigenvalue method

In the last section we showed that through a particular choice of $T_0[\mu|\sigma]$ we could eliminate all non-Markovian behavior in our RSRG transformation for uncoupled cells. We show in this section how one can eliminate non-Markovian behavior to all orders in perturbation theory in the expansion parameter λ introduced in Eqs. (4.1) and (4.2). Similar ideas were used elsewhere in the context of RSRG methods for treating quantum spin systems.[23] Let us assume that we can find a $T[\mu|\sigma]$ satisfying the eigenvalue like equation

$$\tilde{D}[\sigma|\bar{\sigma}]T[\mu|\bar{\sigma}] = \Sigma[\mu|\bar{\mu}]T[\bar{\mu}|\sigma] \ , \tag{4.28}$$

and the normalization condition Eq. (3.18). Using Eq. (4.28) in Eqs. (3.31) and (3.32) we easily find that

$$D^c[\mu|\mu';z] = 0 \ , \tag{4.29}$$

and

$$D[\mu|\mu'] = D^s[\mu|\mu'] = \Sigma[\mu|\mu'] \ . \tag{4.30}$$

Using Eqs. (4.28), (4.30), and (3.18) in Eq. (3.16) leads directly to the very nice result

$$G_t[\mu|\mu'] = e^{D_{\mu'}}\delta_{\mu,\mu'}P[\mu] \ . \tag{4.31}$$

The key result of this paper is that we can obtain a Markovian RSRG transformation mapping D_σ onto D_μ by solving the eigenvalue equation

$$\tilde{D}_\sigma T[\mu|\sigma] = D_\mu T[\mu|\sigma] \tag{4.32a}$$

consistent with the normalization conditions

$$\sum_\mu T[\mu|\sigma] = 1 \ , \tag{4.32b}$$

and

$$\langle T[\mu|\sigma] T[\mu'|\sigma]\rangle = \delta_{\mu,\mu'}P[\mu] \ . \tag{4.32c}$$

The question now is whether we can practically find a $T[\mu|\sigma]$ satisfying Eqs. (4.28), (4.32b), and (4.32c). We discuss here the construction of T using perturbation theory.

We assume that $T[\mu|\sigma]$ and D_μ can be expanded in a power series in λ just as D_σ is expanded in Eq. (4.2). After substituting these expansions into Eq. (4.32) and equating the coefficients of powers of λ we obtain[24]

$$\tilde{D}^0[\sigma|\bar{\sigma}] T_0[\mu|\bar{\sigma}] = D^0[\mu|\bar{\mu}] T_0[\bar{\mu}|\sigma] \ , \tag{4.33}$$

$$\tilde{D}^0[\sigma|\bar{\sigma}] T^{(1)}[\mu|\bar{\sigma}] - D^0[\mu|\bar{\mu}] T^{(1)}[\bar{\mu}|\sigma] = D^{(1)}[\mu|\bar{\mu}] T_0[\bar{\mu}|\sigma] - \tilde{D}^{(1)}[\sigma|\bar{\sigma}] T_0[\mu|\bar{\sigma}] \ , \tag{4.34}$$

etc.

Clearly Eq. (4.33) is equivalent to the zeroth-order result (4.24) and we assume, therefore, that $T_0[\mu|\sigma]$ and $D^0[\mu|\mu']$ are known. The problem is then completely analogous to standard Schrödinger perturbation theory, D_μ corresponding to the eigenvalue, and T to the eigenfunction. In the ordinary perturbation case, one can always choose the higher-order corrections to a given eigenfunction to be orthogonal to the zeroth-order part. This is also the case here. Specifically starting from any zero-order transformation T_0 we can build an operator $\bar{T}[\mu|\sigma]$ which satisfies Eqs. (4.33), (4.34), etc., with $D_\mu^{(n)} \to \bar{D}_\mu^{(n)}$ and the normalization conditions

$$\langle \bar{T}^{(n)}[\mu|\sigma] T_0[\mu'\sigma]\rangle_0 = 0, \quad n > 0 \ , \tag{4.35}$$

$$\langle T_0[\mu|\sigma] T_0[\mu'|\sigma]\rangle_0 = \delta_{\mu,\mu'}P_0[\mu] \ , \tag{4.36}$$

and where $\bar{T}_0 = T_0$. If we then multiply Eq. (4.34) by $T_0[\mu'|\sigma]$ and average over $P_0[\sigma]$ we obtain

$$\sum_\sigma \sum_{\sigma'} P_0[\sigma] T_0[\mu'|\sigma] \tilde{D}^0[\sigma|\sigma'] \bar{T}^{(1)}[\mu|\sigma'] - D^0[\mu|\bar{\mu}] \langle T_0[\mu'|\sigma] \bar{T}^{(1)}[\bar{\mu}|\sigma]\rangle_0 = \bar{D}^{(1)}[\mu|\bar{\mu}] \langle T_0[\mu'|\sigma] T_0[\bar{\mu}|\sigma]\rangle_0 - \sum_\sigma \sum_{\sigma'} P_0[\sigma] T_0[\mu'|\sigma] \tilde{D}^{(1)}[\sigma|\sigma'] T_0[\mu|\sigma'] \ . \tag{4.37}$$

By using the adjoint property of $\tilde{D}^0$ and Eqs. (4.33) and (4.35), it is found that the first term on the left of Eq. (4.37) vanishes. The second term vanishes also because of Eq. (4.35) and we are left with:

$$\bar{D}^{(1)}[\mu|\mu'] P_0[\mu'] = \langle T_0[\mu'|\sigma] \tilde{D}^{(1)} T_0[\mu|\sigma]\rangle_0 \ . \tag{4.38}$$

So, knowing $\bar{D}_\mu^{(1)}$, we can go back to Eq. (4.34) and determine $\bar{T}^{(1)}$. This requires inverting the matrix

$$\bar{D}^0[\sigma|\sigma']\delta_{\mu,\mu'} - D^0[\mu|\mu']\delta_{\sigma,\sigma'} \ ,$$

all of which can be done by using straightforward perturbation theory techniques. The calculations are rather long and they are sketched in the Appendix, where the general expression for $\bar{T}^{(1)}$ is obtained. Of course, to calculate D_μ to first order, one does not need $\bar{T}^{(1)}$, just as one does not need the first-order eigenfunctions to calculate the energy levels to first order. But $\bar{T}^{(1)}$ is needed to obtain $D[\mu|\mu']$ to second order. Once $\bar{T}^{(1)}$ is found, an analysis of the second-order term identical to that carried out above for Eq. (4.34) yields:

$$\bar{D}^{(2)}[\mu|\mu'] P_0[\mu'] = \langle T_0[\mu'|\sigma] \tilde{D}_\sigma^{(2)} T_0[\mu|\sigma]\rangle_0 + \langle T_0[\mu'|\sigma] \tilde{D}_\sigma^{(1)} \bar{T}^{(1)}[\mu|\sigma]\rangle_0 \ . \tag{4.39}$$

It is clear that this procedure can be carried on to any order desired.

There is, however, an additional problem left and that is the transformation function $\bar{T}[\mu|\sigma]$ we have constructed satisfying the normalization conditions (4.35) and (4.36) will not in general satisfy Eq. (3.18). This complication can be remedied by rotating $\bar{T}[\mu|\sigma]$ in μ space into $T[\mu|\sigma]$:

$$T[\mu|\sigma] = S[\mu|\bar{\mu}] \bar{T}[\bar{\mu}|\sigma] \ , \tag{4.40}$$

and determining S through the normalization conditions (3.18) and (3.2) and the sensible requirement that S be a symmetric matrix. In practice the determination of S in a power series in λ is straightfor-

ward. We note then that $T[\mu|\sigma]$ satisfies Eq. (4.32) with

$$D[\mu|\mu'] = S[\mu|\bar{\mu}]\bar{D}[\bar{\mu}|\bar{\mu}']S[\bar{\mu}'|\mu'] \ , \qquad (4.41)$$

and we can easily evaluate $D[\mu|\mu']$ as a power series in λ once the power series in λ for S and $\bar{D}$ are known. This finishes the formal prescription for constructing the new SFO D_μ in perturbation theory.

We have developed in this section a general formalism for carrying out our dynamic RSRG transformation in a way that eliminates all non-Markovian effects thus preserving the time-independent nature of the initial spin-flip operator. The above considerations (together with the Appendix) show that our method can readily be carried out in practice. Furthermore, the physical interpretation of our transformation is transparent: the zeroth-order transformation picks up the slowest independent cell modes. The interested reader can verify that inclusion of $T^{(1)}$ ensures that the transformation selects the slowest two cell mode if the intercell coupling is taken as a perturbation.

Specific calculations using the techniques introduced here are presented in Ref. 17. Additional applications will be given in future work.

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APPENDIX A

Our purpose in this Appendix is to construct the transformation operator $\bar{T}^{(1)}[\mu|\sigma]$, defined by Eqs. (4.34), (4.35), and (4.36). The problem reduces, essentially, to that of finding the inverse operator to $D^0_\sigma - D^0_\mu$. Of course, this operator has $T_0[\mu|\sigma]$ as an eigenvector, with zero eigenvalue. We, therefore, want to project out any component "along T_0" [this is expressed by Eqs. (4.35) and (4.36)]. Hence, we introduce the "transverse" δ function:

$$\delta^T_{\sigma,\sigma'} = \delta_{\sigma,\sigma'} - T_0[\bar{\mu}|\sigma]P_0^{-1}[\bar{\mu}]T_0[\bar{\mu}|\sigma']P_0[\sigma'] \ , \qquad (A1)$$

where sum over barred configurations is implied. We see that δ^T satisfies the condition $\langle T^0\delta^T\rangle_0 = 0$. Then, after using Eq. (4.35) we can write the solution to Eq. (4.34) as:

$$\bar{T}^{(1)}[\mu|\sigma] = G[\sigma\mu|\bar{\sigma}\bar{\mu}] \times (\bar{D}^{(1)}[\bar{\mu}|\bar{\mu}']\delta_{\bar{\sigma},\bar{\sigma}'} - \tilde{D}^{(1)}[\bar{\sigma}|\bar{\sigma}']\delta_{\bar{\sigma},\bar{\sigma}'}) \times T_0[\bar{\mu}'|\bar{\delta}'] \ , \qquad (A2)$$

where $G[\sigma\mu|\sigma'\mu']$ is the Green function

$$K[\sigma\mu|\bar{\sigma}\bar{\mu}]G[\bar{\sigma}\bar{\mu}|\sigma'\mu'] \equiv (\tilde{D}_0[\sigma|\bar{\sigma}]\delta_{\mu,\bar{\mu}} - D^0[\mu|\bar{\mu}]\delta_{\sigma,\bar{\sigma}})G[\bar{\sigma}\bar{\mu}|\sigma'\mu'] = \delta^T_{\sigma,\sigma'}\delta_{\mu'\mu'} \ . \qquad (A3)$$

Formally, the solution to Eq. (A3) is:

$$G[\sigma\mu|\sigma'\mu'] = -\int_0^\infty d\tau e^{K\sigma\mu^\tau}\delta^T_{\sigma,\sigma'}\delta_{\mu,\mu'} \equiv -\int_0^\infty d\tau G[\sigma\mu|\sigma'\mu';\tau] \ . \qquad (A4)$$

During all formal manipulations we can assume that a large negative constant is added, if necessary, to $K[\sigma\mu|\sigma'\mu']$ to ensure convergence. At the end of the calculation, it is set equal to zero. Note that D^0_σ, D^0_μ, and $K_{\sigma\mu}$ are of the form Eq. (4.1). Therefore we can write

$$G[\sigma\mu|\sigma'\mu';\tau] = \prod_i G_i[\sigma\mu|\sigma'\mu';\tau] - \prod_i H_i[\sigma\mu|\sigma'\mu';\tau] \ , \qquad (A5)$$

where i is the cell index. To solve for G_i, we expand in terms of the complete set of cell eigenfunctions $\{\psi^l_i(\sigma)\}$ of $\tilde{D}^i_0$. We then obtain after some algebra the result:

$$G_i[\sigma\mu|\sigma'\mu';\tau] = \sum_l \tfrac{1}{2}e^{-\lambda_l\tau}P^i_0[\sigma']\psi^l_i(\sigma)\psi^l_i(\sigma')(1+e^{\lambda_1\tau}\mu_i\mu_i') \ . \qquad (A6)$$

In a completely similar fashion, we can solve for H_i. The result is the same, except that the sum over the eigenvalue index l is restricted to the $l=0$ ($\lambda_0=0$) and $l=1$ terms only. This completes our solution for $G[\sigma\mu|\sigma'\mu']$ to be used in Eq. (A2). Let us briefly consider the other quantity in Eq. (A2) namely $\tilde{D}^{(1)}_\sigma\delta_{\mu,\mu'} - \bar{D}^{(1)}\delta_{\sigma,\sigma'}$.

The operator $\tilde{D}^{(1)}[\sigma|\sigma']$ in many cases can be written in the form

$$\tilde{D}^{(1)}[\sigma|\sigma'] = -\sum_{i\neq j}\Lambda^{(i,j)}_{\sigma,\sigma'}\tilde{D}^{ij}[\sigma|\sigma'] \ , \qquad (A7)$$

where i and j are neighboring cells. Using the expression (A7) to compute $\tilde{D}^{(1)}_\sigma T_0$, and Eq. (4.38) we

obtain

$$\tilde{D}_{\sigma}^{(1)}[\sigma|\bar{\sigma}]T_0[\mu|\bar{\sigma}]-\tilde{D}^{(1)}[\mu|\bar{\mu}]T_0[\bar{\mu}|\sigma]=-\sum_{i\neq j}T_0^{(i,j)}[\mu|\sigma]\bar{C}_{ij}[\mu|\sigma]\ ,$$
$$\bar{C}_{ij}[\mu|\sigma']=\delta^{T,ij}_{\bar{\sigma},\sigma'}\tilde{D}^{ij}[\sigma|\bar{\sigma}]T_0^{ij}[\mu|\bar{\sigma}]\ . \tag{A8}$$

Substituting the results (A8) and (A6) in Eq. (A2) we obtain

$$\bar{T}^{(1)}[\mu|\sigma]=-\sum_{i\neq j}T_0^{(i,j)}[\mu|\sigma]\bar{C}_{ij}[\bar{\mu}|\bar{\sigma}]\times U^{ij}[\sigma\mu|\bar{\sigma}\bar{\mu}]\ , \tag{A9}$$

where the coefficient U^{ij} is given by, after rather lengthy, but straightforward manipulations

$$U^{ij}[\sigma\mu|\sigma'\mu']=\int_0^{\infty}d\tau\,\tfrac{1}{4}(1+e^{\lambda_1\tau}\mu_i\mu_i')\times(1+e^{\lambda_1\tau}\mu_j\mu_j')e^{\tilde{D}_{ij}\tau}\delta^{T,ij}_{\sigma,\sigma'}\ . \tag{A10}$$

Substituting this expression, and that for $\bar{C}$ [Eq. (A8)] into Eq. (A9) we obtain the result in $\bar{T}^{(1)}$:

$$\bar{T}^{(1)}[\mu|\sigma]=\sum_{i\neq 1}T_0^{[ij]}[\mu|\sigma]t_{\mu}^{ij}(\sigma)\ , \tag{A11}$$

where the matrix elements, $t_{\mu}^{ij}(\sigma)$ are found to be:

$$t_{\mu}^{ij}(\sigma)=\tfrac{1}{4}\sum_{l,m}\psi_i^l(\sigma)\psi_j^m(\sigma)Q(l,m)\left[\frac{1}{\lambda_l+\lambda_m-\lambda_1}(\langle lm|\tilde{D}^{ij}|10\rangle\mu_i+\langle lm|\tilde{D}^{ij}|01\rangle\mu_j)+\frac{\mu_i\mu_j}{\lambda_l+\lambda_m-2\lambda_1}\langle lm|\tilde{D}^{ij}|11\rangle\right]\ . \tag{A12}$$

The matrix elements of $\tilde{D}$ are given by

$$\langle lm|\tilde{D}^{ij}|l'm'\rangle=\sum_{\sigma}\sum_{\sigma'}P_0^l[\sigma]P_0^{l'}[\sigma]\psi_i^l(\sigma)\psi_j^m(\sigma)\tilde{D}^{ij}[\sigma|\sigma']\psi_i^{l'}(\sigma')\psi_j^{m'}(\sigma')\ , \tag{A13}$$

and

$$Q(l,m)=1-(\delta_{l,0}+\delta_{l,1})(\delta_{m,0}+\delta_{m,1})\ . \tag{A14}$$

Equations (A11) and (A12) constitute the final result of this Appendix.

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