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Multiresolution analysis in statistical mechanics. I. Using wavelets to calculate thermodynamic properties

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The wavelet transform, a family of orthonormal bases, is introduced as a technique for performing multiresolution analysis in statistical mechanics. The wavelet transform is a hierarchical technique designed to separate data sets into sets representing local averages and local differences. Although one-to-one transformations of data sets are possible, the advantage of the wavelet transform is as an approximation scheme for the efficient calculation of thermodynamic and ensemble properties. Even under the most drastic of approximations, the resulting errors in the values obtained for average absolute magnetization, free energy, and heat capacity are on the order of 10%, with a corresponding computational efficiency gain of two orders of magnitude for a system such as a 4×4 Ising lattice. In addition, the errors in the results tend toward zero in the neighborhood of fixed points, as determined by renormalization group theory. © *2003 American Institute of Physics.*
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I. INTRODUCTION

Spin models are popular tools for theoretical calculations and for numerical simulations, as their universality classes allow a huge range of different systems—as varied as binary metal alloys, surface adsorption, and neural networks—to be modeled simultaneously. For example, even the ''trivial'' one-dimensional Ising model can be used to model the helix–coil transition in biopolymers; the deep connection between magnetic models and polymer chains allow us to predict scaling behavior and other properties across an even wider range of materials.[1] Lattice models are still widely used in modeling the thermodynamics of complex systems, because their regular structure simplifies the type and nature of interactions among components of the system. Moreover, the difficulty in obtaining analytical solutions of lattice systems, and the relative ease of computational simulations thereof, make them ideal test cases for new simulation algorithms.

Although simulations of lattice models are relatively straightforward to implement, they share the same drawbacks as off-lattice models. The chief drawback is that as the number of particles grows large, the time required to sample the system accurately increases rapidly. A popular approach for addressing this problem is to *coarse-grain* the system; that is, we ''rescale'' the problem by increasing the basic size of a simulation element. For example, we might coarse-grain an atomic representation of a polymer chain into a ''united atom'' model, where a chain molecule is treated as if it consisted only of the backbone. More creative approaches redefine the problem to be addressed; for example, Mattice and co-workers have produced a method which maps a polymer chain atomistically onto a high-coordination lattice. This lattice is then used as the basis for a Monte Carlo simulation; the resulting configuration is then used to map back to continuous space to provide ''evolution in time.'' [2–5]

This paper illustrates the use of the wavelet transform as a mathematical basis for performing thermodynamic computations of lattice models. The wavelet transform is an important tool in *multiresolution analysis*, which analyzes a system simultaneously at several length or frequency scales selected to reflect the actual physical processes underlying the observed behavior as closely as possible. The wavelet transform possesses a number of convenient properties, including orthogonality, compactness, and reconstruction; we will make these concepts more precise in Sec. II B below. The orthogonal nature of most wavelet constructions makes them a logical choice for use in *ab initio* density-matrix quantum chemistry computations, in which the selection of an accurate basis set is crucial to the convergence and efficiency of the calculations.[6–8] Wavelet decompositions have been applied principally in electrical engineering, particularly in the field of signal processing. In this context, white noise and Markov processes have been studied using multiscale methods.[9,10] To date, however, wavelet analysis does not seem to have been extensively applied to models in statistical mechanics. Huang uses wavelet analysis to observe the statistical distribution of multiplicity fluctuations in a lattice gas,[11] while Gamero *et al.* employ wavelets to introduce their notion of *multiresolution entropy*, although their primary goal is dynamic signal analysis rather than statistical mechanics simulations,[12] while O'Carroll attempts to establish a theoretical foundation connecting wavelets to the block renormalization group.[13,14] A more in-depth review of the connection between wavelets and renormalization theory is provided in a recent monograph by Battle.[15]

II. WAVELET TRANSFORM FUNDAMENTALS

A. The conceptual picture

The wavelet transform is a hierarchical method for decomposing a data set into averages and differences. Like the Fourier transform, it can be used to provide a decomposition

in both real space and reciprocal space (**k**-space), or time space and frequency space. Unlike the Fourier transform, however, it is capable of providing simultaneously localized transformations in both real and reciprocal space. A function localized in position space, such as a finite impulse function, cannot be represented by a few terms of its Fourier series; many terms are required before good convergence is achieved. By contrast, in wavelet space, this same function can be almost completely described by just a handful of wavelet coefficients. Although the first wavelet was discovered almost a century ago by Haar,[16] they have become an important computational technique only in the last decade, following the work of Mallat,[17,18] Daubechies,[19] and others.[20–22]

The wavelet transform, like any other transform, takes a mathematical object and transforms it into another; we can represent its action by writing

$$\tilde{u} = \mathcal{W}[u]; \tag{1}$$

the specific form of $\mathcal{W}$ depends both on the type of wavelet we have selected, and the object u which we wish to transform. All versions of the wavelet transform $\mathcal{W}$, however, are derived from the same source: a set of coefficients which define the transform. If u is a discrete data set, such as a signal sampled at regular intervals, then $\mathcal{W}$ is usually represented as a matrix; if u represents a continuous data set, such as the same signal measured at all times, then $\mathcal{W}$ acts as an integral operator. While the matrix form of $\mathcal{W}$ is often called a ''filter bank'' and the integral form a ''wavelet transform,'' we will not distinguish between them in what follows, as the theory developed here for discrete lattices and filter banks should carry over to continuous systems and wavelet transforms essentially unchanged.

Similar to the Fourier transform, the wavelet transform decomposes the object x into two separate components, as two different functions, a scaling function ϕ and a wavelet function ψ, both operate on x. However, the two functions separate its components not into cosines and sines, but into averages and differences, with a ''wavelength'' equal to the ''window'' over which the scaling and wavelet functions are nonzero. In another important distinction, the wavelet transform is *recursive*, so that it can be applied in succession to any set of averages which is produced using that wavelet transform, to produce another level of averages and another level of details.

We shall now make the above concepts more mathematically precise. Let us define u to be a discrete set of samples $u=(u(1),u(2),\ldots,u(n))$. Then applying the scaling and wavelet functions ϕ and ψ to u creates a set of averages $s(i)$ and a set of differences $\delta(i)$,

$$s(i) = \sum_{k=0}^{r-1} \phi(k) u(i+k), \tag{2}$$

$$\delta(i) = \sum_{k=0}^{r-1} \psi(k) u(i+k), \tag{3}$$

where r is a finite integer which defines the length scale, often referred to as the ''size of the support,'' over which ϕ and ψ are nonzero. The index i runs from 1 to n; generally the data set is padded with zeros to ensure that all sums in Eqs. (2) and (3) are well-defined, although periodicity is sometimes used instead.[23] The coefficients $\phi(k)$ and $\psi(k)$ in Eqs. (2) and (3) are related,[19,23] and are central in controlling the features of the wavelet transform. Note the wavelet transform is inherently redundant; for every sample $u(i)$ in the original set u, we now have two values, a local average $s(i)$ and a local difference $\delta(i)$. Since the new data are simply linear combinations of the original values, it is superfluous to retain both sets; at the same time, it is obvious that we cannot simply discard one set of data and recover all the original information using only the other data set. Instead, we choose to keep only the odd-numbered $s(i)$'s and $\delta(i)$'s, eliminating the even-numbered samples; this process is called *downsampling*.[23] Downsampling removes half of the $s(i)$ and half of the $\delta(i)$, regardless of the length r of the wavelet. Now we are left with n data: $s(1),s(3),\ldots,s(n-1)$ and $\delta(1),\delta(3),\ldots,\delta(n-1)$. These n data points can be stored as the level-one wavelet transform $\tilde{u}$ of u, by assigning $s(1),s(3),\ldots,s(n-1)$ to $\tilde{u}^{(1)}(1),\tilde{u}^{(1)}(2),\ldots,\tilde{u}^{(1)}(n/2)$, and the corresponding $\delta(i)$'s as $\tilde{u}^{(1)}(n/2+1),\ldots,\tilde{u}^{(1)}(n)$. [The superscript (1) denotes that the wavelet transform has been applied once to this data set.] We can either stop at this level of description, or continue by further decomposing the averages: then the new object $u^{(1)}$ to be transformed is $u^{(1)}(1)=\tilde{u}(1),\ldots,u^{(1)}(n/2)=\tilde{u}(n/2)$, and so on. Note that although $\tilde{u}^{(1)}$ contains the averages $s(i)$'s and the differences $\delta(i)$'s obtained in the previous step, successive transforms only apply to averages obtained in the previous step. This process can be repeated until we have reduced our set of averages to a single point; no further averaging is possible. We assume henceforth that the data set $u^{(k)}$ has been sufficiently downsampled to retain only the minimum data set required.

B. Properties and examples of wavelet and scaling functions

Until this point, we have not introduced any specific wavelet or scaling functions. Before we do so, we note that the choice of a wavelet transform to apply to a given system usually hinges on the desired properties which one wishes to include in the transformed data. Three principal properties are almost universally required for filter banks and wavelet families:[19,23]

(1) *Perfect reconstruction*: No data are distorted by performing analysis followed by synthesis, so that the only permissible change is a delay in recovery of the original sample.
(2) *Orthogonality*: Wavelets computed at different length scales or at different spatial locations are mutually orthogonal; thus fluctuations in the system are localized at the scales where they are most relevant.
(3) *Compact support*: Properly designed wavelets are identically zero except for a finite interval, which means that exact results can be obtained using only a finite number of terms.

Other properties, such as orthonormality, symmetry in

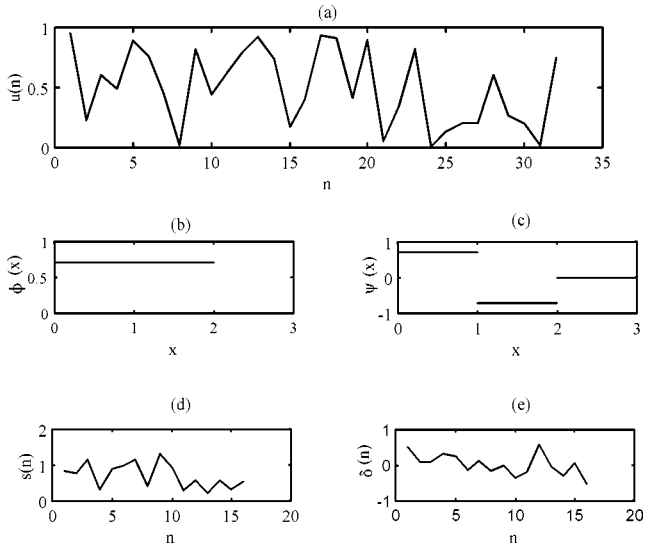

FIG. 1. (a) A sample signal $u(n)$. (b), (c) The one-dimensional Haar scaling function $\phi(x)$ and wavelet (differencing) function $\psi(x)$. (d), (e) The first-level scaling coefficients $s(n)$ and $\delta(n)$ produced from the original signal $u(n)$ using the Haar pair, following downsampling of the signal.

the functional form of the wavelet or a certain number of vanishing moments, can be taken into account when constructing the wavelet transform.[24]

The two most commonly encountered selections are the Haar and Daubechies wavelets, named after their respective discoverers. The Haar pair is the oldest and simplest set of wavelets:[16] the coefficients of the scaling function are $\phi=(\phi(0),\phi(1))=(1/\sqrt{2})\,(1,1)$, while the coefficients of the wavelet function are $\psi=(\psi(0),\psi(1))=1/\sqrt{2}\,(-1,1)$. No other wavelet can be described with two points, and therefore no other wavelet has a support as compact as the Haar wavelet. The scaling function ϕ simply averages the values stored at neighboring points, while ψ finds the difference between those values; the extra factor of $\sqrt{2}$ is incorporated to ensure orthonormality between overlapping $\phi(k)$ and $\psi(k)$. A simple example of the action of the Haar wavelet is shown in Fig. 1.

The Daubechies wavelets are a family of orthonormal functions whose construction was explicitly designed to have orthogonality as well as vanishing higher-order moments.[25] Daubechies was able to show that the Haar wavelet is in fact the "first" member of the Daubechies family; that is, the Haar wavelet is the Daubechies wavelet with the shortest support. The second such member has four terms in its definition; the scaling function is defined by $\phi=(\phi(0),\phi(1),\phi(2),\phi(3))=(1/4\sqrt{2})(1+\sqrt{3},3+\sqrt{3},3-\sqrt{3},1-\sqrt{3})$. The wavelet function reverses the order of the coefficients and inverts the sign of every other component, which allows the orthonormality properties to be satisfied: $\psi=(\psi(0),\psi(1),\psi(2),\psi(3))=(-\phi(3),\phi(2),-\phi(1),\phi(0))$. We can see that the Haar wavelet obeys the same pattern as the Daubechies wavelet, $\psi_H=(-\phi(1),\phi(0))$. This pattern can be extended, using different coefficients but the same general sign rules, for wavelets with 6, 8, 10, ... coefficients. The resulting wavelet and scaling functions become increasingly smooth, and therefore are better suited for data sets in which there is only a gradual change in the data set with position—in thermodynamic systems, this would be more useful for, say, a spin-N Ising model than a spin-$\frac{1}{2}$ Ising model (presuming that $N\gg\frac{1}{2}$).

C. Matrix formulation of the wavelet transform

For discrete systems, a conceptually simple method of implementing the wavelet transform is to set up the transform as a matrix equation. The input u is converted into a column vector $\mathbf{u}$, so that the elements $s(i)$ and $\delta(i)$ are obtained via the dot product of $\mathbf{u}$ with vectors $\mathbf{h}(i)$ and $\mathbf{l}(i)$, where the vectors are padded so that the first nonzero element is located at position i,

$$\mathbf{h}(i)=(0,\ldots,0,\phi(0),\phi(1),\ldots,\phi(r-1),0,\ldots,0),$$

$$\mathbf{l}(i)=(0,\ldots,0,\psi(0),\psi(1),\ldots,\psi(r-1),0,\ldots,0).$$

The vectors $\mathbf{s}$ and $\boldsymbol{\delta}$, which contain the wavelet-transformed coefficients of the decomposition, can be obtained by forming the matrices $\mathbf{H}$ and $\mathbf{L}$ and right-multiplying by the vector $\mathbf{u}$,

$$\mathbf{s}=\mathbf{H}\mathbf{u} \quad \text{and} \quad \boldsymbol{\delta}=\mathbf{L}\mathbf{u},$$

where the rows of the matrices $\mathbf{H}$ and $\mathbf{L}$ are the vectors $(\mathbf{h}(1),\ldots,\mathbf{h}(n))$ and $(\mathbf{l}(1),\ldots,\mathbf{l}(n))$, respectively. As mentioned in the previous section, we do not need to keep all of the $s(i)$'s and $\delta(i)$'s in order to obtain perfect reconstruction of our signal; thus, we can obtain all the necessary coefficients in a single matrix multiplication by combining the relevant rows of $\mathbf{H}$ and $\mathbf{L}$ into a single matrix $\mathbf{W}^{(1)}$, whose rows are $(\mathbf{h}(1),\mathbf{h}(3),\ldots,\mathbf{h}(n-1),\mathbf{l}(1),\mathbf{l}(3),\ldots,\mathbf{l}(n-1))$. Thus, the wavelet transformation (1) can be written as

$$\begin{bmatrix} s(1) \\ \vdots \\ s(n-1) \\ \delta(1) \\ \vdots \\ \delta(n-1) \end{bmatrix} = \begin{bmatrix} \mathbf{h}(1) \\ \vdots \\ \mathbf{h}(n-1) \\ \mathbf{l}(1) \\ \vdots \\ \mathbf{l}(n-1) \end{bmatrix} \begin{bmatrix} u(1) \\ u(2) \\ \\ \vdots \\ \\ u(n) \end{bmatrix}. \tag{4}$$

We will denote the product on the left-hand side of (4) as $\tilde{\mathbf{u}}$.

As stated above, the wavelet process can be applied recursively: the set of averages $(s(1),s(3),\ldots,s(n-1))$ can be treated as a new data sample $\mathbf{u}^{(1)}=(u^{(1)}(1),\ldots,u^{(1)}(n/2))$, and operated on by an $(N/2)\times(N/2)$ reduction of $\mathbf{W}^{(1)}$, which we denote $\mathbf{W}^{(2)}$, to produce a new set of $n/4$ averages $(s^{(2)}(1),s^{(2)}(3),\ldots,s^{(2)}(n/2-1))$ and corresponding new set of $n/4$ differences $(\delta^{(2)}(1),\delta^{(2)}(3),\ldots,\delta^{(2)}(n/2-1))$. To reconstruct the original data set, we combine these $n/2$ values along with the $n/2$ differences $(\delta^{(1)}(1),\delta^{(1)}(3),\ldots,\delta^{(1)}(n-1))$ obtained from applying $\mathbf{W}^{(1)}$. This process can be repeated as many times as desired, dividing the m nondownsampled averages $\mathbf{s}^{(k)}$ into $m/2$ averages $\mathbf{s}^{(k+1)}$ and $m/2$ differences $\delta^{(k+1)}$. However, since at each iteration the matrix $\mathbf{W}^{(k)}$ only operates on selected elements of the vector $\tilde{\mathbf{u}}^{(k)}=\mathbf{W}^{(k-1)}\mathbf{u}^{(k-1)}$, computations for multiple levels can be performed at the same time. Thus, if we wish to apply the wavelet transform K times, we can write this operation as an extended matrix product,[26]

$$\tilde{\mathbf{u}}^{(K)} = \mathbf{W}\mathbf{u} = \prod_{k=1}^{K} \mathbf{Q}^{(k)}\mathbf{u}, \tag{5}$$

where the $\mathbf{Q}^{(k)}$ are a family of matrices of the form,

$$\mathbf{Q}^{(k)} = \begin{bmatrix} \mathbf{W}^{(k)} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}. \tag{6}$$

In (6), $\mathbf{Q}^{(k)}$ is always an $N \times N$ matrix, while the matrix $\mathbf{W}^{(k)}$ has size $(N/2^{k-1}) \times (N/2^{k-1})$.

To recover the original data sample $\mathbf{u}$ following a wavelet transform $\mathbf{W}$, we can simply multiply $\tilde{\mathbf{u}}$ by the inverse of the wavelet matrix $\mathbf{W}$. The matrix $\mathbf{W}$ is unitary, that is, its inverse $\mathbf{W}^{-1}$ is equal to its transpose $\mathbf{W}^{T}$. Consequently, if $\mathbf{W}$ is known, all that is necessary to reverse the transformation is to left-multiply $\tilde{\mathbf{u}}^{(k)}$ by the transpose $\mathbf{W}^{T}$. Moreover, the computation (4) of the wavelet transform can usually be carried out ''in place'' by manipulating local coordinates; in this manner, the computation is carried out even more rapidly than a standard multiplication, and without the increased storage costs associated with matrix multiplications.[27,28]

D. Multidimensional wavelet transforms

Since virtually all problems in lattice thermodynamics are in multiple dimensions, it is necessary to take the wavelet transform of a multivariate function or data set. Several methods have been developed to carry out such transformations; among them are Cohen and Daubechies's *separable wavelets*, which form the multidimensional scaling and wavelet functions $\phi(x,y)$, $\psi_{xx}(x,y)$, $\psi_{xy}(x,y)$, and $\psi_{yy}(x,y)$ from products of the one-dimensional scaling and wavelet functions $\phi(x)$ and $\psi(x)$.[20] A more general algorithm, the *lifting algorithm*, has been developed by Sweldens.[29,30] It divides the wavelet transform into two steps: the first computes the wavelet coefficients $\delta(i)$; the second step uses the wavelet coefficients to speed up the calculation of the scaling coefficients. ''Initialization'' of the lifting algorithm requires the use of an appropriately selected basis function.

A particularly convenient basis function for the multidimensional lifting transform is the generalized orthogonal Haar wavelets outlined by Sweldens.[29] An extension of the one-dimensional wavelet transform, they can be created in any number of dimensions, and have the same basic orthonormality properties as the one-dimensional Haar functions, although the orthonormality constant becomes $2^{-d/2}$, where d is the dimensionality of the system. (The two-dimensional version is shown in Fig. 2.) Moreover, the use of the Haar wavelets as a starting point for further iterations of the lifting algorithm allows the development of additional, ''better'' lifted wavelets with more desirable properties, such as smoothness.

It can further be seen that the ''oversampling'' problem which exists in one dimension will be magnified in multiple dimensions; since the number of wavelet functions which are produced from each data point increases by a factor of 2 with each additional dimension added, we must reduce the number of points maintained for each wavelet function by that same factor. Thus, in two dimensions, we keep only every fourth point; in three dimensions, every eighth point, and so on. The wavelet transform for multidimensional systems can thus still be written in the form of (5) and (6), after we have written the multidimensional data set in terms of a column vector. This can be accomplished by wrapping around the edges of the matrix in creating $\mathbf{u}$; for example, after inserting element $(1,N)$ of a two-dimensional data set into $\mathbf{u}$, we next store element (2,1), and so forth. The other significant difference in the structure of these equations is that the size of the submatrix $\mathbf{W}^{(k)}$ in (6) is now $N/2^{(k-1)d} \times N/2^{(k-1)d}$ instead of $N/2^{k-1} \times N/2^{k-1}$.

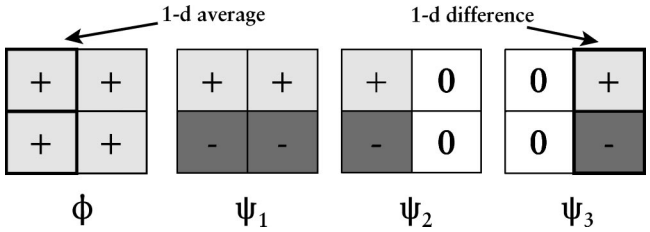

FIG. 2. The two-dimensional orthogonal Haar wavelets. The coefficient in all cases is 1/2, times the sign indicated in each quadrant. Note that the scaling function ϕ is built from the one-dimensional Haar scaling function, while the wavelet functions are built from the one-dimensional wavelet function.

III. WAVELET ANALYSIS OF LATTICE THERMODYNAMICS

A. Applying the wavelet transform to Hamiltonians

The standard model for studying the thermodynamic behavior of lattice systems is the spin-$\frac{1}{2}$ Ising model, which contains both nearest-neighbor pairwise interactions as well as interactions between lattice sites and an external field. The Hamiltonian for this system is normally written in the form,

$$-\beta\mathcal{H} = h\sum_{i} \sigma_i + J\sum_{\langle ij \rangle} \sigma_i\sigma_j, \tag{7}$$

where h is the strength of the external field in the direction of the spins σ_i, and J is the strength of the interaction between nearest-neighbor pairs of spins on the lattice; these pairs are indicated by the subscript $\langle ij \rangle$ in the second summation in Eq. (7). The inverse temperature $\beta = (k_B T)^{-1}$; for convenience we let $k_B = 1$, so that temperature, external field, and nearest-neighbor interactions are all dimensionless quantities. The model can be further extended by the inclusion of a position-dependent external field, or by the inclusion of pairwise interactions beyond nearest neighbors. In this case, Eq. (7) can be written in the more general form,

$$-\beta\mathcal{H} = \sum_{i} h_i\sigma_i + \sum_{i}\sum_{j} J_{ij}\sigma_i\sigma_j, \tag{8}$$

where in Eq. (8) h_i is the strength of the external field at lattice site i, and J_{ij} is the strength of the interaction between sites i and j. Analytical solutions of Eq. (7) are well-known for one-dimensional systems and two-dimensional systems when $h = 0$;[31,32] it has recently been suggested that analytic solutions do not exist for more complicated systems.[33]

While Eqs. (7) and (8) are compact representations of the Hamiltonian of the system, the expansion of the lattice variables σ_i and σ_j as a sum of wavelet coefficients makes these equations impractical for applying the wavelet transformation. Since the system is described discretely, we want to use discrete wavelets, and therefore a matrix formulation of the Hamiltonian would be convenient. Using graph theory,[34] this is readily accomplished. Let the vectors $\mathbf{u}=(\sigma_1,\sigma_2,\ldots,\sigma_N)$ and $\mathbf{h}=(h_1,\ldots,h_N)$ denote the values of each of the N lattice variables in the system and the set of external-field interaction strengths, respectively, constructed in the rowwise manner described in the previous section. Furthermore, define the matrix $\mathbf{J}$ such that element J_{ij} is the strength of the interaction between site i and site j. If these sites do not interact, then $J_{ij}=0$. Then, the Hamiltonian (8) can be written in the form of a matrix equation,

$$-\beta\mathcal{H}=\mathbf{h}^T\mathbf{u}+\mathbf{u}^T\mathbf{J}\mathbf{u}, \tag{9}$$

where the superscript T denotes the transpose of the vector (or matrix) which precedes it.

The matrix $\mathbf{W}$ which defines the wavelet transform satisfies by construction $\mathbf{W}^T\mathbf{W}=\mathbf{I}$, where $\mathbf{I}$ is the identity matrix. Therefore, to apply the wavelet transform, we simply insert $\mathbf{W}^T\mathbf{W}$ between each pair of terms in Eq. (9), thereby obtaining

$$-\beta\mathcal{H}=(\mathbf{h}^T\mathbf{W}^T)(\mathbf{W}\mathbf{u})+(\mathbf{u}^T\mathbf{W}^T)(\mathbf{W}\mathbf{J}\mathbf{W}^T)(\mathbf{W}\mathbf{u}). \tag{10}$$

Using the general matrix property that $\mathbf{B}^T\mathbf{A}^T=(\mathbf{A}\mathbf{B})^T$, Eq. (10) can be rewritten in terms of the wavelet-transformed vectors $\tilde{\mathbf{h}}^{(K)}=\mathbf{W}\mathbf{h}$, $\tilde{\mathbf{u}}^{(K)}=\mathbf{W}\mathbf{u}$, and the wavelet-transformed matrix $\tilde{\mathbf{J}}^{(K)}=\mathbf{W}\mathbf{J}\mathbf{W}^T$,

$$-\beta\tilde{\mathcal{H}}=(\tilde{\mathbf{h}}^{(K)})^T\tilde{\mathbf{u}}^{(K)}+(\tilde{\mathbf{u}}^{(K)})^T\tilde{\mathbf{J}}^{(K)}\tilde{\mathbf{u}}^{(K)}. \tag{11}$$

It is important to note that in writing Eq. (11), we have not made any explicit assumptions about the form of the matrix $\mathbf{W}$, other than to require it to be a matrix describing a wavelet transform. As a result, we can perform several levels of multiresolution simultaneously through appropriate preparation of the matrix $\mathbf{W}$ in the manner outlined above. Using the inverse wavelet transform $\mathbf{W}^{-1}=\mathbf{W}^T$ to recover an original configuration $\mathbf{u}$ is a one-to-one mapping only if we are provided with n distinct data points, as contained in $\tilde{\mathbf{u}}^{(K)}$.

Examining Eq. (11), we see that the result of applying the wavelet transform to a set of spins $\mathbf{u}$ is to create a new representation $\tilde{\mathbf{u}}^{(K)}$, which contains the same information about the spins as does the original state vector $\mathbf{u}$. However, the vector $\tilde{\mathbf{u}}^{(K)}$ contains $n/2^{dK}$ averages, where d is the dimensionality of the lattice; these averages can be viewed as ''block spins'' in a sense similar to that of Kadanoff.[35] The remaining elements of $\tilde{\mathbf{u}}^{(K)}$ contain the local differences in the spins; that is, they can be used to describe the specific set of spins which give rise to a particular block spin $\tilde{s}_i^{(K)}$.

B. Computing thermodynamic functions

The canonical partition function,

$$Z=\sum_{\mathbf{u}\in\mathbb{S}}\exp(-\beta\mathcal{H}(\mathbf{u})), \tag{12}$$

where $\mathbb{S}$ is the configuration space of the system, can be used to derive all the thermodynamic properties of a lattice system. Applying the wavelet transform $\mathbf{W}$ to the state vector $\mathbf{u}$ results in a new state vector $\tilde{\mathbf{u}}^{(K)}$ belonging to the configuration space $\tilde{\mathbb{S}}^{(K)}$. Provided that $\mathbf{W}$ satisfies the perfect reconstruction property, if the summation over $\mathbf{u}\in\tilde{\mathbb{S}}$ in Eq. (12) is replaced with the summation over $\tilde{\mathbf{u}}^{(K)}\in\tilde{\mathbb{S}}^{(K)}$, the results will be identical. This result follows naturally, since perfect reconstruction necessarily implies that there is a unique state vector $\tilde{\mathbf{u}}^{(K)}\in\tilde{\mathbb{S}}^{(K)}$ for each state vector $\mathbf{u}\in\mathbb{S}$, and by construction of the wavelet-transformed Hamiltonian (11), $-\beta\mathcal{H}=-\beta\tilde{\mathcal{H}}^{(K)}$.

Ensemble averages involving wavelet-transformed variables are in general no more complicated than computations involving the original variables. In general, the transformation of a function (or functional) of the original variables $f(\mathbf{u})$ or $f[u]$ will generally have the same characteristics after applying the wavelet transform to obtain $\tilde{f}^{(K)}(\tilde{\mathbf{u}}^{(K)})$ or $\tilde{f}^{(K)}[\tilde{u}^{(K)}]$. Moreover, the standard properties of ensemble averaging, such as linearity, also apply, which makes calculations of moments of the distribution particularly simple.

The above formulation can be applied to any system whose Hamiltonian can be written in the form of Eq. (8), or as the sum of contributions, each of which is of that form. While the wavelet transform can be applied to any lattice system whose Hamiltonian is a function of the components of the state vector $\mathbf{u}$—or, indeed, to any Hamiltonian which is a functional of $\mathbf{u}(\mathbf{r})$ for continuous systems—in most of these cases, it is necessary to rely on the more cumbersome series expansions, or integral transforms in the case of continuous systems.

In addition, for Ising spin variables, the use of the wavelet transform poses an additional challenge. While it is entirely straightforward to describe the possible values an individual lattice site can take—for a spin-q Ising model, the allowed values of an individual spin σ are $-q$, $-q+1,\ldots,q-1$, q—the rules which determine whether an arbitrarily selected ''transformed'' state vector $\tilde{\mathbf{u}}^{(K)}$ represents a real state vector $\mathbf{u}$ are cumbersome to manipulate and to implement, and have proven a formidable challenge in prior research as well.[36]

IV. ANALYSIS

In this section, we use two variants of the two-dimensional Ising model as a basis for our calculations: we look at 4×4 and 32×32 Ising lattices; the former is used for calculations when it is desired to perform calculations over all states explicitly, while the latter is illustrative of larger systems, for which exact calculations are intractable. The emphasis in this paper will be on the use of wavelets to yield approximate answers in significantly faster time than is possible with a Monte Carlo simulation incorporating all degrees of freedom explicitly. The methodology by which the wavelet transform can be extended to Monte Carlo simulations of lattice systems is the focus of the companion paper.[37]

Before proceeding to the results of the calculations, we make note of the time required to execute the simulations.

Each of Figs. 3–6 plots the observed variables in the temperature range $T=0.50$ to $T=5.00$, with a step size of $\Delta T=0.01$. The computations for the original problem, with $2^{16}=65\,536$ states to consider explicitly, required more than 6.8 s per point to execute the required calculations on a 733 MHz Pentium III; the same calculations using one and two applications of the wavelet transform required just 0.061 and 0.026 s per point to consider $5^4=625$ and 17 states, respectively.

A. Weighting functions for wavelet-transformed statistics

Until now, we have worked with wavelet transforms which preserve the number of degrees of freedom between the original and transformed problems. This approach yields results for the wavelet-transformed system in exact agreement with those for the original system. However, as mentioned above, in such cases the transformed equations are usually harder to model than the original ones. Hence it is desirable to use the wavelet transform not only as a means of describing a lattice system, but also to derive an approximation scheme whereby estimates of thermodynamic properties can be made efficiently, while still offering error estimates that bound the true results.

The approach we adopt in this paper is to ignore all local differences, that is, we assume that $\delta_i^{(k)}=0$ for all values of i and k. As a secondary assumption, we assume that correlation functions which include wavelet coefficients are also equal to zero, that is, we assume $\langle \delta_i^{(k)} A(\cdot)\rangle=0$ for any choice of property $A(\cdot)$. These extreme assumptions represent a ''worst-case scenario'' for the use of the wavelet transform method; any more accurate representation of the behavior of the wavelet coefficients will lead to similarly more accurate results in the calculations we present below. Note that under certain circumstances, these approximations are accurate; for Hamiltonians of the form (8) which do not exhibit interactions with an external field, there exist configurations with equal energies but opposite signs for $\delta_i^{(k)}$; consequently, when we take the average over all configurations, the ensemble average of $\delta_i^{(k)}$ will vanish.

Let us assume that we have applied the wavelet transform to our original Hamiltonian, $\mathcal{H}(\mathbf{s})$, and have obtained a new function $\tilde{\mathcal{H}}^{(K)}(\tilde{\mathbf{u}}^{(K)})$. If we then make our approximation that all the wavelet coefficients are negligible, we can reduce $\tilde{\mathcal{H}}^{(K)}(\tilde{\mathbf{u}}^{(K)})$ to a new function $\tilde{\mathcal{H}}^{(K)}(\tilde{\mathbf{s}}^{(K)})$, where $\tilde{\mathbf{s}}^{(K)}$ represents the set of all averages $(s_1^{(K)},\ldots,s_m^{(K)})$ that were preserved by the wavelet transform. We know that the partition function of the system before we performed the wavelet transform is given by Eq. (12); after using the wavelet transform, we hypothesize that the partition function of the new system is given by

$$\tilde{Z}=\sum_{\tilde{\mathbf{s}}^{(K)}\in\tilde{\mathbb{S}}^{(K)}} w(\tilde{\mathbf{s}}^{(K)})\exp(-\beta\tilde{\mathcal{H}}^{(K)}(\tilde{\mathbf{s}}^{(K)})), \tag{13}$$

where the $w(\tilde{\mathbf{s}}^{(K)})$ is the weight of configuration $\tilde{\mathbf{s}}^{(K)}$ in the configuration space $\tilde{\mathbb{S}}^{(K)}$. Since multiple configurations $\mathbf{u}\in\mathbb{S}$ can correspond to the same $\tilde{\mathbf{s}}^{(K)}$, we cannot set $w(\tilde{\mathbf{s}}^{(K)})=1$ as we did in the untransformed Ising model. Clearly, the new partition function (13) will be identical to the original partition function (12) if we define

$$w(\tilde{\mathbf{s}})=\sum_{\mathbf{u}:\mathbf{u}\to\tilde{\mathbf{s}}^{(K)}} \exp[-\beta(\mathcal{H}(\mathbf{u})-\tilde{\mathcal{H}}^{(K)}(\tilde{\mathbf{s}}^{(K)}))], \tag{14}$$

where the notation $\mathbf{u}:\mathbf{u}\to\tilde{\mathbf{s}}^{(K)}$ denotes that the sum is to be performed over all configurations $\mathbf{u}$ which have the same set of wavelet-transformed averages $\tilde{\mathbf{s}}^{(K)}$. However, evaluating (14) to obtain the weighting functions is no more tractable than the computation of the original partition function. Thus, any computational efficiency to be gained is by finding an economical approximation for Eq. (14). One such approach is to take $w(\tilde{\mathbf{s}}^{(K)})$ to be equal to the number of states $\mathbf{s}$ whose wavelet transform yields $\tilde{\mathbf{s}}^{(K)}$, so that Eq. (13) is the standard form of the canonical partition function for a system with degenerate energy levels. Let us call the number of such states $\mathbf{s}$ with equivalent averages $\tilde{\mathbf{s}}^{(K)}$ the degeneracy of state $\tilde{\mathbf{s}}^{(K)}$, and denote this degeneracy as $g(\tilde{\mathbf{s}}^{(K)})$. The restriction of $\tilde{\mathbf{u}}^{(K)}$ to the averages $\tilde{\mathbf{s}}^{(K)}$ prevents a unique reconstruction of $\mathbf{u}$, unless $g(\tilde{\mathbf{s}}^{(K)})=1$.

B. Order parameter

A natural variable to compute is the order parameter, generically denoted η, which for lattice spin systems is the average magnetization,

$$m=\frac{1}{N}\left\langle \sum_i \sigma_i \right\rangle; \tag{15}$$

for other members of the Ising universality class, the order parameter can represent the overall density ρ or the difference between the densities of two phases.[38] While the computation of the order parameter is straightforward in simulations, its calculation can be made difficult in the case of zero external field because of symmetries in the configuration space; for every configuration with magnetization m_i, there exists another configuration with the same energy and magnetization $-m_i$. As a result, when all the states are combined using Eq. (15), we do not observe spontaneous magnetization, but instead find $m=0$ at all temperatures. Thus, we consider the absolute value of the magnetization, $|m|$, in place of the magnetization m. The results of this calculation for the 4×4 Ising model with the wavelet transform, setting all $\delta_i^{(k)}$'s to zero, and without the wavelet transform are shown in Fig. 3. We note that the error is essentially negligible for temperatures below $T=1$, and decreases again for large values of T, where differences in energy levels become negligible and the average magnetization of a state is the only contributing factor to $|m|$.

C. Free-energy considerations

The Helmholtz free energy is just the logarithm of the partition function, $A=-k_BT\ln Z$; if we estimate the partition function using an expression such as Eq. (13), we naturally expect the approximated value A to differ from its true value. When we examine the behavior of the 4×4 Ising model under the wavelet transform, we find as expected that the two free energy surfaces are similar, although they are clearly not

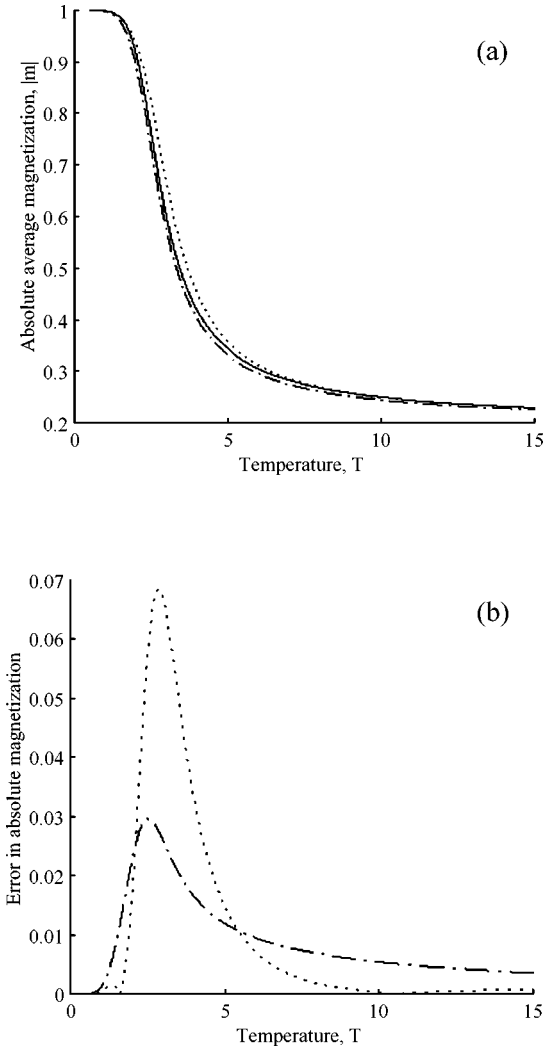

FIG. 3. (a) Average absolute magnetization $|m|=\Sigma_i|\sigma_i|$ of the 4×4 Ising model at zero external field as a function of temperature, as computed by an exact enumeration using no wavelet transform (solid line), and using one and two iterations of the two-dimensional Haar wavelet (dot-dashed and dotted lines, respectively). (b) Error in the average absolute magnetization of the 4×4 Ising model for one and two iterations of the two-dimensional Haar wavelet vs an exact enumeration.

identical. In particular, the exact numerical values obtained from the two equations are not the same. However, since the assignment $A=0$ is arbitrary in any system, we can choose to define $A=0$ as either the maximum or the minimum free energy obtained in each system. Under these conditions, the energy scales for the exact calculation and the wavelet transform calculation are essentially identical, particularly at the so-called ''fixed points'' of the system—that is, for points which are not affected by renormalization transformations.[39] For the two-dimensional Ising model, these points are at $T=0$, and at infinite (positive or negative) values of the external field interaction h.

This agreement at the fixed points should not be surprising; the fixed points correspond to unique configurations of the system, such that for the configurations $\tilde{\mathbf{s}}^{(K)}$ which result from the wavelet transform of the fixed points $\mathbf{u}^*$, the degeneracy of the states is unity. Consequently, the approximation $w(\tilde{\mathbf{s}}^{(K)})=g(\tilde{\mathbf{s}}^{(K)})$ is correct for the dominant configuration in the system, and therefore the behavior of the approximate partition function Z' is almost identical to that of the true partition function Z in the vicinity of the fixed points.

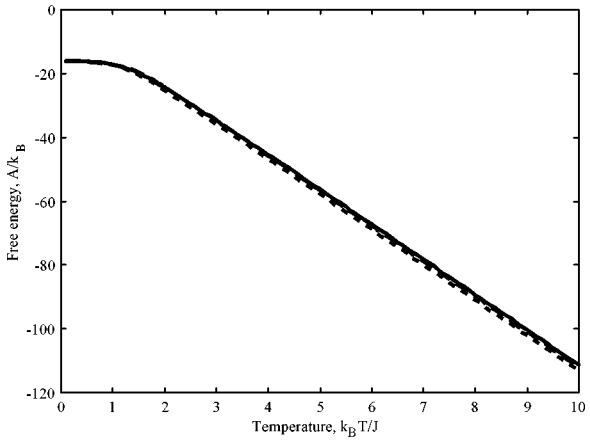

FIG. 4. Free energy A of the 4×4 Ising model at zero external field as a function of temperature, as computed by an exact enumeration using no wavelet transform (solid line), and using one and two iterations of the two-dimensional Haar wavelet (dashed and dot-dashed lines, respectively).

As can be seen in Fig. 4, the free energy converges to the same values in the low-temperature limit, where only a few states which are essentially unaffected by the wavelet transform contribute to the partition function of the system. At high temperatures, the agreement is less exact, because of the approximations made in evaluating the Boltzmann factors of the block spin configurations.

D. Entropy of a wavelet-transformed lattice system

It is relatively straightforward to show that coarse-graining a system with a countable phase space—that is, a phase space whose states can be completely enumerated—requires a correction factor to ensure satisfactory agreement with results from the fine-scale system. As an example, consider the entropy of a wavelet-transformed spin-$\frac{1}{2}$ Ising model. The original lattice has 2^{N_t} total configurations, and therefore in the high-temperature limit, the entropy approaches

$$S_{\max}=k_B N_t \ln 2. \tag{16}$$

If we ignore the weighting factor of the wavelet-transformed system by setting $w(\tilde{\mathbf{s}}^{(K)})=1$ for all states $\tilde{\mathbf{s}}^{(K)}$, the resulting system will have $(1+\Pi_{i=1}^{K-1}N^{(i)})^{N^{(K)}}$, and the maximum possible entropy for this system is

$$S_{\max}^{(K)}=k_B N^{(K)} \ln\left(\prod_{i=1}^{K-1} N^{(k)}+1\right). \tag{17}$$

Comparing Eq. (17) to the original limit of $S_{\max}=k_B N_t \ln 2$, we must have $S_{\max}>S_{\max}^{(K)}$, since the configuration space is smaller, which indicates that our coarse-graining has effectively reduced the available entropy of the system. We can conclude from this that unless the volume of phase space is conserved by the coarse-graining procedure, some entropy will be lost at high temperatures, regardless of the accuracy of the coarse-graining. Our choice of the degeneracy $g(\tilde{\mathbf{s}}^{(K)})$

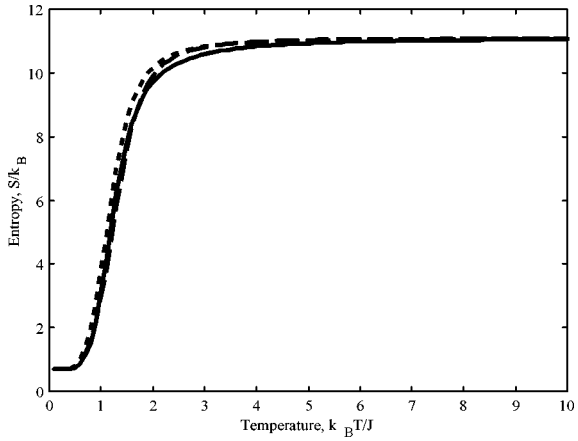

FIG. 5. Entropy of the 4×4 Ising model at zero external field as a function of temperature, as computed by an exact enumeration using no wavelet transform (solid line), and using one and two iterations of the two-dimensional Haar wavelet (dashed and dot-dashed lines, respectively). The bottom of the y-axis corresponds to the zero-temperature limit of $S=\ln 2$.

for the weighting function $w(\tilde{\mathbf{s}}^{(K)})$ preserves the volume of phase space in the limit of $T\to\infty$ for the systems under study here.

Looking at the specific case of the 4×4 Ising model, we compute the entropy as a function of temperature for zero external field for the exact problem, and for the wavelet-transformed problem using one and two iterations of the two-dimensional Haar wavelet. The results are shown in Fig. 5. As before, we find that errors vanish in the low-temperature limit, where only the lowest-energy states make a contribution to the partition function; since there are two such states, namely those with all spins up and all spins down, we find that the $T\to0$ limit of the entropy is

$$S(T\to0)\approx-\sum_{i=1}^{2}\tfrac{1}{2}\ln\tfrac{1}{2}=\ln 2.$$

In the high-temperature limit, the entropies agree because, by construction, we have $\Sigma_{\tilde{\mathbf{s}}\in\tilde{\mathbb{S}}}w(\tilde{\mathbf{s}})=2^{16}$, and therefore, since the Boltzmann factor goes to unity for all states as $T\to\infty$, $Z\to\Sigma_{\tilde{\mathbf{s}}\in\tilde{\mathbb{S}}}w(\tilde{\mathbf{s}})$, and the entropy tends toward the value $S_{\max}$ given by Eq. (16). Disagreement in the intermediate temperature regime is largely the result of grouping together states with different energies into a single transformed state with a single energy. In particular, the mapping of higher-energy states to a lower energy increases the probability of being in those states, and therefore increases the total entropy of the system. This explains the seemingly anomalous result of coarse-graining increasing the entropy at intermediate temperatures observed in Fig. 5.

For more general systems, we can consider the formal definition of the entropy for a continuous distribution,

$$S=-k_B\int_{\mathbf{u}\in\mathbb{S}}d\mathbf{u}p(\mathbf{u})\ln p(\mathbf{u}), \tag{18}$$

where $p(\mathbf{u})$ is the probability of observing the configuration $\mathbf{u}$. For the original Ising model, each configuration $\mathbf{u}$ is unique, and therefore the probability $p(\mathbf{u})$ is just the Boltzmann weight $Z^{-1}\exp(-\beta\mathcal{H}(\mathbf{u}))$, and thus the entropy is given by

$$S=k_B\ln Z+\frac{k_B}{Z}\int_{\mathbf{u}\in\mathbb{S}}d\mathbf{u}\beta\mathcal{H}(\mathbf{u})\exp(-\beta\mathcal{H}(\mathbf{u})). \tag{19}$$

After performing the wavelet transform, and discarding finer-scale details, we must account for the weighting factor $w(\tilde{\mathbf{s}})$ in our expression for the entropy. Consequently, the entropy for such a system is given by

$$\begin{aligned}S^{(K)}&=-k_B\int_{\tilde{\mathbf{s}}\in\tilde{\mathbb{S}}}d\tilde{\mathbf{s}}w(\tilde{\mathbf{s}})p(\tilde{\mathbf{s}})\ln p(\tilde{\mathbf{s}})\\&=k_B\ln\tilde{Z}+\frac{k_B}{\tilde{Z}}\int_{\tilde{\mathbf{s}}\in\tilde{\mathbb{S}}}d\tilde{\mathbf{s}}w(\tilde{\mathbf{s}})\beta\tilde{\mathcal{H}}^{(K)}(\tilde{\mathbf{s}}^{(K)})\\&\quad\times e^{-\beta\tilde{\mathcal{H}}^{(K)}(\tilde{\mathbf{s}}^{(K)})},\end{aligned} \tag{20}$$

where the coarse-grained partition function $\tilde{Z}$ is given by Eq. (13).

E. Fluctuation properties

For a given thermodynamic system, the constant-volume heat capacity C is defined as the fluctuation in the internal energy of the system,

$$C=\frac{\langle E^2\rangle-\langle E\rangle^2}{k_BT^2}. \tag{21}$$

It is well-known that in the vicinity of a continuous phase transition, the heat capacity C diverges. At the same time, it is also known that no system of finite size can have $C\to\infty$, since the energy, and hence the variance $\langle E^2\rangle-\langle E\rangle^2$ in the energy of the system will also remain finite. However, we can still observe evidence of power-law divergence near the critical temperature.[40] For small finite systems, we do not observe evidence of a divergence in the heat capacity; instead, the heat capacity is a smooth function of temperature T. The wavelet transform largely preserves the behavior of the original model; we observe the same general functional form in both the original model as well as the transformed systems, as seen in Fig. 6. However, for large finite systems, we can still detect the characteristic power-law divergence in the vicinity of the critical point; such a divergence is shown for a 32×32 Ising model as Fig. 7.

Applying the wavelet transform to a given thermodynamic system, we expect that we will still find evidence of a critical point; however, because of the mean-field-like behavior of the wavelet transform method, the critical point should be found at a higher temperature in the wavelet-transformed system than in the original system. Computing the heat capacity for large lattices cannot be done by exhaustive enumeration; therefore, we save discussion of our numerical results for a subsequent paper,[37] and present a brief heuristic argument. As the size of a block spin increases, corresponding to a greater number of iterations of the wavelet transform, we expect that the suppression of fluctuations in the system will lead to an increase in the temperature of the

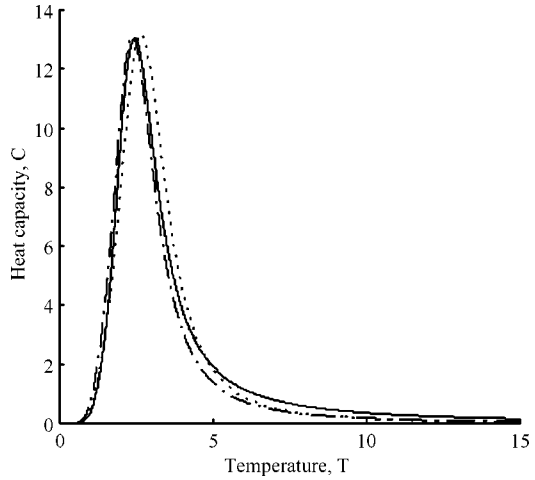

FIG. 6. Heat capacity of the 4×4 Ising model at zero external field as a function of temperature, as computed by an exact enumeration using no wavelet transform (solid line), and using one and two iterations of the two-dimensional Haar wavelet (dashed and dot-dashed lines, respectively).

phase transition, while the actual numerical value of the heat capacity itself decreases. The decrease in the number of degrees of freedom in the system is accompanied by an increasing trend towards homogeneity of the system—the remaining configurations begin to look more and more similar to one another. As a result, the variance measured by $\langle E^2\rangle-\langle E\rangle^2$ decreases with increasing amounts of coarse-graining. This trend is much less pronounced for small systems, as shown in Fig. 6. When the number of degrees of freedom is small, the ability to perform an exact enumeration ensures that the only errors observed are those introduced by the wavelet approximation itself. Thus, since the free energy and entropy of small systems are accurately reproduced by the transform, only minor deviations in the phase transition temperature for small systems are expected.

V. SIMILARITIES TO RENORMALIZATION GROUP THEORIES

It should already be apparent that close affinities exist between the method described here and position-space renormalization methods. The construction of wavelet-based averages naturally corresponds to Kadanoff's concept of a ''block spin'' transformation;[35] both the present method and Kadanoff's approach rely on combining a region of contiguous spins into a single new ''block spin.'' However, with the approach outlined above, we do not seek to impose the requirement that the block spins must be restricted to have the same spin values as the original spins. For example, in a wavelet-transformed spin-$\frac{1}{2}$ Ising model, the block spins can take on values other than $+1$ and -1. In addition, we do not impose ''majority rules'' or other ''tiebreakers'' in the case where there are equal numbers of ''up'' and ''down'' spins contained in a single block.

A less apparent connection can also be established with Migdal's ''bond-moving'' approximation,[41,42] or similarly with Wilson's recursion method.[43] In particular, Migdal's method can be compared to applying a separable wavelet transformation, in that the recursion is performed in only one spatial direction at a time. However, using the methods of either Migdal or Wilson, after performing the bond-moving or decimation transformation, the new interaction strengths J'_{ij} are determined by manipulating the resulting Hamiltonian and recasting it in the form of the original, leading at times to very complicated, nonlinear formulas for the J'_{ij} as a function of J_{ij}. By contrast, using wavelets, the values for the transformed coupling coefficients $\tilde{J}_{ij}$ are obtained directly by transforming the interaction matrix $\mathbf{J}$, since $\tilde{\mathbf{J}}=\mathbf{WJW}^T$. The trade-off that must be made for the algorithmic transparency of obtaining the new coupling constants via a matrix multiplication is that we cannot solve for the fixed points of the recursion relation, which makes the production of a renormalization ''flow diagram'' using the wavelet method a difficult problem.

The behavior of the wavelet transform and of the renormalization group differs in another, important manner. By the nature of its construction, the group of renormalization transformations is only a *semigroup*, inasmuch as reversing the mapping to move from a coarsened description to a more detailed description is impossible.[44,45] Using the wavelet transform, a reverse mapping is theoretically possible: reversibility fails because of the approximations invoked to reduce the number of wavelet coefficients which are kept, rather than as an inherent limitation of the wavelet transform itself.

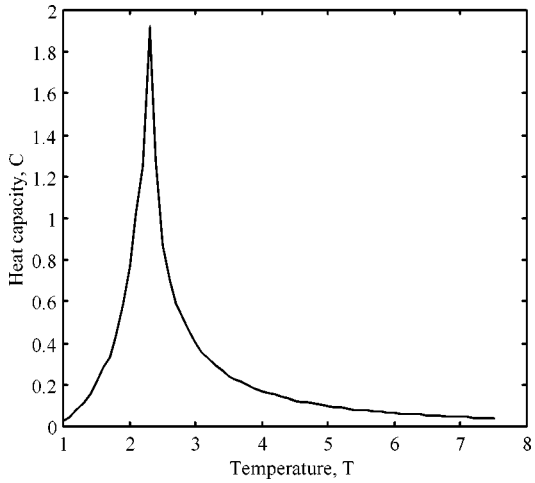

FIG. 7. Heat capacity of a 32×32 Ising model, illustrating the power-law divergence in the vicinity of the critical point.

VI. CONCLUSIONS

Using the wavelet transform as a basis for calculations of lattice systems yields an impressive reduction in the computational time required to obtain estimates of thermodynamic properties, at the price of modest errors in accuracy, given the relatively small size of the systems considered here, and the approximations introduced to simplify our calculations. The wavelet transform provides a systematic approach to coarse-grain systems to any level of resolution. The method produces correct results in the vicinity of fixed attractors, with decreasing accuracy as one approaches the critical point in parameter space.

In addition, the use of the wavelet transform on such systems is simple to implement; after selecting a particular set of wavelets, all of the operations can be reduced to matrix multiplications, as shown in Sec. III A. The computational requirements needed to implement the transformation are small; if the transformation cannot be accomplished in the explicit form of a matrix multiplication, it is possible to organize the calculation to be performed in-place.[29] Moreover, the amount of coarse-graining that can be achieved using the wavelet transform can be adjusted dynamically. These properties of the wavelet transform lead naturally to an extension of the method to systems for which simulations are required; the resulting algorithm is the focus of the companion paper.[37]

ACKNOWLEDGMENTS

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