A One-Dimensional Statistical Mechanics Model with Exact Transfer Integral Solution

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A simple one-dimensional model with scalar variables $-1 \leq s_n \leq +1$, coupled according to a Hamiltonian, $H = -J\sum_n |s_n - s_{n+1}|$, is presented. This Ising-like model is an interesting example of a graduate-level statistical mechanics problem where the eigenfunctions and eigenvalues of an *integral* operator, the transfer integral, can be determined exactly. This can be contrasted with the determination of eigenfunctions and eigenvalues of *differential* operators, such as the quantum mechanical finite-depth square well. In this problem transcendental equations leading to the eigenvalues and eigenfunctions are also obtained. The largest eigenvalue is identified and the free energy is determined. The thermodynamic properties depend on the *sign* of J, unlike classical Ising or Heisenberg models.

I. Introduction

There is always interest in statistical mechanics models with exact solutions, even in one dimension (1D), with the hope that the insight gained may be useful for solving the higher dimensional model, or perhaps relate to some other problem indirectly. Here I want to discuss a simple 1D model based on an Ising model[1] where the "spins" don't have just two states, but instead, a continuum of states over a finite range of a scalar spin variable s. This might be thought of as similar to taking a quantum spin$-S$ model, perhaps Heisenberg ($J\mathbf{S}_n \cdot \mathbf{S}_{n+1}$ near-neighbor Hamiltonian) or XY interaction (only couple the x and y spin components), and letting $S \rightarrow \infty$, $J \rightarrow 0$, while the product JS^2 remains finite. Of course doing this sort of limiting process leads to a *vector* classical spin variable $\mathbf{S}$, with two degrees of freedom, relating to the two angles needed to specify its direction. That would then be the classical Heisenberg or XY model, both of which have exact solutions in one dimension.[2,3]

Instead, I am now interested in making it a *scalar* "spin" model, where the variables s_n at each site have the range,

$$-1 \leq s_n \leq +1. \tag{1}$$

An equivalent parameterization with a more obvious physical interpretation would be to use $0 \leq s_n \leq +1$, if for instance the variables s_n represented occupation probabilities or perhaps sticking probabilities for atoms on the sites. I shall use the symmetric -1 to +1 range because of its mathematical simplicity; a change of variables can easily be used to get the other parameterization. The same idea is used in mapping the Ising model into lattice gas models.

The model to be considered, with a nearly linear interaction, is found to be exactly solvable using the transfer integral method. This is an interesting problem for learning about transfer integral eigenequations, with a completely determined spectrum. It is also interesting to compare the method of solution with that for mathematically similar problems such as the finite depth quantum square well.[4] The similarity comes about because the transfer integral eigenvalues are determined from transcendental equations with multiple solutions that are reminiscent of the square well problem.

Consider constructing an interaction between these continuum variables s_n, that may be vaguely equivalent to the Ising interaction, with possibilities of ferromagnetic (neighboring sites similar) or antiferromagnetic (neighboring sites opposite) forms. I do not simply use the Ising model itself and change the variables from discrete to continuum, because that problem is analytically difficult. In extending to continuum variables, there may be many different interactions whose limits in some sense are equivalent to the discrete-valued Ising model. One popular choice has been the ϕ^4 model used by Wilson, Fisher and others in renormalization group analyses.[5] The discrete Ising model was derived as a limit of the continuum ϕ^4 model, to which the renormalization group techniques could be more directly applied. The purpose here is simply to point out that a simpler interaction with effectively ferromagnetic or antiferromagnetic coupling has an exact solution in one dimension. However, there is not a smooth procedure for obtaining the discrete Ising model as a limit when some parameter goes to a particular value.

The Hamiltonian under consideration is

$$H = -J \sum_{n=1}^{N} |s_n - s_{n+1}|, \tag{2}$$

where the s_n are continuum variables with a finite range (Eq. 1) and piecewise linear coupling. The absolute-value interaction corresponds to having a force ($-\delta H/\delta s_n$) acting between the spins that has only two equal but opposite values (repulsive or attractive). $J < 0$ corresponds to an effective ferromagnetic coupling, where neighboring sites prefer to be "aligned", with neighboring s_n taking on similar values. $J > 0$ corresponds to an effective antiferromagnetic coupling, where neighboring sites prefer to be opposite, with the s_n alternately +1 and -1. In the lattice gas language, $J < 0$ means neighboring sites prefer to have the same occupation, while $J > 0$ means neighboring sites prefer to be alternately occupied and unoccupied.

One-dimensional models such as this have been considered previously.[6] Most of the interest concerned looking for models that would exhibit transitions to a phase with long range order, in the thermodynamic limit (number of paricles goes to infinity). Tonks[7] introduced a model of a one-dimensional gas of atoms, interacting by nearest neighbor hard core pair potentials. For a 1D gas there is a restriction on the atomic positions x_n such that atom $n + 1$ is to the right of atom n, i.e., $x_n < x_{n+1}$. Takahashi[8] showed how to find the partition function for a chain of such atoms with arbitrary pair potentials of finite range, by solving the transfer integral problem using a Laplace transform. He demonstrated that there could be no phase transition in the model. Later, Van Hove[9] proved that more general 1D gas models with pairwise interactions acting out to some finite cutoff distance (finite range potentials acting beyond nearest neighbors) cannot exhibit phase transitions. However, he did not give any general solution for these models.

Kac[10] introduced a 1D gas model with long range exponentially decaying attractive interactions combined with a hard core repulsion. He showed that there is also no phase transition in this model, for any finite values of the parameters in the potential. However, Baker[11] looked at the model more fully and found that in a special limit, where the range of the attractive interaction is allowed to diverge while its strength goes to zero, the model is seen to exhibit a Van der Waals type phase transition. In general, it is now understood that these types of gas models will not exhibit phase transitions unless there is an infinite range or cluster potential involved.[12]

Feynman[13] considered 1D gas models with a potential of the form $e^{-|s_{n+1}-s_n|}$ but the solution is difficult because it leads to a complicated integral eigenvalue equation. A model whose potential bears more resemblance to the model considered here is the 1D Coulomb gas.[14,15] The interaction potential in that case is via an absolute value of the difference of positions, however, the positions are allowed to have arbitrary values, and the forces may be repulsive or attractive depending on the signs of the charges involved. A mass was also assumed for the charged particles, leading to a kinetic term in the Hamiltonian. Here we include no kinetic energy and consequently no real dynamics. Van Hove's theorem applies to this model and there is no phase transition; the model is useful as a good example where the transfer integral method can be applied to obtain any thermodynamic quantities of interest as well as correlation functions and related probability distributions of the s_n.

II. Short Finite Chain Solutions

Consider a chain of length N with open ended boundaries. The canonical partition function is given by the integral,

$$Z_N = \int_{-1}^{1} ds_1 \int_{-1}^{1} ds_2 ... \int_{-1}^{1} ds_N e^{\beta|s_1-s_2|} e^{\beta|s_2-s_3|} ... e^{\beta|s_{N-1}-s_N|} \tag{3}$$

where $\beta \equiv J/kT$ is the coupling scaled by the temperature and Boltzmann's constant k. The integral can be evaluated by sequentially performing each integration, or, by making a coordinate transformation which effectively decouples the sites. Consider the transformation to variables σ_n, defined by

$$\sigma_1 = s_1,$$

$$\sigma_2 = -s_1 + s_2,$$

$$\sigma_3 = -s_2 + s_3, \tag{4}$$

and in general, $\sigma_n = s_n - s_{n-1}$. The corresponding inverse transformation is

$$s_1 = \sigma_1,$$

$$s_2 = \sigma_1 + \sigma_2,$$

$$s_3 = \sigma_1 + \sigma_2 + \sigma_3, \tag{5}$$

and in general, $s_n = \sum_{i=1}^{n} \sigma_i$. The Jacobian of the transformation is unity. The decoupling has been done at the expense of more complicated boudaries of integration. The original cubic boundaries of integration over the s_n variables convert to

$$-1 \le \sigma_1 \le 1,$$

$$-1 - \sigma_1 \le \sigma_2 \le 1 - \sigma_1,$$

$$-1 - \sigma_1 - \sigma_2 \le \sigma_3 \le 1 - \sigma_1 - \sigma_2, \tag{6}$$

and so on. For example, the three site problem is solved by the integral

$$Z_3 = \int_{-1}^{1} d\sigma_1 \int_{-1-\sigma_1}^{1-\sigma_1} d\sigma_2 \;\; e^{\beta|\sigma_2|} \int_{-1-\sigma_1-\sigma_2}^{1-\sigma_1-\sigma_2} d\sigma_3 \;\; e^{\beta|\sigma_3|}. \tag{7}$$

In this case there are only two bonds with an interaction, the coupling between s_1 and s_2, and the coupling between s_2 and s_3. By separating each integration into $\sigma < 0$ and $\sigma > 0$ regions, all the integrations are trivial, and we directly find the following results for the shortest possible chains:

$$Z_1 = 2$$

$$Z_2 = -4/\beta + 2(e^{2\beta} - 1)/\beta^2$$

$$Z_3 = (8 + 4e^{2\beta})/\beta^2 + (7 - 8e^{2\beta} + e^{4\beta})/\beta^3. \tag{8}$$

The tedium of the algebra increases dramatically with increasing N. These results for finite systems do not demonstrate that there must be a closed-form solution in the thermodynamic limit $N \to \infty$, but they are suggestive that this almost linear (actually, piecewise linear) interaction is analytically tractable. Of course, being able to solve finite chains doesn't really tell us anything about how to get the thermodynamic limit. Clearly, solutions for finite systems for the usual Ising model could be obtained in any dimensions if the system is small enough, but the thermodynamic limit has been obtained only for one and two dimensions.[16]

III.A The Transfer Integral Method

In this section the partition function is developed in terms of the eigenfunctions and eigenvalues of a *transfer integral* operator, a formalism in which the thermodynamic limit is greatly simplified.[17] We can also consider how the eigenspectrum can be used to get various probabilty distributions for the spin variables. It turns out that the eigenfunctions of this transfer operator contain all the information needed to describe how the spins are distributed and how they are correlated with their neighbors, and so on.

Suppose we have the n$^{\text{th}}$ *partial* partition function $z_n(s_n)$, where all of the spins up to s_{n-1} (in Eq. 3) have been integrated out, and the last spin is in the state s_n. The total partition function for a chain of n sites would be determined by integration over the n$^{\text{th}}$ site:

$$Z_n = \int_{-1}^{1} ds_n \; z_n(s_n). \tag{9}$$

A subsequent partial partition function $z_{n+1}(s_{n+1})$ is generated by adding the spin s_{n+1} and integrating over its interaction with s_n, defining the transfer integral operation,

$$z_{n+1}(s_{n+1}) = \int_{-1}^{1} ds_n \; z_n(s_n) \; e^{\beta|s_n - s_{n+1}|}. \tag{10}$$

Or, we may just write this in terms of the transfer integral operator T as

$$z_{n+1}(s_{n+1}) = T\{z_n(s_n)\}. \tag{11}$$

One obtains the N-particle partition function Z_N by repeated application of this operation onto $z_1(s_1) = 1$, with an integration over the states of the last particle,

$$Z_N = \int_{-1}^{1} ds_N \quad T^{N-1}\{z_1(s_1)\} \tag{12}$$

This operation is characterized by the eigenspectrum of the transfer operator T. If z_1 is expanded in the eigenspectrum of the transfer operator, with eigenfunctions u_i and corresponding eigenvalues λ_i, we can write

$$z_1(s) = 1 = \sum_i c_i \; u_i(s), \tag{13}$$

where the c_i are the expansion coefficients, and the sum is over the complete set of eigenfunctions (an infinite set). The eigenspectrum itself is determined by solutions of the following integral equation:

$$T\{u_i(s')\} = \int_{-1}^{1} ds' e^{\beta|s-s'|} u_i(s') = \lambda_i u_i(s). \tag{14}$$

The transfer operation (10) has a symmetric kernel, $e^{\beta|s_n - s_{n+1}|}$, and is self-adjoint. As a result, its eigenfunctions can be made orthonormal;

$$\int_{-1}^{+1} ds \; u_i(s) \; u_j(s) = \delta_{ij}. \tag{15}$$

With this orthogonality condition the expansion coefficients in (13) are determined to be

$$c_i = \int_{-1}^{+1} ds \; u_i(s). \tag{16}$$

Using the expansion (13), and the above constants c_i, repeated application of the transfer operation gives Z_N for a chain of N sites,

$$Z_N = \int_{-1}^{1} ds_N \sum_i c_i \lambda_i^{N-1} \; u_i(s_N) = \sum_i c_i^2 \lambda_i^{N-1}. \tag{17}$$

In the thermodynamic limit $N \rightarrow \infty$, the free energy per particle is proportional to the largest eigenvalue of T;

$$F/N = -(kT/N)\ln Z_N \rightarrow -kT \ln \lambda_{max}, \tag{18}$$

where λ_{max} is the largest eigenvalue of the integral equation (14). Then once the free energy is known, any desired thermodynamic quantities can be obtained through appropriate derivatives.

The above calculation can also be made alternatively by rewriting the kernel in terms of the eigenfunctions, which makes the calculation even easier. Using an expansion as in (13), one finds for the kernel,

$$e^{\beta|s_1-s_2|} = \sum_i \ \lambda_i \ u_i(s_1) \ u_i(s_2). \tag{19}$$

Then sequentially integrating over s_1, s_2, and so on, and making use of the fact that N-1 of the integrations in the definition of Z_N (Eq. 3) are just transfer operations on eigenfunctions, again (17) results for the chain's partition function. The added bonus of this method is that it also makes the calculation for a ring of N sites (i.e., N sites with periodic boundary conditions) simplify. With the help of (19) the result for a ring of N sites is easily found to be

$$Z_N = \sum_i \lambda_i^N, \tag{20}$$

and again in the thermodynamic limit, the free energy is given by the logarithm of the largest eigenvalue, Eq. (18).

While the largest eigenvalue of the transfer operation determines the free energy, the corresponding eigenfunction determines the probability distribution for the spin variables. The probability distribution for a single site, $p_N(s_n)$, is defined by integrating over all sites except the one of interest in Eq. (3), and then normalizing by Z_N. For a closed ring of N sites, we have for the distribution of site 1,

$$p_N(s_1) \equiv Z_N^{-1} \int_{-1}^{1} ds_2 \int_{-1}^{1} ds_3 ... \int_{-1}^{1} ds_N e^{\beta|s_1-s_2|} e^{\beta|s_2-s_3|} ... e^{\beta|s_N-s_1|} \tag{21}$$

But again using the expansion (19) for the $s_1 - s_2$ interaction converts the subsequent integrations over s_2, s_3, etc., into transfer operations. Finally there results,

$$p_N(s) = Z_N^{-1} \sum_i \lambda_i^N u_i^2(s). \tag{22}$$

The subscript on s_1 was dropped since it is clear that all sites are equivalent. In the thermodynamic limit, the sum is dominated by the largest eigenvalue, with corresponding eigenfunction $u_{max}(s)$, and

$$p(s) = u_{max}^2(s). \tag{23}$$

This result also holds for the infinite length *chain* of sites. However, for the finite chain there results for $p_N(s_n)$, with $1 \leq n \leq N$,

$$p_N(s_n) \equiv Z_N^{-1} \int_{-1}^{1} ds_1 \int_{-1}^{1} ds_2 ... \int_{-1}^{1} ds_{n-1} \int_{-1}^{1} ds_{n+1} ... \int_{-1}^{1} ds_N$$

$$e^{\beta|s_1-s_2|} e^{\beta|s_2-s_3|} ... e^{\beta|s_{N-1}-s_N|}$$

$$= Z_N^{-1} \sum_i \sum_j \ \lambda_i^{n-1} c_i u_i(s_n) \ \lambda_j^{N-n} c_j u_j(s_n). \tag{24}$$

For the finite chain the probabilty distribution does indeed depend on the particular site.

Other higher order probability distributions can be defined, such as a two-site distribution that could be used to get correlation functions. Simply generalizing the one-site distribution's definition into one for a two-site joint distribution suggests the definition (for a ring of sites)

$$p_N(s_1, s_{1+n}) \equiv Z_N^{-1} \int_{-1}^{1} ds_2 \int_{-1}^{1} ds_3 ... \int_{-1}^{1} ds_n \int_{-1}^{1} ds_{n+2} ... \int_{-1}^{1} ds_N$$

$$e^{\beta|s_1-s_2|} e^{\beta|s_2-s_3|} ... e^{\beta|s_N-s_1|} \tag{25}$$

The spatial separation of the sites is chosen to be n, and it is interesting to consider the dependence of this function on n. Once again employing the kernel expansion (19) leads to

$$p_N(s_1, s_{1+n}) = Z_N^{-1} \sum_i \sum_j \lambda_i^n \lambda_j^{N-n} \ u_i(s_1) u_j(s_1) \ u_i(s_{1+n}) u_j(s_{1+n}). \tag{26}$$

In the thermodynamic limit, this function's dependence on the separation n is dominated by the ratio of the first *two* largest magnitude eigenvalues, λ_{max}, and λ_{max-1};

$$p(s_1, s_{1+n}) \approx u_{max}(s_1) u_{max}(s_{1+n}) \times$$

$$\left[u_{max}(s_1) u_{max}(s_{1+n}) + (\lambda_{max-1}/\lambda_{max})^n \ u_{max-1}(s_1) u_{max-1}(s_{1+n}) \right]. \tag{27}$$

This exponential distance dependence on n will also appear in any correlation functions that are defined, and leads to a correlation length ξ given by

$$\xi^{-1} = \ln |\lambda_{max}/\lambda_{max-1}|. \tag{28}$$

The other important point to note about Eq. (27) is that the sign of $\lambda_{max-1}/\lambda_{max}$ indicates what kind of short range order is present. When this ratio is positive, neighboring sites tend to be alike, as in a ferromagnetic sense. When the ratio is negative, however, it means that correlation functions will oscillate with a factor $(-1)^n$, and neighboring sites will tend to be opposite, in an antiferromagnetic sense.

The function $p(s_1, s_{1+n})$ can be used to compute probability distributions for other quantities of interest. For example, the correlations between two sites might be characterized by the difference, $y_n \equiv |s_1 - s_{1+n}|$. Then the probability distribution $d(y_n)$ for y_n is derived using a delta function:

$$d(y_n) \equiv \int_{-1}^{+1} ds_1 \int_{-1}^{+1} ds_{1+n} \ \ p_N(s_1, s_{1+n}) \ \delta(y_n - |s_1 - s_{1+n}|). \tag{29}$$

It is clear that $p_N(s_1, s_{1+n})$ can be used for the calculation of any desired probability distribution involving s_1 and s_{1+n} via similar definitions. To get explicit expressions for such objects, the eigenfunctions $u_i(s)$ must first be determined, as developed in the following section.

III.B The Transfer Integral Solution

The absolute value interaction suggests splitting the integral in (14) into two regimes:

$$T\{u(s')\} = \int_{-1}^{s} ds' e^{\beta(s-s')} u(s') + \int_{s}^{1} ds' e^{-\beta(s-s')} u(s') = \lambda u(s). \tag{30}$$

This equation can be converted to a *nearly* equivalent differential equation for the eigenfunctions. For instance, multiply Eq. (14) by $e^{\beta s}$ and take the derivative d/ds, giving

$$\int_{-1}^{s} ds' e^{-\beta s'} u(s') = (\lambda/2\beta) e^{-2\beta s} (d/ds)[e^{\beta s} u(s)] \tag{31}$$

Differentiating once more with respect to s gives

$$u(s) = (\lambda/2\beta) e^{\beta s} (d/ds)\{e^{-2\beta s} (d/ds)[e^{\beta s} u(s)]\}. \tag{32}$$

This is equivalent to the elementary differential equation,

$$\frac{d^2 u}{ds^2} = (\beta^2 + 2\beta/\lambda) u. \tag{33}$$

The equation has the fundamental solution

$$u(s) = A e^{\alpha s} + B e^{-\alpha s}, \tag{34}$$

where

$$\alpha = (\beta^2 + 2\beta/\lambda)^{1/2}. \tag{35}$$

The constant coefficients A and B and the eigenvalue λ are yet to be determined. This has an interesting contrast with the usual differential equation eigenvalue problems encountered in quantum mechanics or electrostatics that we are more familiar with. For differential equation eigenvalue problems, once the general form of the solution is known, the eigenvalues and constant coefficients are determined by forcing the solution to satisfy appropriate *boundary* conditions. However, for integral equation eigenvalue problems such as this, instead the eigenvalues are determined by an *integral* or *global* condition, which is the integral equation itself acting as a constraint. Applying the transfer operation Eq. (14) to the fundamental solution Eq. (34) gives

$$T\{A e^{\alpha s'} + B e^{\alpha s'}\} = \frac{2\beta}{\alpha^2 - \beta^2} (A e^{\alpha s} + B e^{\alpha s})$$

$$+ [(\frac{e^{\alpha}}{\alpha + \beta}) A - (\frac{e^{-\alpha}}{\alpha - \beta}) B] e^{\beta} e^{-\beta s} - [(\frac{e^{-\alpha}}{\alpha - \beta}) A - (\frac{e^{\alpha}}{\alpha + \beta}) B] e^{\beta} e^{\beta s} \tag{36}$$

The operation reproduces the original function plus two extra dependences on s. In order to enforce that we have an eigenfunction, there are the conditions that the coefficients of the extra terms vanish (the global constraint referred to above),

$$(\frac{e^{\alpha}}{\alpha + \beta}) A - (\frac{e^{-\alpha}}{\alpha - \beta}) B = 0,$$

$$(\frac{e^{-\alpha}}{\alpha - \beta}) A - (\frac{e^{\alpha}}{\alpha + \beta}) B = 0. \tag{37}$$

The eigenvalue is identified as

$$\lambda = 2\beta/(\alpha^2 - \beta^2). \tag{38}$$

This last equation just reproduces Eq. (35). The homogeneous Eq. (37) has nontrivial solutions only when the determinant of the coefficients vanishes. This leads to two types of solutions, even or odd, which have either $A/B = +1$ or $A/B = -1$, respectively. Correspondingly, there result transcendental equations for the parameter α, which then implicitly defines the eigenvalues λ and thus the free energy. The even symmetry solutions are determined according to

$$u^+(s) = \cosh \alpha s, \tag{39a}$$

$$\alpha \tanh \alpha = \beta, \tag{39b}$$

$$\lambda = 2\beta^{-1} \sinh^2 \alpha, \tag{39c}$$

and the odd symmetry solutions are determined by

$$u^-(s) = \sinh \alpha s, \tag{40a}$$

$$\alpha \coth \alpha = \beta, \tag{40b}$$

$$\lambda = -2\beta^{-1} \cosh^2 \alpha. \tag{40c}$$

These implicitly represent the solution for the eigenvalues, which must be derived by first solving for α. The original integral operator is self-adjoint, ensuring that the eigenvalues are real. This further implies via Eq. (35) that α must be pure real or pure imaginary, leading to either hyperbolic functions or to sinusoidal functions, respectively. With these points in mind, these transcendental equations are seen to have an infinite set of solutions, corresponding to a complete set of eigenfunctions, mutually orthogonal on the interval from $s = -1$ to $s = +1$. This whole process through which the eigenspectrum is identified is very similar to the solution of the quantum 1-D finite square potential problem, except that here we are considering an integral operator rather than a differential operator.

IV.A The Eigenvalues, Eigenfunctions

The eigenvalues α are found as indicated graphically in Figures 1 and 2, by plotting the LHS vs. the RHS of Equations (39b) and (40b), and looking for points at which the curves cross. First consider the *even* symmetry eigenfunctions for $\beta > 0$. The LHS of Eq. (39b) increases monotonically, implying that there is only one solution where α is real, see Fig. 1a. Note that this solution exists *only* when $\beta > 0$, for the effective antiferromagnetic coupling. This solution will be refered to as $u_0^+(s)$, with eigenvalue λ_0^+;

$$u_0^+(s) = \cosh \alpha_0^+ s, \tag{41}$$

where α_0^+ is the only real solution to Eq. (39b). However, it is realized that Eq. (39b) also has an infinite set of solutions where α is pure imaginary, e.g., $\alpha = ia$ with a real. These will be cosinusoidal eigenfunctions:

$$u_l^+(s) = \cos a_l^+ s, \tag{42a}$$

$$a_l^+ \tan a_l^+ = -\beta, \tag{42b}$$

$$\lambda_l^+ = -2\beta^{-1} \sin^2 a_l^+. \tag{42c}$$

The index l refers to the lth root of Eq. (42b), suggested graphically in Fig. 1b. As $l \to \infty$, subsequent α_l^+ increment by π. It is also interesting to note that when β changes sign from positive to negative, the real α_0^+ solution disappears while an additional a_l^+ solution appears at $a = 0$. In this sense the number of solutions (which is infinite) is independent of β.

Similar statements apply to the odd symmetry solutions. For $\beta > 1$, there will be only one real solution to Eq. (40b) (Fig. 2a), denoted α_0^-, with eigenvalue λ_0^- and eigenfunction

$$u_0^-(s) = \sinh \alpha_0^- s. \tag{43}$$

This solution exists *only* for $\beta > 1$. There are additionally pure imaginary solutions to Eq. (40b) (Fig. 2b). Again putting $\alpha = ia$, with a pure real, these must satisfy

$$u_l^-(s) = \sin a_l^- s, \tag{44a}$$

$$a_l^- \cot a_l^- = \beta, \tag{44b}$$

$$\lambda_l^- = -2\beta^{-1} \cos^2 a_l^- \tag{44c}$$

The graphical solutions are depicted in Fig. 2. Again, at the point $\beta = 1$ where the real solution disappears, an extra imaginary solution appears.

IV.B The Largest Eigenvalue

Now we can determine the largest eigenvalue. In fact all that is needed is the largest *positive* eigenvalue, since it is clear that $Z_N \approx \lambda_{max}^N$ must be positive definite, regardless of whether N is even or odd. First we consider $\beta > 0$.

For the imaginary solutions, the eigenvalues can be written as $\lambda = -2\beta/(a^2 + \beta^2)$, so that the eigenvalue with the largest magnitude must have the smallest a. However, these are always negative for $\beta > 0$. Therefore, if $\beta > 1$, the largest eigenvalue must be either λ_0^+ or λ_0^-. A short analysis shows that in the limit $\beta \to \infty$, these have asymptotic forms

$$\lambda_0^+ \approx \left(e^{2\beta} + 4\beta - 1\right)/(2\beta), \tag{45a}$$

$$\lambda_0^- \approx -\left(e^{2\beta} - 4\beta + 1\right)/(2\beta). \tag{45b}$$

In fact, λ_0^- is always negative, and therefore λ_0^+ is *always* the largest eigenvalue for the entire range $\beta > 0$, i.e., for antiferromagnetic coupling, with corresponding hyperbolic cosine eigenfunction, Eq. (41). When $\beta > 1$, the second largest eigenvalue is λ_0^-, so that the ratio $\lambda_{max-1}/\lambda_{max} = \lambda_0^-/\lambda_0^+ < 0$, and neighboring sites exhibit short range antiferromagnetic order. For $0 < \beta < 1$, the second largest eigenvalue becomes λ_1^+, which is also negative, and the short range ordering is still antiferromagnetic.

When $\beta < 0$, only the imaginary solutions exist. It is easily seen in Figs. 1 and 2 that the the solution with the minimum value of a is $\lambda_1^+ \leq \pi/2$, with corresponding cosinusoidal eigenfunction, Eq. (42a). This remains the largest eigenvalue for all $\beta < 0$. It is also clear that the lowest odd imaginary solution, λ_1^-, is the second largest eigenvalue, and is also positive. With the ratio $\lambda_{max-1}/\lambda_{max} = \lambda_1^-/\lambda_1^+ > 0$, neighboring sites exhibit short range ferromagnetic order for all $\beta < 0$.

Therefore, for any temperature we have the largest eigenvalue of the transfer operator, and thus the resulting equilibrium thermodynamic functions can be found in the usual way, through derivatives of the free energy. Additionally, since the second largest eigenvalue also is known, information about correlations, such as the correlation length, Eq. (28), can be extracted.

Thermodynamic Results and Conclusions

Quantities such as the internal energy per site can be found via derivatives of the partition function, $Z \approx \lambda_{max}^N$. For example, for the internal energy per site U and the specific heat per site C, we have

$$U = -\lim_{N\to\infty}(J/N)(\partial/\partial\beta)\ln Z_N(\beta) = (J/\lambda_{max})(\partial\lambda_{max}/\partial\beta), \tag{46a}$$

$$C = \partial U/\partial T. \tag{46b}$$

The latter partial derivative of λ_{max} can be evaluated in terms of β and α, producing the following results using Eq. (37) and Eq. (40):

$$U = \frac{J}{\beta}\left(\frac{\alpha_0^{+\,2} + \beta^2 - \beta}{-\alpha_0^{+\,2} + \beta^2 - \beta}\right) \qquad \text{for} \quad \beta > 0, \tag{47a}$$

$$U = \frac{J}{\beta}\left(\frac{-a_1^{+\,2} + \beta^2 - \beta}{a_1^{+\,2} + \beta^2 - \beta}\right) \qquad \text{for} \quad \beta < 0, \tag{47b}$$

Alternatively, the derivatives can be found from numerical differentiation. For results shown here, λ_{max} was determined numerically using a Newton's method to solve for $\alpha(\beta)$, then these partial derivatives were evaluated numerically. I do not give more complete analytic expressions for the thermodynamic quantities—however, they can be evaluated to any desired degree of accuracy without using statistical methods such as Monte Carlo. In this sense the calculation is exact.

These results are shown in Fig. 3, for positive and for negative J. A comparison with the 1D Ising model can be made, also shown in Fig. 3, for which $U = -J\tanh(\beta)$, and $C = \beta^2\mathrm{sech}^2(\beta)$. An obvious difference between the two is that the sign of J is irrelevant for the Ising model, while it plays a crucial role in the model discussed here. This can be understood by looking at the transfer integral eigenfunctions. For $\beta > 0$ $(J > 0)$, according to the discussion in Section III.A, the probability distribution for the spin at a single site is determined from the normalized eigenfunction with largest eigenvalue,

$$p(s) = u_0^+(s)^2 = \frac{2\alpha_0^+\cosh^2\alpha_0^+ s}{2\alpha_0^+ + \sinh 2\alpha_0^+}. \tag{48}$$

This distribution is shown in Fig. 4a, for high and low temperatures. At very low temperatures, $(\beta \to \infty)$, to a very good approximation, $\alpha_0^+ \approx \beta$. Then the distribution is concentrated symmetrically at $s \approx \pm 1$, and approaches a pair of delta functions at ± 1. This is an antiferromagnetic situation, with the sites alternately +1 and -1.

For $\beta < 0$ $(J < 0)$, the probability distribution changes to

$$p(s) = u_1^+(s)^2 = \frac{2a_1^+\cos^2 a_1^+ s}{2a_1^+ + \sin 2a_1^+}. \tag{49}$$

This is shown in Fig. 4b. For low temperatures, with $\beta \to -\infty$, the parameter $a_1^+ \to \pi/2$. Then the distribution goes to zero at $s = \pm 1$, and the most probable value is $s = 0$. The s_n, however, do not concentrate at $s = 0$, rather, there is an appreciable population on both sides of zero. This is in sharp contrast to the case with $J > 0$, and is responsible for the dependence on the sign of J.

To summarize, the model given by Hamiltonian (1) represents an interesting example for application of the transfer integral method to one-dimensional continuous variable systems. Thermodynamic functions and correlation functions can be found from the knowledge of the eigenspectrum of the transfer operator. The eigenfunctions contain information about the probability distributions for the spin variables, which leads directly to desired correlation functions.

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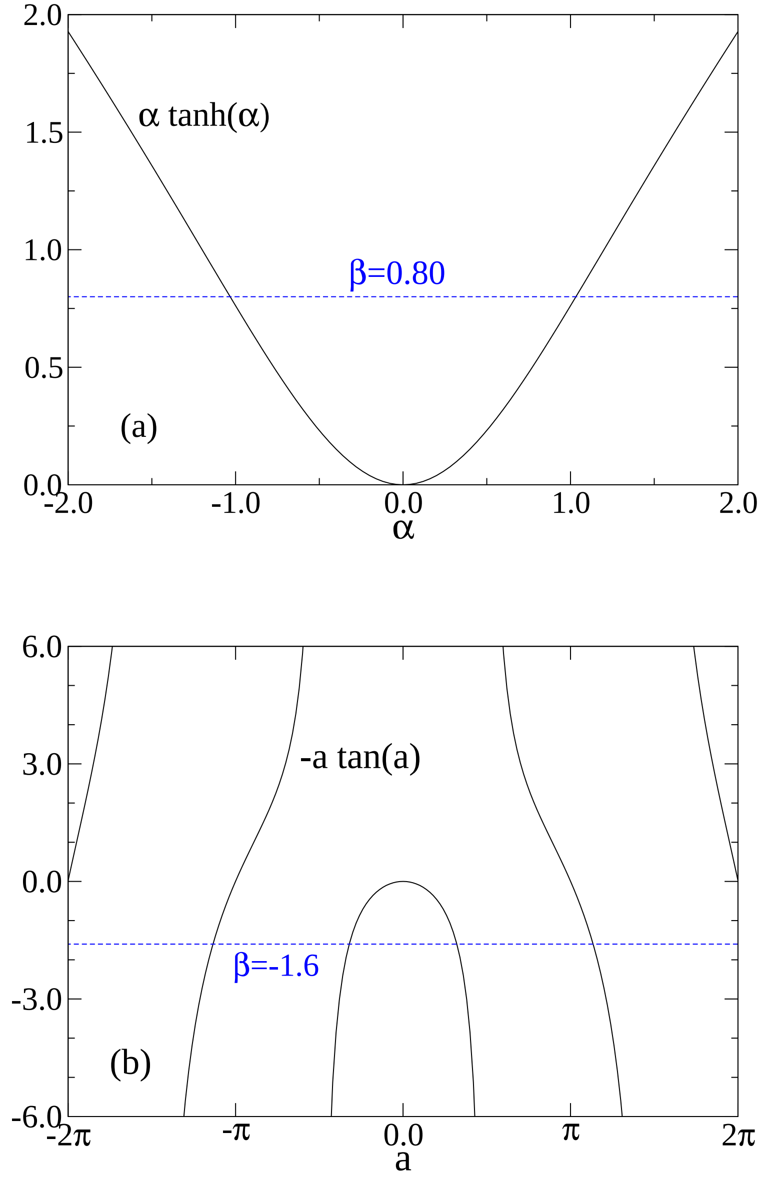


Fig. 1. Graphical solutions for the values of α corresponding to *even* symmetry eigenfunctions. In a), the real solution α_0^+ for the eigenfunction $u_0^+(s) = \cosh \alpha_0^+ s$ is determined by using Eq. (39b). The intersections with horizontal lines at the given value for $\beta = J/T$ determine the solutions. Only positive values for α need to be considered. The real solution α_0^+ exists only for $\beta > 0$. In b), a_l^+ for the eigenfunction $\cos a_l^+ s$ is determined by using Eq. (42b), with $\alpha = ia$. Here and in Fig. 2b there are an infinite number of intersections with a line at constant β, corresponding to an infinite set of eigenvalues and eigenfunctions.

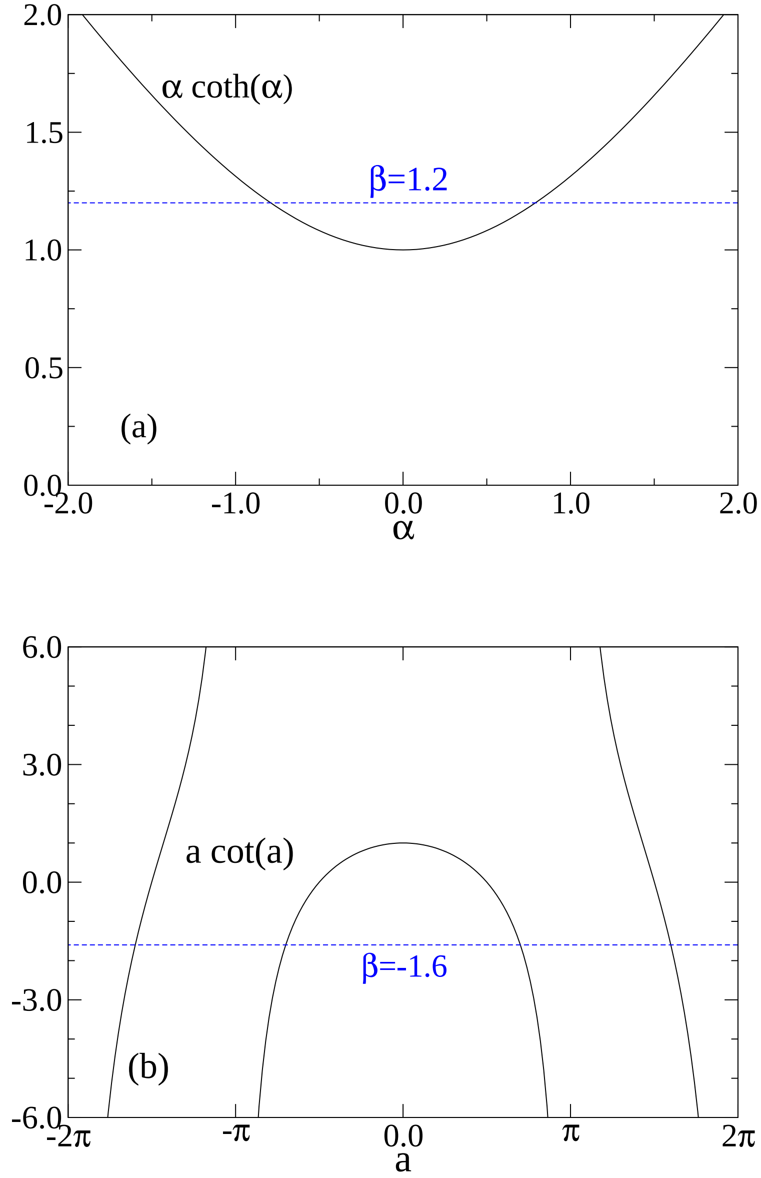
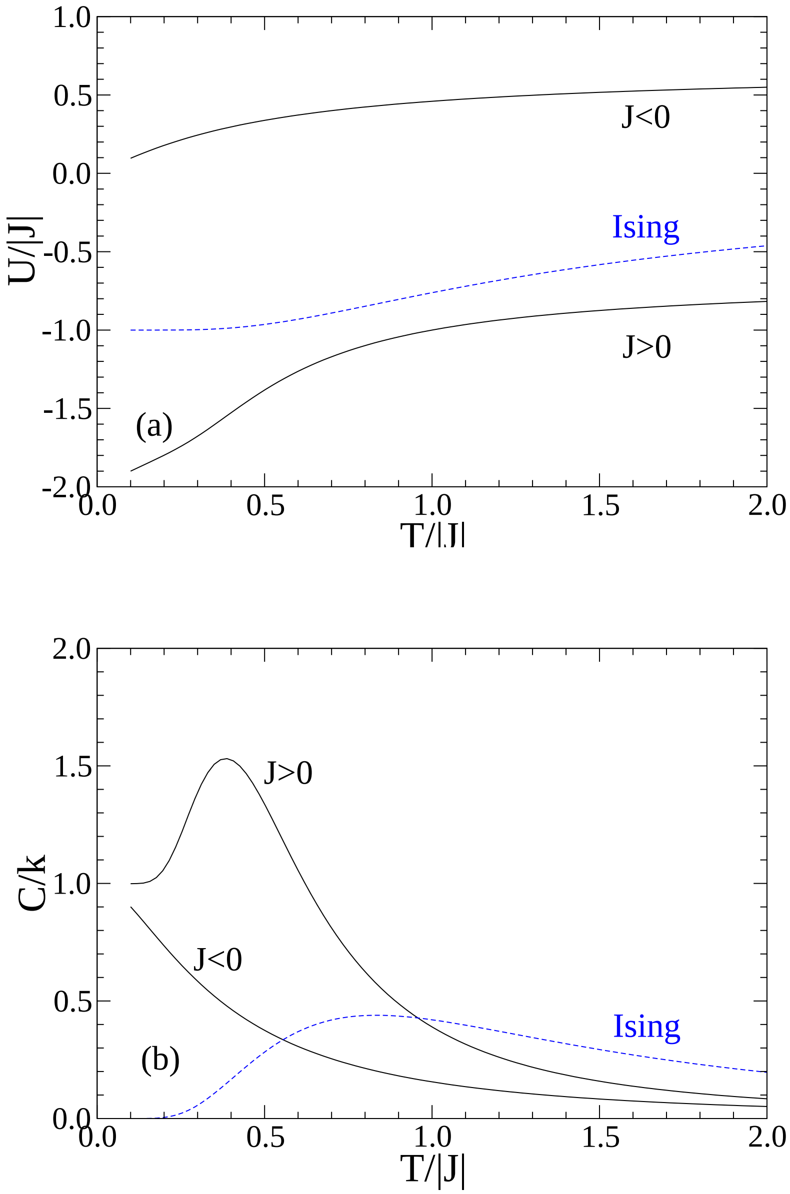
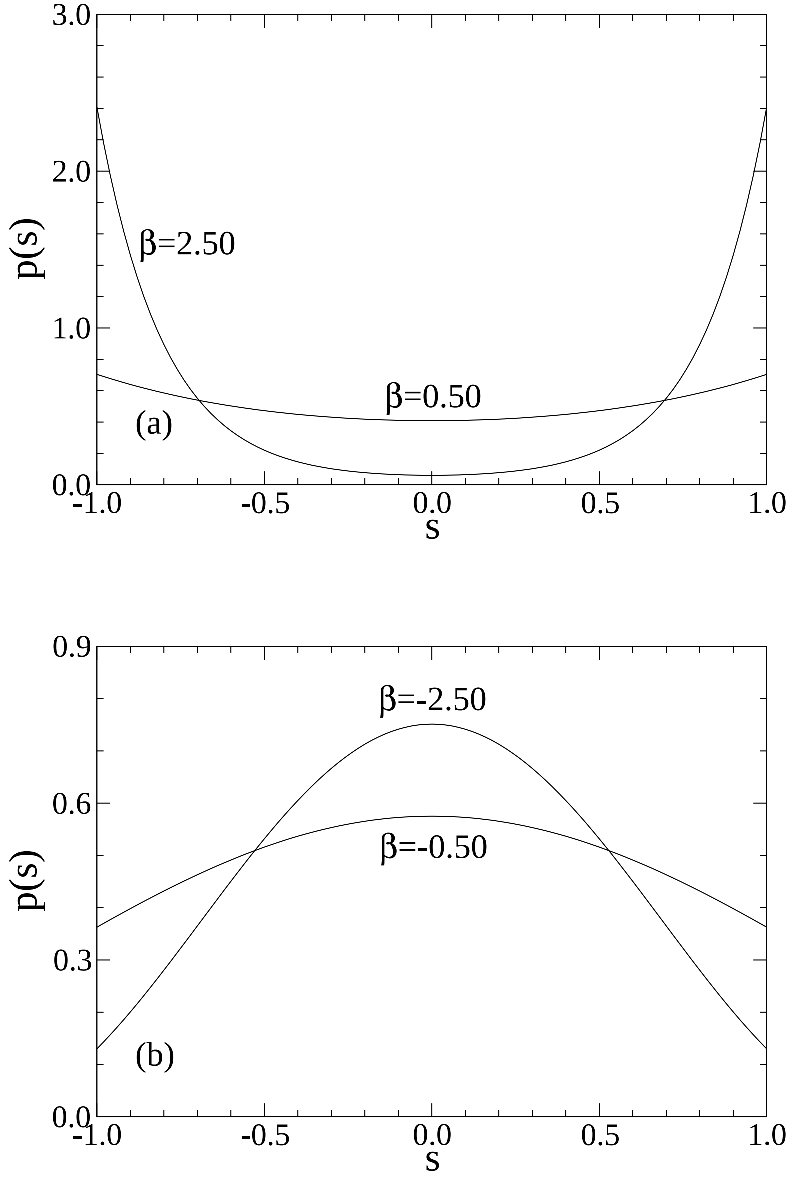


Fig. 2. Graphical solutions for the values of α corresponding to *odd* symmetry eigenfunctions. In a), the real solution α_0^- for the eigenfunction $u_0^-(s) = \sinh \alpha_0^- s$ is determined by using Eq. (40b). This solution exists only for $\beta > 1$. In b), a_l^- for the eigenfunction $\sin a_l^- s$ is determined by using Eq. (44b), with $\alpha = ia$.



3. Results for (a) internal energy per site U and (b) specific heat per site C. The dashed curves represent the 1D Ising model for comparison.



4. The single site spin distribution for (a) $J > 0$ and (b) $J < 0$. The curves are described by Eqs. (48) and (49).

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