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Abstract. Numerical evaluation of functional integrals usually involves a finite (L-slice) discretization of the imaginary-time axis. In the auxiliary-field method, the L-slice approximant to the density matrix can be evaluated as a function of inverse temperature at any finite L as $\hat{\rho}_L(\beta) = [\hat{\rho}_1(\beta/L)]^L$, if the density matrix $\hat{\rho}_1(\beta)$ in the static approximation is known. We investigate the convergence of the partition function $Z_L(\beta) \equiv \text{Tr}\, \hat{\rho}_L(\beta)$, the internal energy and the density of states $g_L(E)$ (the inverse Laplace transform of Z_L), as $L \to \infty$. For the simple harmonic oscillator, $g_L(E)$ is a normalized truncated Fourier series for the exact density of states. When the auxiliary-field approach is applied to spin systems, approximants to the density of states and heat capacity can be negative. Approximants to the density matrix for a spin-$\frac{1}{2}$ dimer are found in closed form for all L by appending a self-interaction to the divergent Gaussian integral and analytically continuing to zero self-interaction. Because of this continuation, the coefficient of the singlet projector in the approximate density matrix can be negative. For a spin dimer, Z_L is an even function of the coupling constant for $L < 3$: ferromagnetic and antiferromagnetic coupling can be distinguished only for $L \geqslant 3$, where a Berry phase appears in the functional integral. At any non-zero temperature, the exact partition function is recovered as $L \to \infty$.

1. Introduction

Functional integration is a long-established technique in quantum mechanics [1]. More recently, advances in computing power have allowed direct Monte Carlo evaluation of such integrals for many-body systems [2]. Such algorithms are often based on an auxiliary-field functional integral, which is used in areas as diverse as strongly correlated electron systems [3], spin systems [4] and nuclear structure [5]. The statistical mechanics of a many-body system on a d-dimensional lattice is mapped onto that of a classical field $u(r, \tau)$ (the *auxiliary field*) in a $(d + 1)$-dimensional slab of extension $0 \leqslant \tau \leqslant \beta = 1/kT$ in the imaginary time dimension. The many-body system reduces to a system of non-interacting particles moving in a time-dependent auxiliary field. To evaluate the integral over all time evolutions, it is necessary to sample the field at a finite number L of imaginary times—not necessarily uniformly or deterministically spaced—and extrapolate to the continuum limit $L \to \infty$. The $L = 1$, or *static*, approximation maps the system onto classical statistical mechanics in d dimensions. The ground state in this approximation for many-fermion systems is a single Slater determinant, typically corresponding to the Hartree–Fock solution; for spin models it is the mean-field ground state. For $L > 2$, closed paths may enclose an area, breaking time-reversal invariance and thereby contributing a sign or Berry phase factor to the integral. This factor has some important consequences. It restores quantization: correlation between phases on neighbouring sites discriminates between the classically equivalent ferromagnets and unfrustrated antiferromagnets [6]. The large-L limit must also restore symmetry if the

auxiliary fields do not have the full local symmetry (such as in the Ising decomposition of the Hubbard model) [7]. On the other hand, the resulting rapid oscillation of the integrand (the notorious sign problem) seriously restricts convergence of Monte Carlo simulations at low temperatures. The present author has shown how the distributions of the auxiliary fields tend to the appropriate quantum distribution (the Wigner function) with increasing L, while numerical convergence becomes increasingly problematical [8]. For repulsive interactions, an imaginary auxiliary field is required, resulting in a sign problem even in the static approximation.

Since numerical studies of the auxiliary-field functional integral are frequently hampered by the sign problem, it is of value to investigate toy models in which the finite-L approximants may be evaluated in closed form. This paper is a framework for discussion of these approximants, specifically for simple spin systems. This differs from finite-size scaling in real space; while a lattice truncated in real space is a cluster, and therefore physically realizable, the time-discretized system may possess unphysical properties vanishing only in the continuum limit. Indeed, in a number of examples the static approximants to the heat capacity and density of states are not positive-definite [9]. The static approximation (and other finite-L approximations) give a saddle-point approximation, usually a variational overestimate, of the ground state energy, but are correct in the high-temperature limit. The heat capacity shows competition between the recovery of quantum fluctuations, which give a negative contribution at low temperatures, and true thermal fluctuations, which give a positive contribution (exponentially small if there is a gap).

To motivate this work, at this point we recall the path integral of a simple harmonic oscillator in the frequency domain (which does not suffer from the above problem). The partition function is [1]

$$Z(\beta) = \int \mathcal{D}x \exp\left(-\int_0^\beta d\tau \left[\frac{m}{2\hbar^2}\left(\frac{dx}{d\tau}\right)^2 + \frac{1}{2}m\omega^2 x^2\right]\right). \tag{1}$$

We impose a frequency cut-off, restricting the function space to paths with L Matsubara frequencies (L odd):

$$x(\tau) = \sum_{n=(1-L)/2}^{(L-1)/2} a_n e^{2\pi i n k T \tau}. \tag{2}$$

The resulting Lth approximant to the partition function is [10, 11]

$$Z_L(\beta) = \frac{1}{\beta\hbar\omega} \prod_{n=1}^{(L-1)/2} \left[1 + \left(\frac{\beta\hbar\omega}{2\pi n}\right)^2\right]^{-1}, \tag{3}$$

with poles at $\beta = 2\pi i n/\hbar\omega$, $(1 - L)/2 \leqslant n \leqslant (L - 1)/2$. The inverse Laplace transform of Z_L gives the Lth approximant to the density of states:

$$g_L(E) = \frac{2^{L-1}\left([(L-1)/2]!\right)^2}{(L-1)!\hbar\omega} \sin^{L-1}(\pi E/\hbar\omega)\Theta(E) \tag{4}$$

where Θ is the Heaviside step function. The approximants have the following limits:

$$g_1(E) = \Theta(E) \tag{5}$$

$$\lim_{L\to\infty} g_L(E) \to \sum_{n=0}^{\infty} \delta\left(E - \left(n + \tfrac{1}{2}\right)\hbar\omega\right) \tag{6}$$

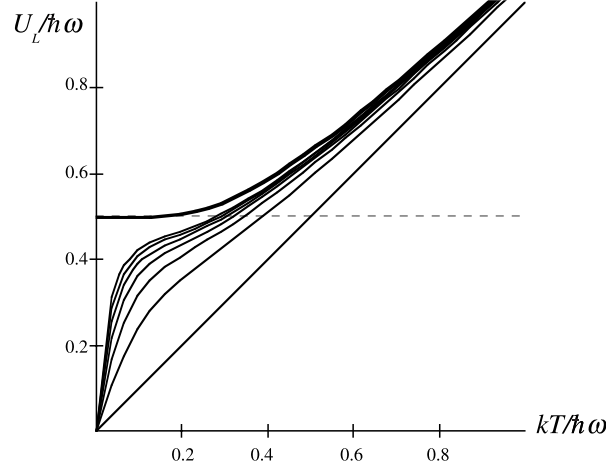$$g_L(E) \sim E^{L-1}, \qquad E \to 0_+. \tag{7}$$

Figure 1. Internal energy for simple harmonic oscillator showing approximants with $L = 1, 3, 5, 7, 9, 11, 13$ Matsubara frequencies converging to the exact (bold) energy.

In particular, equation (6) verifies the emergence of the correct density of states in the continuum limit. Figure 1 shows the convergence of the internal energy U_L, obtained from Z_L (3), to the exact result $(\hbar\omega/2)\coth(\hbar\omega/2kT)$ for any fixed positive temperature. The ground state energy vanishes for all L, and the low-temperature heat capacity is Lk; the zero-point energy is recovered with increasing temperature. In this case the finite-L approximants to the partition function represent physically realizable systems (ensembles of harmonic oscillators of the same frequency with a distribution of energy shifts). This is to be compared with the results to be shown in figures 2 and 3, which do not exhibit this behaviour.

Of more relevance to the present paper would be a time discretization of the path integral (1). The resulting approximants to the partition function have a similar form to (3), although the poles are non-uniformly spaced [10, 12, 13]. The approximant to the density of states has a less transparent form than (4), being quasiperiodic rather than periodic, but still converges with L in any finite energy interval.

Section 2 presents the auxiliary field formalism used in this work. Two case studies of toy spin models in section 3 show how truncation of the functional integral gives a sequence of approximants which, although they converge to the correct value, do not themselves represent any physical system. Section 4 discusses possible wider applicability of the features of these models.

2. Theory

The general Hamiltonian with two-body interactions is of the form

$$\hat{H} = -\sum_{\mu=1}^{N}(K_\mu \hat{A}_\mu + K_\mu^* \hat{A}_\mu^\dagger) - \sum_{\mu,\nu=1}^{N} J_{\mu\nu} \hat{A}_\mu^\dagger \hat{A}_\nu. \tag{8}$$

Here $\hat{A} = \{\hat{A}_\mu, \mu = 1, \ldots, N\}$ are single-particle operators generating a closed algebra; they will be spin operators in the examples studied here, but might, for example, represent hopping or pairing operators, $c_{i\uparrow}^\dagger c_{j\uparrow}$ or $c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger$. To avoid notational complications, we assume

the operators to be Hermitian. This can be achieved by changing the basis to $\hat{A}_\mu^\dagger + \hat{A}_\mu$ and $i(\hat{A}_\mu^\dagger - \hat{A}_\mu)$. To obtain the functional integral, we separate the density matrix into L time slices,

$$\hat{\rho}(\beta) \equiv e^{-\beta\hat{H}} = \left(e^{-\beta\hat{H}/L}\right)^L \tag{9}$$

and apply the Hubbard–Stratonovich transformation to each time slice:

$$\exp(-\beta\hat{H}/L) = \frac{\int d^N u \exp(-\beta u \cdot J^{-1} u/4L) \exp(\beta(K+u) \cdot \hat{A}/L)}{\sqrt{\det(4\pi J L/\beta)}} + O(L^{-2}). \tag{10}$$

This is a formal expression, convergent only for a positive interaction matrix J. In general, one needs to reduce the matrix into positive, zero and negative blocks and treat each separately, omitting the auxiliary fields in the zero block and using an imaginary auxiliary field in the negative block [14]. An alternative is to add a multiple of a positive matrix to J. In the latter case, this addition may correspond to a constant or one-body term, which can be absorbed into K, at the cost of introducing a fictitious self-interaction; the functional integration will have to work harder to remove this self-interaction. The coefficient of the additional term may be analytically continued or extrapolated to zero [15]; it is this approach we shall use here. The Lth approximant to the density matrix is then

$$\hat{\rho}_L(\beta) = \prod_{n=1}^{L} \frac{\int d^N u_n \exp(-\beta u_n \cdot J^{-1} u_n/4L) \exp(\beta(K+u_n) \cdot \hat{A}/L)}{\sqrt{[\det(4\pi L J/\beta)]}}. \tag{11}$$

This can be obtained from the density matrix in the static approximation

$$\hat{\rho}_L(\beta) = [\hat{\rho}_1(\beta/L)]^L \tag{12}$$

and tends to the exact density matrix as $L \to \infty$. We shall subsequently refer to the Lth approximant of the 'function' (obtained by replacing the exact density matrix with its approximant (11)) as the L-'function'.

The L-partition function is

$$Z_L(\beta) = \text{Tr}\,\hat{\rho}_L(\beta). \tag{13}$$

Approximants to the internal energy may be computed directly from approximants to the partition function,

$$U_L(\beta) = -\frac{\partial}{\partial\beta} \ln Z_L(\beta), \tag{14}$$

which is an average of the one-body (auxiliary-field) Hamiltonian:

$$U_L(\beta) = -\tfrac{1}{2}LkT + \left(\text{Tr}\left\{\int \prod_{n=1}^{L}[e^{-\beta(u_n \cdot J^{-1} u_n/4 - (K+u_n) \cdot \hat{A})/L}\, d^N u_n]\right.\right.$$
$$\left.\times [u_1 \cdot J^{-1} u_1/4 - (K+u_1) \cdot \hat{A}]\right\}\Big)$$
$$\times \left(\text{Tr}\left\{\int \prod_{n=1}^{L}[e^{-\beta(u_n \cdot J^{-1} u_n/4 - (K+u_n) \cdot \hat{A})/L}\, d^N u_n]\right\}\right)^{-1}. \tag{15}$$

This will therefore tend to the expectation of the auxiliary field Hamiltonian at low temperatures, typically a mean-field energy.

Since it is difficult to extract the partition function from importance-sampled Monte Carlo calculations, the form (14) is impractical. It is possible to calculate the energy as a thermal average of the true Hamiltonian

$$\tilde{U}_L(\beta) = Z_L(\beta)^{-1} \text{Tr}[\hat{\rho}_L(\beta)\hat{H}]. \tag{16}$$

This is a variational approximation to the ground state energy, which might be expected to be bounded below by the ground state energy. The example in section 3.2 below shows that this natural assumption is not always justified for these approximants. The forms (14) and (16) are not equivalent; the latter is usually a better approximation. Heat capacities will be defined as temperature derivatives of these energies, although these may be calculated in other ways [16].

The partition function is the Laplace transform of the density of states $g_L(E)$. The L-density of states, $g_L(E)$, is defined implicitly by

$$Z_L(\beta) = \int_{-\infty}^{\infty} e^{-\beta E} g_L(E) \, dE. \tag{17}$$

The spectrum is bounded below but, if necessary, the origin of E can be shifted to ensure that $g_L(E) = 0$ for $E < 0$. Such densities of states have been studied in the nuclear shell model [17], although in that case the partition function is derived by integration of the measured energy (16) in (14) and the inverse Laplace transform is computed within the saddle-point approximation (which is appropriate for a large density of states). The propagator may also be determined by a similar inverse transform of the density matrix. The L-partition function $Z_L(\beta)$ converges pointwise to the partition function $Z(\beta)$ as $L \to \infty$ at any non-zero temperature. The L-density of states converges to the true density of states in the distributional sense: for any sufficiently smooth function f,

$$\lim_{L \to \infty} \int_{-\infty}^{\infty} f(E) g_L(E) \, dE = \int_{-\infty}^{\infty} f(E) g(E) \, dE. \tag{18}$$

There are now two possibilities. If $\int_{-\infty}^{\infty} f(E) g_L(E) \, dE$ is positive for all positive test functions $f(E)$, the heat capacity is non-negative at all temperatures and we say that the approximant is physical; there can exist a Hermitian Hamiltonian with that thermodynamics. This is evidently the case for the harmonic oscillator discussed in section 1, although this is not related to the auxiliary-field functional integral. If the density of states is non-positive, then we say that the approximant is unphysical. The spin models in the next section provide examples.

3. Examples

3.1. Single spin

A single spin s with self-interaction,

$$\hat{H} = -J\hat{S} \cdot \hat{S} \tag{19}$$

may seem a trivial case, although a similar situation would arise in the study of a Hubbard model with degenerate bands and strong Hund's rule coupling. The static approximation to this has been discussed earlier [9]. Although a scalar auxiliary field does not suffer from this problem, it violates rotational invariance [18]. Clearly, the exact partition function, internal energy and density of states are

$$Z(\beta) = (2s + 1) \exp(\beta J s(s + 1)) \tag{20}$$

$$U(\beta) = -J s(s + 1) \tag{21}$$

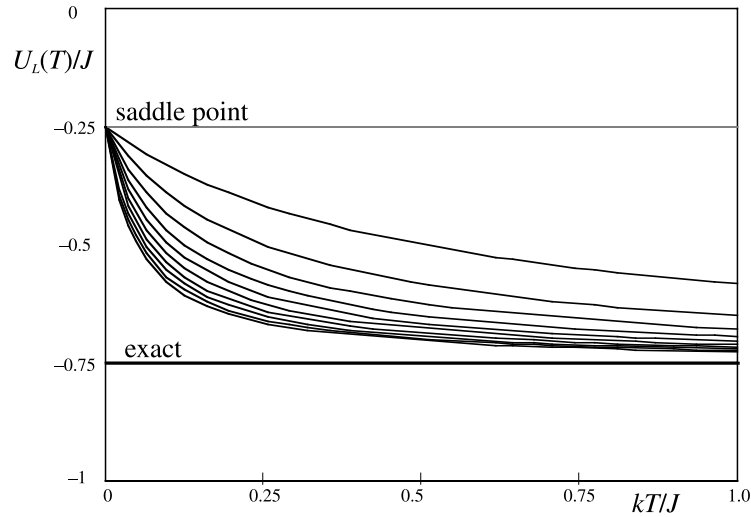$$g(E) = (2s + 1)\delta(E + J s(s + 1)). \tag{22}$$

Figure 2. Internal energy for single spin $\frac{1}{2}$ showing approximants with $L = 1$ (top curve) to 10 (bottom curve) converging to the exact (bold) energy.

Applying the Hubbard–Stratonovich transformation gives the $L = 1$ density matrix as

$$\hat{\rho}_1 = (\beta/4\pi J)^{3/2} \int d^3 u \exp(-\beta u^2/4J) \exp(\beta u \cdot \hat{S}). \tag{23}$$

This is rotationally invariant, and therefore a multiple of the unit matrix. The partition function in the static approximation follows from taking the trace of the exponential and performing the Gaussian integrals [9], giving

$$\hat{\rho}_1(\beta) = \frac{Z_1(\beta)}{2s+1} = \frac{1}{2s+1} \sum_{m=-s}^{s} (1 + 2m^2 \beta J) e^{m^2 \beta J}. \tag{24}$$

The L-partition function is then

$$Z_L(\beta) = (2s+1) \left(\frac{1}{2s+1} \sum_{m=-s}^{s} (1 + 2m^2 \beta J/L) e^{m^2 \beta J/L} \right)^L; \tag{25}$$

this tends to the correct limit (20) as $L \to \infty$. The L-energy (14) is

$$U_L(\beta) = -J \frac{\sum_{m=-s}^{s} (3m^2 + 2m^4 \beta J/L) e^{m^2 \beta J/L}}{\sum_{m=-s}^{s} (1 + 2m^2 \beta J/L) e^{m^2 \beta J/L}} = U_1(\beta/L). \tag{26}$$

This is a monotonically *decreasing* function of temperature, falling from the saddle-point value of $-Js^2$ at $T = 0$ to the correct value of $-Js(s+1)$ at high temperatures. Figure 2 shows the energy for spin $\frac{1}{2}$. The thermal average of the Hamiltonian (16) is trivially $\tilde{U}_L(\beta) = -Js(s+1)$ at all temperatures.

This negative heat capacity implies a non-physical density of states. For spin $\frac{1}{2}$, the approximants to the partition function are

$$Z_L(\beta) = 2(1 + \beta J/2L)^L e^{\beta J/4}, \tag{27}$$

converging to $2e^{3\beta J/4}$ as $L \to \infty$. Its inverse Laplace transform is the L-density of states

$$g_L(E) = 2\left(1 + \frac{J}{2L}\frac{\mathrm{d}}{\mathrm{d}E}\right)^L \delta(E + J/4) \tag{28}$$

which involves L derivatives of the delta function at the saddle-point energy. The formal limit

$$\lim_{L\to\infty} g_L(E) = 2\exp\left(1 + \frac{J}{2}\frac{\mathrm{d}}{\mathrm{d}E}\right)\delta(E + J/4) = 2\delta(E + 3J/4) \tag{29}$$

is correct when applied to a sufficiently good test function (such as a polynomial). In this way expectation values are correct to $O(L^{-1})$, even though the only spectral point is at the classical rather than the quantum ground state energy, and is in error by $O(1)$. For larger spins, this single singularity becomes a discrete spectrum of singularities between $E = -Js^2$ and $E = -J/4$ (half-odd-integer spin) or $E = 0$ (integer spin), all higher than the true energy.

There is a suggestive but probably fortuitous resemblance between the partition function for spin $\frac{1}{2}$ and the q-Laplace transform, recently introduced in the context of non-extensive statistical mechanics [19]. One version of this q-Laplace transform defines a q-partition function as

$$Z_q(\beta) = \int_0^\infty g(E)[1 + (1-q)\beta E]^{1/(1-q)}\,\mathrm{d}E, \tag{30}$$

where q corresponds to $1-1/L$. Negative heat capacities are found in this theory [20] (although the correspondence between Z_q and thermodynamic potentials differs from that in standard thermodynamics).

3.2. Spin-$\frac{1}{2}$ dimer

The highly non-physical behaviour of the approximants to the heat capacity above stems from the emergence of the quantum fluctuations (a negative energy contribution) with increasing temperature. For a single spin in zero field there are no compensating thermal fluctuations. We therefore investigate the spin-$\frac{1}{2}$ dimer,

$$\hat{H} = -J'(\hat{S}_1 \cdot \hat{S}_1 + \hat{S}_2 \cdot \hat{S}_2) - 2J\hat{S}_1 \cdot \hat{S}_2. \tag{31}$$

The self-interaction is added to ensure convergence. The integral (10) only converges for $J' > |J|$, but is analytic in the matrix elements, allowing continuation to $J' = 0$. Manipulation of the Gaussian integrals eventually gives the L-density matrix as

$$\hat{\rho}_L(\beta) = \left[\left(\frac{5}{6} - \frac{J'^2}{6J^2} + \frac{\beta(J+J')^2}{3LJ}\right)e^{\beta J/2L} + \left(\frac{1}{6} + \frac{J'^2}{6J^2} - \frac{\beta(J-J')^2}{6LJ}\right)e^{-\beta J/2L}\right]^L e^{\beta J'/2}\hat{P}_1$$

$$+ \left[\left(-\frac{1}{2} + \frac{J'^2}{2J^2}\right)e^{\beta J/2L} + \left(\frac{3}{2} - \frac{J'^2}{2J^2} - \frac{\beta(J-J')^2}{2LJ}\right)e^{-\beta J/2L}\right]^L e^{\beta J'/2}\hat{P}_0. \tag{32}$$

This is an entire function of both J and J'. Taking $J \to 0$ gives the direct product of two one-particle density matrices (25). More importantly, we can remove the interaction by setting $J' = 0$ to obtain

$$\hat{\rho}_L(\beta) = \left[\left(\frac{5}{6} + \frac{\beta J}{3L}\right)e^{\beta J/2L} + \left(\frac{1}{6} - \frac{\beta J}{6L}\right)e^{-\beta J/2L}\right]^L \hat{P}_1$$

$$+ \left[-\frac{1}{2}e^{\beta J/2L} + \left(\frac{3}{2} - \frac{\beta J}{2L}\right)e^{-\beta J/2L}\right]^L \hat{P}_0 \tag{33}$$
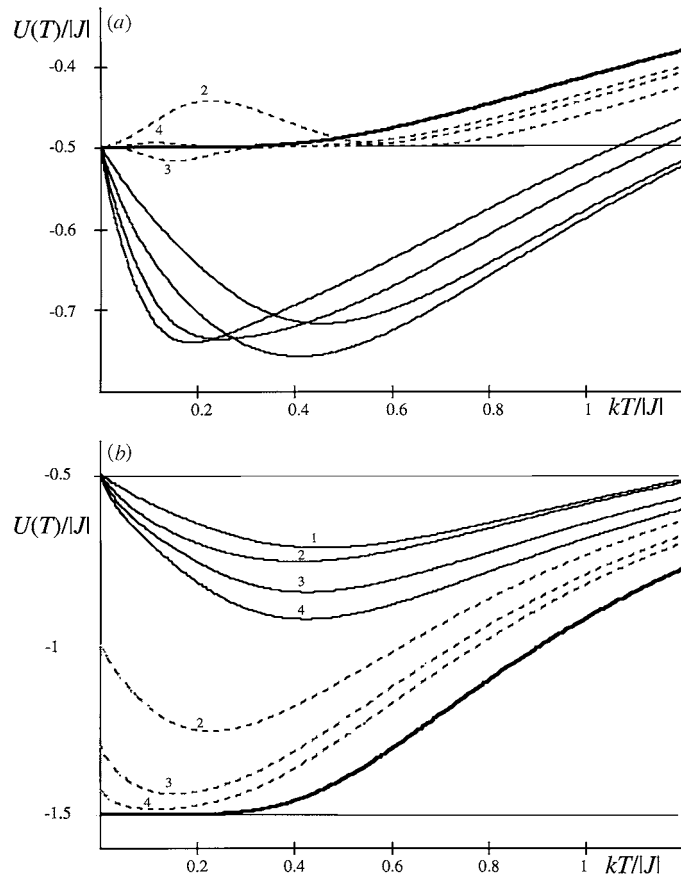
Figure 3. Lth approximant to the energy for the spin-$\frac{1}{2}$ dimer with (*a*) ferromagnetic and (*b*) antiferromagnetic coupling. The bold curve is the exact energy, the full curves are U_L, the derivative of $\ln Z_L$ (14), and the broken curves are $\tilde{U}_L$, the thermal average of the Hamiltonian (16). Curves shown for $L = 1, \ldots, 4$, annotated by L. The energies U_1 and $\tilde{U}_1$ are coincident.

where $\hat{P}_1$ and $\hat{P}_0$ are projections onto the triplet and singlet subspace, respectively. In the large-L limit we recover the correct density matrix:

$$\lim_{L\to\infty} \hat{\rho}_L(\beta) = \lim_{L\to\infty} \left[\left(1 + \frac{\beta J}{2L}\right)^L \hat{P}_1 + \left(1 - \frac{3\beta J}{2L}\right)^L \hat{P}_0 \right] \tag{34}$$

$$= e^{\beta J/2} \hat{P}_1 + e^{-3\beta J/2} \hat{P}_0. \tag{35}$$

It is not possible to distinguish ferromagnetic from antiferromagnetic coupling in the thermodynamics for $L < 3$, where the paths do not enclose an area. Thus the L-partition function is an even function of J for $L = 1, 2$. A high-temperature expansion (Maple) verifies this and shows that the second moment of the density of states is correct for all L:

$$Z_L(\beta) = 4 + \frac{3(\beta J)^2}{2} - \frac{(L-1)(L-2)(\beta J)^3}{2L^2} + \frac{(21L^3 - 72L^2 + 116L - 60)(\beta J)^4}{96L^3} + \cdots. \tag{36}$$

Figure 3 shows approximants to the internal energy for ferromagnetic and antiferromagnetic coupling. U_L, as calculated from the partition function (14), is always equal to its mean-field value $-|J|/2$ at $T = 0$. This is the correct energy only for the ferromagnet. U_1 and U_2, as already discussed, cannot distinguish the ferromagnet and antiferromagnet. The L-heat capacity is negative at low temperatures and positive at higher temperatures. $\tilde{U}_L$, as calculated from the thermal average of the Hamiltonian (16) is, as expected, a better approximation than U_L for $L > 1$, giving improved estimates of the antiferromagnetic ground state energy, although it still shows a small region of negative L-heat capacity.

One at first surprising feature is that in the ferromagnet $\tilde{U}_L$ falls *below* its variational bound $-J/2$ for odd L. This is due to the unphysical form of the L-density matrix itself, and not just to its temperature dependence. As a result of the analytic continuation to $J' = 0$, the coefficient of the singlet projector in (33) is negative at low temperature for odd L, representing a negative weight for the singlet state. The coefficients of both projectors are always positive when $J' > |J|$, the parameter region for which the integral (10) converges. Direct application of the Hubbard–Stratonovich transformation to the Hamiltonian for $J' = 0$ would require an imaginary field coupled to $\hat{S}_1 - \hat{S}_2$, leading to a similar non-classical weight.

The L-density of states is again non-physical and is symmetric for $L < 3$ for the reasons discussed above; there are $L + 1$ singularities in $-J/2 \leqslant E \leqslant J/2$, involving L derivatives of the delta function, for example

$$g_1(E) = 2\left(\delta(E + J/2) + \delta(E - J/2)\right) + J\left(\delta'(E + J/2) - \delta'(E - J/2)\right). \tag{37}$$

For large L, we obtain the correct result (the limit to be understood in the distributional sense)

$$\lim_{L \to \infty} g_L(E) = 3\delta(E + J/2) + \delta(E - 3J/2). \tag{38}$$

4. Discussion

In all of the above, the approximants to thermodynamic functions have an error of $O(L^{-1})$ at any fixed non-zero temperature. In practice, more careful Trotter decompositions and truncations of the density matrix may accelerate the convergence in Monte Carlo simulations [16, 21, 22]. The models discussed, being analytically soluble for all discretizations, are not representative of real applications but may provide a useful test of methods. The main outcome of this work is a pointer to possible difficulties in the use of finite discretizations: underestimated (or negative) heat capacities and non-physical spectral functions. The effects might be largest in strongly correlated systems, or systems with an excitation gap, where the lowest auxiliary field state is a poor approximation to the true ground state. In that case the density of states must suffer substantial distortion to provide the correct thermodynamics; the true ground state energy lies outside the approximate spectrum. More accurate energies are obtained from the thermal average of the Hamiltonian than from the derivative of the partition function.

This work has been in some sense complementary to the sign problem, which can arise for $L \geqslant 3$ or for repulsive interactions [14]: the weight in the functional integral (10) need not be positive, although the physical quantities are correctly obtained. This will arise if the correlations to be calculated are incompatible with a positive distribution for the auxiliary fields [8]. In this case low-L approximations lead to unphysical results, characterized by non-positive distributions in the energy domain. The examples discussed are those with the most acute sign problem: the auxiliary field couples to operators (such as spin components) whose equal-time commutators do not vanish.

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