Hybrid ED/DMRG approach to the thermodynamics of 1D quantum models

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Exact diagonalization (ED) of small model systems gives the thermodynamics of spin chains or quantum cell models at high temperature $T$. Density matrix renormalization group (DMRG) calculations of progressively larger systems are used to obtain excitations up to a cutoff $W_C$ and the low-$T$ thermodynamics. The hybrid approach is applied to the magnetic susceptibility $\chi(T)$ and specific heat $C(T)$ of spin-1/2 chains with isotropic exchange such as the linear Heisenberg antiferromagnet (HAF) and the frustrated $J_1 - J_2$ model with ferromagnetic (F) $J_1 < 0$ and antiferromagnetic (AF) $J_2 > 0$. The hybrid approach is fully validated by comparison with HAF results. It extends $J_1 - J_2$ thermodynamics down to $T \sim 0.01|J_1|$ for $J_2/|J_1| \geq \alpha_c = 1/4$ and is consistent with other methods. The criterion for the cutoff $W_C(N)$ in systems of $N$ spins is discussed. The cutoff leads to bounds for the thermodynamic limit that are best satisfied at a specific $T(N)$ at system size $N$.

I. INTRODUCTION

White introduced the density matrix renormalization group (DMRG) and applied it to the ground state of quantum spin chains [1]. DMRG has become a powerful general method for the ground state and excitation gaps that characterize the quantum ($T = 0$) phases of one-dimensional (1D) models with spin or charge degrees of freedom [2, 3]. The transfer matrix renormalization group (TMRG) is a related approach to finite temperature in which the partition function with increasing system size is followed to lower $T$ [4–6]. White and Feiguin generalized DMRG to finite $T$ by enlarging the Hilbert space [7]. The auxiliary Hamiltonian contains fictitious states in one-to-one correspondence with the physical basis. Karrasch et al. discuss ways to facilitate the calculation of transport properties using the time dependent DMRG at finite $T$ [8]. These methods have strengths and limitations. DMRG has been applied directly to the low-$T$ thermodynamics of gapped chains with two spins per unit cell [9]. The striking success of DMRG at $T = 0$ provides strong incentive for extension to finite $T$. The most challenging systems are gapless chains with one spin per unit cell and quasi-long-range correlations in the ground state.

We develop in this paper a hybrid approach to the thermodynamics of spin chains and quantum cell models. The high-$T$ regime is treated conventionally by exact diagonalization (ED) of small systems. DMRG then gives the low-energy excitations of increasingly large systems. Partition functions based on a few thousand states yield the low-$T$ thermodynamics. The combination of ED and DMRG covers the entire range, down to $T$ set by the accuracy of DMRG excitations, without ever invoking the full spectrum of large systems. The hybrid ED/DMRG approach is general, with DMRG tuned to the low-energy spectrum instead of the ground state.

There are broadly two contexts, mathematical and physical, for discussing spin chains or 1D quantum cell models. The spin-1/2 linear Heisenberg antiferromagnet (HAF) is the oldest and best characterized many-spin system [10, 11]. The spin-1 HAF or other spin-1/2 models have been intensively studied for decades using field theory [12, 13] and numerical methods [14]. Correlated many-spin or many-electron models are intrinsically interesting. The characterization of quasi-1D compounds with linear chains of transition metal ions or organic radical ions has an equally long history [15, 16]. Isotropic exchange is the dominant interaction, but not the only one. Thermodynamics to a factor of two or three lower $T$ than possible by ED would significantly aid the analysis of magnetic data. The $T \to 0$ limit is interesting mathematically.

The $J_1 - J_2$ model, Eq. 3 below, illustrates both contexts. The model has one spin-1/2 per unit cell and isotropic exchange $J_1$ and $J_2 > 0$ with first and second neighbors, respectively. The quantum phases for AF exchange $J_1 > 0$ include the exact ground state at the Majumdar-Ghosh [17] point ($J_2 = J_1/2$) and the critical point [18] $J_2/J_1 = 0.2411$ at the onset of the gapped dimer phase. The quantum phases for F exchange $J_1 < 0$ feature the critical point [19] at $J_2 = |J_1|/4$ between the FM ground state and the gapped incommensurate (IC) singlet ground state [20]. The gapless decoupled phase [21] includes $J_1 = 0$ and lies between IC phases with $J_1 < 0$ and $J_1 > 0$.

The $J_1 - J_2$ model with $J_1 < 0$ is the starting point for the magnetic properties of cupric oxides that contain chains of spin-1/2 Cu(II) ions and have singlet ground states [22–26]. An applied magnetic field of 10 Tesla is sufficient to induce the FM ground state in some cases. The $T$ and field dependencies of the magnetization and magnetic specific heat can be followed in systems with competing F and AF interactions. Present estimates of $J_1$ and $J_2$ in specific materials are rather approximate.
At issue are the low-$T$ thermodynamics of the model, corrections due to spin-orbit coupling and additional (dipolar, hyperfine, interchain) weak interactions. We discuss the zero-field thermodynamics and focus on the magnetic susceptibility and specific heat.

The hybrid ED/DMRG approach is applicable to quantum cell models with a large but finite basis that increases exponentially with system size. There are $(2S + 1)^N$ states in a system of $N$ spins-$S$, and similar expressions hold for models with charge as well as spin degrees of freedom. Here we consider $N$ spins-$1/2$ in models indexed by $\alpha$. The energy spectrum $\{E(\alpha, N)\}$ has $2^N$ states for any $\alpha$. The thermodynamics is governed by the canonical partitions function

$$Q(T, \alpha, N) = \sum \exp (-\beta E_j(\alpha, N)),$$

where $T$ is the absolute temperature, $\beta = 1/k_B T$, $k_B$ is the Boltzmann constant, the sum is over all states, and $E_j(\alpha, N)$ is relative to the ground state energy. The per spin result of the infinite chain is

$$N^{-1} \ln Q(T, \alpha, N) \to \ln Q(T, \alpha).$$

The problem is to obtain or approximate the thermodynamic limit.

Our basic premise is that the full spectrum $\{E(\alpha, N)\}$ of large systems is never needed. The most demanding cases are gapless chains with quasi-long-range order in the ground state or chains with exponentially small gaps. Even then, thermal fluctuations suppress correlations between distant spins and the system size becomes irrelevant when $N$ is several times the correlation length. ED yields the full spectrum $\{E(\alpha, N)\}$ up to $N$, here to $N = 24$ for spin-$1/2$ chains. We can always find $T_n(\alpha, N)$ such that the thermodynamic limit is satisfied at $T > T_n(\alpha, 24)$ for the quantity of interest. The low energy part of $\{E(\alpha, N)\}$ for larger $N$ is required at lower $T$, and DMRG is well suited for low-energy excitations. In principle, the problems are to obtain the low-energy excitations and to combine them with ED results.

The same conclusion follows from the increasing density of states with system size and the passage from a sum in $Q(T, \alpha, N)$ to an integral over excitations. The Boltzmann factor varies smoothly at high $T$ but is strongly peaked at low $T$. We expect and find lower $T_n(\alpha, N)$ in models with a high density of low-energy excitations. The normalized density of excitations, $\rho(\varepsilon, \alpha)$ with $\varepsilon = E(\alpha, N)/N|J_1|$, is shown in Fig. 1 for $N = 16, 20$ and $24$ spins in the HAF and $J_1 - J_2$ models with $J_1 < 0$ and $\alpha = J_2/|J_1|$. We obtained $\rho(\varepsilon, \alpha)$ for $N = 16$ and $20$ as the number of states in $40 - 50$ bins of equal width. We took narrower bins for $N = 24$ and averaged over several adjacent bins to get relatively smooth curves.

A triplet at $E_T(\alpha, N)$ is typically the lowest excitation of spin chains with a singlet ground state. The size dependence of $E_T(\alpha, N)$ has been extensively discussed for the HAF and half-filled Hubbard or extended Hubbard models. The spin chains we consider have frustrated exchange interactions that shift the density of excitations to lower energy in Fig. 1. We shall be comparing systems with similar finite-size gaps but different thermodynamics that reflects the excitation spectrum $\rho(\varepsilon, \alpha)$.

The paper is organized as follows. Section II presents the hybrid ED/DMRG procedure, starting with the DMRG calculation of excitation energies, moving on to truncation and ending with comparison with HAF thermodynamics. We turn in Section III to the $J_1 - J_2$ model with F exchange $J_1 < 0$ and AF exchange $J_2 > 0$. We compare results on the $J_1 < 0$ side with field theory and TMRG. ED to $N = 24$ accounts well for the spin susceptibility $\chi(T)$ and specific heat $C(T)$ per site at the critical point, $\alpha_c = 1/4$. DMRG extends the thermodynamics of F/AF chains to $T \sim 0.01$ in units of $|J_1|$, the largest exchange. Section IV is a brief discussion of the method and its scope.

II. THERMODYNAMICS, TRUNCATION AND EXTRAPOLATION

We develop in this Section the thermodynamics of spin chains without invoking the full energy spectrum $\{E(\alpha, N)\}$. In II A we obtain the low-energy states $E_j(\alpha, N)$ of models $\alpha$ with $N$ spins. In II B we truncate the partition function $Q(T, \alpha, N)$ in Eq. 1 at $E_j(\alpha, N) \leq W_c(\alpha, N)$ and discuss the choice of the energy cutoff. Extrapolation to the thermodynamic limit is demonstrated in II C against exact HAF results. The applications in Section III are to $J_1 - J_2$ models for which numerical analysis is more difficult and exact results are limited to $T = 0$. 

![FIG. 1. Normalized density of excitations, $\rho(\varepsilon, \alpha)$ with $\varepsilon = E(\alpha, N)/N|J_1|$, for three models of $N$ spins. The ground state is a singlet ($S = 0$) at $\varepsilon = 0$. The Néel state ($\ldots \alpha\beta\alpha\beta \ldots$) has excitation energy $\varepsilon_N = 1/2$ for the $\alpha_c$ model while the FM state ($\ldots \alpha\alpha\alpha \ldots$) has $\varepsilon_F = \ln 2$ for the HAF.](image-url)
The $J_1 - J_2$ model has isotropic exchange $J_1$, $J_2/|J_1| = \alpha$ and is frustrated for either sign of $J_1$. We consider $J_1 < 0$ and set $|J_1| = 1$ as the unit of energy in chains of $N = 4n$ spins-1/2 with periodic boundary conditions. The model Hamiltonians $\alpha$ are

$$H(\alpha) = -\sum_r \tilde{S}_r \cdot \tilde{S}_{r+1} + \alpha \sum_r \tilde{S}_r \cdot \tilde{S}_{r+2}. \quad (3)$$

The ground state is a singlet, total $S = 0$, for $\alpha > \alpha_c = 1/4$. The singlet and FM states are degenerate at the exact quantum critical point $\alpha_c$ [19]. The degeneracy at $\alpha_c$ is also exact for finite $N = 4n$ [27]. The HAF has AF exchange $J_1 = 1$ and $\alpha = 0$ in Eq. 3. Exact, field theoretical and numerical results for its thermodynamics in zero field are summarized in detail in Ref. 11. Although there are open questions, especially in finite field, nowadays the HAF provides convenient tests of numerical methods.

### A. DMRG

We use the efficient DMRG algorithm for periodic boundary conditions in Ref. 28, where it was applied to the ground state energy and lowest excitation of HAFs with spin-1/2 and 1. The superblock in this method has two new sites in addition to the left and right blocks. Since Eq. 3 has second neighbor interactions, we take new blocks of two sites in order to avoid interaction terms between old blocks. Four sites are added in each block at every step of infinite DMRG. The accuracy and computational costs are similar to matrix product state calculations [28].

Infinite DMRG is used to generate the desired system of $N = 4n$ spins. Some 5-10 sweeps of finite DMRG are then performed. In most calculations we kept $m = 400$ eigenvectors that correspond to highest eigenvalues of the system block density matrix. The superblock Hamiltonian has dimension $m^2 2^4$. The ground state $E_1(N)$ is taken as zero. The states $j > 1$ have excitation energies $E_j(N) > 0$. The DMRG partition function with $\ell$ states of the superblock Hamiltonian is

$$Q_\ell(T, N) = \sum_{j=1}^\ell \exp(-\beta E_j(N)). \quad (4)$$

We later consider truncated partition functions $Q_C(T, N)$ with $E_j(N) \leq W_C(N)$ at energy cutoff $W_C(N)$.

We introduce in this paper several modifications that are tailored for finite systems. The focus is on excitations rather than the ground state. To improve the accuracy of the spectrum, we construct the system block density matrices $\rho_j(N)$ for the $\ell$ levels at system size $N$ and define an effective density matrix $\rho'(\beta', \ell)$

$$\rho'(\beta', \ell, N) = \sum_{j=1}^\ell \rho_j(N) \exp(-\beta' E_j(N)) / Q_\ell(T, N). \quad (5)$$

The $l = 1$ case is simply $\rho'(\beta', 1) = \rho_1$ when the ground state is sought. Contributions for $l > 1$ are governed by $\beta'$, an effective inverse $T$. We set $\beta' = 10$ (in units of $1/|J_1|$) since $T \sim 0.1$ is the range of interest. Variations of $\beta'$ by 10 to 20% hardly change the accuracy of the spectrum. The effective density matrix becomes important when the lowest excitations are closely spaced.

The system block Hamiltonian and all operators are renormalized by $\rho'(\beta', l, N)$ to obtain the energy spectrum the model Hamiltonian at system size $N$. We perform two calculations. We first take $l = 5$ or 10 in order to obtain the lowest excitations very accurately. The second calculation has $l > 100$. The entire spectrum is red shifted by an approximately constant amount because the density matrix now has projections from many excited states. Accordingly, we shift the spectrum by a constant and use the first calculation for the lowest excitations.

To illustrate the accuracy, we compare DMRG excitation energies for $l = 400$ and $\beta' = 10$ with exact results. The lowest 10 levels are listed in Table I for $N = 24$ and 32 at $\alpha = 2/3$ in Eq. 3. The starred excitation is the lowest singlet, $S = 0$.

| Level no. | $N = 24$ | $N = 32$ |
|----------|----------|----------|
| 2        | 0.1256   | 0.1256   |
| 3        | 0.1256   | 0.1256   |
| 4        | 0.1256   | 0.1256   |
| 5        | 0.1256   | 0.1256   |
| 6        | 0.1256   | 0.1256   |
| 7        | 0.1256   | 0.1256   |
| 8        | 0.1256   | 0.1256   |
| 9        | 0.1256   | 0.1256   |
| 10       | 0.1256   | 0.1256   |

Table II. Exact (ED) and DMRG excitation energies for $N = 24$ and 32 at $\alpha = 1/2$ in Eq. 3. The starred excitation is the lowest singlet, $S = 0$.

| Level no. | $N = 24$ | $N = 32$ |
|----------|----------|----------|
| 2        | 0.0114*  | 0.0114*  |
| 3        | 0.0114*  | 0.0114*  |
| 4        | 0.0114*  | 0.0114*  |
| 5        | 0.0114*  | 0.0114*  |
| 6        | 0.0114*  | 0.0114*  |
| 7        | 0.0114*  | 0.0114*  |
| 8        | 0.0114*  | 0.0114*  |
| 9        | 0.0114*  | 0.0114*  |
| 10       | 0.0114*  | 0.0114*  |

The $l = 1$ case is simply $\rho'(\beta', 1) = \rho_1$ when the ground state is sought. Contributions for $l > 1$ are governed by $\beta'$, an effective inverse $T$. We set $\beta' = 10$ (in units of $1/|J_1|$) since $T \sim 0.1$ is the range of interest. Variations of $\beta'$ by 10 to 20% hardly change the accuracy of the spectrum. The effective density matrix becomes important when the lowest excitations are closely spaced.

The system block Hamiltonian and all operators are renormalized by $\rho'(\beta', l, N)$ to obtain the energy spectrum the model Hamiltonian at system size $N$. We perform two calculations. We first take $l = 5$ or 10 in order to obtain the lowest excitations very accurately. The second calculation has $l > 100$. The entire spectrum is red shifted by an approximately constant amount because the density matrix now has projections from many excited states. Accordingly, we shift the spectrum by a constant and use the first calculation for the lowest excitations.

To illustrate the accuracy, we compare DMRG excitation energies for $l = 400$ and $\beta' = 10$ with exact results. The lowest 10 levels are listed in Table I for $N = 24$ and 32 at $\alpha = 2/3$, and in Table II at $\alpha = 1/2$. The $\alpha = 1/2$ levels are clearly denser than the $\alpha = 2/3$ levels that in turn are denser than the corresponding HAF levels (not listed). Translational symmetry for periodic boundary conditions makes possible the ED results in the Tables.
The accuracy of the lowest 5 excitations is about 1 and 1.5%, respectively, for $\alpha = 2/3$ and $1/2$. The HAF accuracy is better than 1%. The accuracy up to level 100 is better than 5% and better than 10% for levels far higher than 100. Truncated partition functions are limited to $T \sim T'(N)$ that depends on system size as discussed below. Since the cutoff $W_C(N)$ is more than $10T'(N)$, the Boltzmann factors are very small. Accurate excitation energies are essential at low $T$.

To summarize, DMRG yields the excitations $E_j(\alpha, N) \leq W_C(\alpha, N)$ in models $\alpha$ with $N$ spins in Eq. 3. Calculations are performed in sectors with Zeeman component $S^z = M$. The absolute ground state is in the $M = 0$ sector for $\alpha > \alpha_c$ and the $E_j(M, \alpha, N)$ are relative to $E_1(\alpha, N) = 0$.

**B. Thermodynamics**

The evolution of any thermodynamic quantity can be followed as the cutoff $W_C(N)$ is increased. The truncated partition function $Q_C(T, N)$ with $E_j(N) \leq W_C(N)$ in Eq. 4 is accurate at low $T$ and merges with ED at $T > T_c(N)$ when the full spectrum is retained. However, computational resources limit $W_C(N)$ and thermodynamics to $T < T_c(N)$, as seen explicitly for ED at $N = 24$. We need a criterion for choosing the cutoff. $W_C(N)$ leads to $R_C(M, N)$ states in sectors with $S^z = M$. Since $S$ is conserved, the total number of states is

$$R_C(N) = R_C(0, N) + \sum_{M=1}^{N/2} 2R_C(M, N). \quad (6)$$

The number of states in the $M = 0$ sector is more convenient and intuitive than $W_C(N)$ for discussing thermodynamics. We retain $10^3 - 10^4$ states at low $T$ out of $2^N$ states.

We chose $W_C(N)$ based on the maxima of $S_C(T, N)/T$ and $\chi_C(T, N)$, where $S_C(T, N)$ is the entropy per spin and $\chi_C(T, N)$ is the magnetic susceptibility per spin. Both are reduced at low $T$ by finite size gaps and at high $T$ by truncation.

Fig. 2 illustrates the convergence of $S_C(T, N)/T$ and $\chi_C(T, N)$ for $N = 48$ and 64 at $\alpha = 2/3$ in Eq. 3. The logarithmic scale is to emphasize low $T$. The cut-off governs the number of states in the $M = 0$ sector. $R_C(0, N) = 400$ ensures adequate convergence with respect to finite size gaps. The truncated partition function has $R_C(N) = 1563$ and 1818 states, respectively, at $N = 48$ and 64.

Fig. 3 shows the same functions for $\alpha = 1/2$ in Eq. 3. The maxima of $S_C(T, N)/T$ and $\chi_C(T, N)$ are about twice as high and are shifted to lower $T$ compared to $\alpha = 2/3$. However, the maxima are again converged with $R_C(0, N) = 400$ states. Now the truncated partition function has $R_C(N) = 1832$ and 2200 states, respectively, at $N = 48$ and 64. As implied by the $S(T)/T$ panel, there are many states with $E_j(64) < 0.01$ where the numerical accuracy has to be considered. The $\alpha = 1/3$ spectrum has even smaller and denser excitations.

The full and truncated partition functions are given in Eq. 1 and Eq. 4. Truncation always reduces $Q(T, N)$. It also reduces the internal energy $E(T, N)$ as shown by taking the difference and noting that the sum below is
over \( E_j(N) > W_C(N) > E_C(T, N) \),
\[
E(T, N) - E_C(T, N) = \frac{1}{Q(T, N)} \times \\
\sum_j \left( E_j(N) - E_C(T, N) \right) \exp \left( -\beta E_j(N) \right).
\]
(7)

It follows that truncation also reduces the entropy
\( S(T, N) = k_B \ln Q(T, N)/N + E(T, N)/NT \). Truncation is arbitrarily accurate for \( \beta W_C(N) \gg 1 \) and inevitably fails at high \( T \).

We will necessarily be working with \( S_C(T, N) \) in large systems. The function \( S_C(T, N)/T \) has a maximum at \( T'(N) \) where
\[
S_C(T', N) = T'(N)S_C(T', N).
\]
(8)

The same relation holds for the maximum of \( S(T, N)/T \) or of \( S(T)/T \). The maxima at \( S_C(T', N)/T' \) in Fig. 2 and Fig. 3 are lower bounds on \( S(T)/T \) in the thermodynamic limit. They are the most accurate approximation at truncation \( W_C(N) \). Accordingly, the cutoff criterion is convergence at the maximum.

Truncation reduces the entropy but not necessarily the susceptibility. The difference between the full and truncated magnetic susceptibility per site is
\[
\chi(T, N) - \chi_C(T, N) = \frac{1}{NTQ(T, N)} \times \\
\sum_j \left( M_j^2(N) - M_j^2(T, N) \right) \exp \left( -\beta E_j(N) \right).
\]
(9)

The sum is over states \( E_j(N) > W_C(N) \) with Zeeman components \( S^z = M_k \), and \( M_j^2(T, N) \) is the average value of \( M_j^2 \) over \( E_j(N) \leq W_C(N) \). There is no guarantee that the sum is positive. However, we are always using a tiny fraction of states close to the singlet ground state and find that \( \chi_C(T, N) \) converges from below with increasing \( W_C(N) \). A satisfactory cutoff converges \( \chi_C(T, N) \) to its peak. The \( \chi_C(T, N) \) maxima in Fig. 2 and Fig. 3 are less converged than the \( S_C(T, N)/T \) maxima.

The spectrum in the \( M = 0 \) sector is the densest since it includes a Zeeman component of all states with \( S > 0 \), and it has the largest truncation error. The following results are mostly based on cutoffs \( W_C(\alpha, N) \) that retain 10 states with \( M = 5 \) and none with \( M > 5 \). The \( M = 0 \) and 1 sectors contain more than 400 states, nearly 1000 states, when the Zeeman components include the projection from sectors with higher \( M \) within cutoff \( W_C(\alpha, N) \). The total number of states is \( R_C = 4532 \) and 2705 for \( N = 48 \) and 64, respectively at \( \alpha = 2/3 \), and 3647 and 2239 at 48 and 64 at \( \alpha = 1/2 \). The results are not sensitive to \( W_C(N) \) provided the cutoff is high enough to enforce convergence at the maxima in Fig. 2 and Fig. 3.

C. Extrapolation

Fig. 4 shows the absolute spin susceptibility \( \chi(T) \) and specific heat \( C(T) \) of the HAF. \( N_A \) is Avogadro’s number, \( \mu_B \) is the Bohr magneton and \( g \) is the electronic g factor. We use reduced units from here on and label the axes of subsequent graphs as \( \chi(T) \) or \( S'(T) = C(T)/T \) vs. \( T \).

ED (solid lines) clearly indicates converged \( \chi(T) \) at \( T > T_n = 0.20 \). The peak at \( T_m = 0.641 \) and \( \chi(T_m) = 0.147 \) in the upper panel are quantitative [11]. DMRG (dashed lines) extends \( \chi(T) \) to lower \( T \) and illustrates once again that finite-size gaps decrease with increasing system size. The squares on the DMRG curves \( \chi'(T', N) \) evaluated at \( T'(N) \), the maximum of \( S_C(T, N)/T \), open symbols are quantum Monte Carlo (QMC) calculations following Ref. 14 at \( N = 48 \), 100 and 256. The arrow marks the exact \( \chi(0) = 1/\pi^2 \). There are logarithmic corrections [11] at \( k_B T / J_1 < 0.005 \).

The lower panel of Fig. 4 shows the entropy derivative, \( S'(T') = C(T)/T \), over the same range. The area under ED (solid) lines is \( \ln 2 \) and ED again converges for \( T > 0.20 \). The peak at \( T^* = 0.307 \) and \( S'(T^*) = 0.897 \) are quantitative [11]. The arrow marks the exact \( S'(0) = 2/3 \). DMRG (dashed lines) terminate at \( T'(N) \), shown as open circles. The \( S'(T', N) \) maxima are at \( T_m(N) < T'(N) \). We return later to the squares. DMRG and truncation is almost quantitative up to \( T'(N) \), as seen from ED at \( N = 24 \). That is also the case for \( \chi(T) \) at \( T'(N) \) in the upper panel.

There are far fewer published \( C(T, N) \) than \( \chi(T, N) \) curves. Moreover, \( C(T, N) \) plots completely obscure the behavior at low \( T \) where finite size effects are responsible for deviations from linearity. QMC works beautifully for
\( \chi(T) \) but produces scatter plots for \( C(T, N)/T \) at low \( T \); it is ill suited for narrow features such as the \( T_m(N) \) peaks. Finite size effects are readily understood. Since \( S(T_n) \) is in the thermodynamic limit and finite systems have \( S'(0, N) = 0 \), reduced \( S'(T, N) \) at low \( T \) must be compensated by increased \( S'(T, N) \) at \( T < T_n \). The truncated \( S'(T, N) \) have maxima at \( T_m(N) \) where

\[
S'_c(T_m, N) = \frac{C_c(T_m, N)}{T_m} > S'(T_m)
\]  

(10)

Convergence of \( S'_c(T, N) \) to the thermodynamic limit is from above while \( S_c(T, N) \) converges from below.

In order to extract the thermodynamic limit of \( S'(T) \), we note that its maximum \( T^* \) is above \( T_n \). The \( S'(T, N) \) peaks are superimposed on a smooth background that we take as \( S'(T) = a(1 + bT + c^2T^4) \) for \( T \leq T_n \). There are three parameters, \( a, b, \) and \( c \). Two are fixed by \( S(T_n) \) and \( S'(T_n) \). The third is fixed by the scaling \( x(N) = S'(T_m)/S'(T_m, N) \) for each truncated spectrum. We sought parameters for which \( x(N) \) is size independent. The best choice had \( x < 68.5 \) and 69.4\% for the \( T_m(N) \) peaks from \( N = 24 \) to 96. The resulting \( S'(T) = C(T)/T \) is the \( T < T_n \) line in Fig. 4. We find \( S'(0) = 0.659 \) and very small \( b = 10^{-5} \). The exact result is \( S'(0) = 2/3 \) and \( S'(T) \) is quadratic at low \( T \) [11] aside from logarithmic corrections below \( T = 0.005 \).

We conclude that hybrid ED/DMRG works well for the HAF’s spin susceptibility and specific heat. The HAF is especially simple: spin-1/2, one spin per unit cell, one exchange and hence no frustration. We did not appreciate that improved extrapolation is needed for the frustrated \( J_1 - J_2 \) model in Eq. 3. The \( S'(T, \alpha)/T \) peak at \( T^*(\alpha) \) shifts to \( T < T_n(\alpha) \) and reaches \( T = 0 \) near the critical point \( \alpha_c \). Agreement with the HAF is necessary but not sufficient.

### III. THERMODYNAMICS OF \( J_1 - J_2 \) MODELS

In this section we study the \( J_1 - J_2 \) model with \( \alpha \geq \alpha_c = 1/4 \) in Eq. 3. Its quantum phases have already been mentioned. The general TMRG study of Lu et al. [29] has results for \( J_1, J_2 \) of either sign and discusses the thermodynamics of both singlet and FM phases. Sirker [30] later applied TMRG to the singlet phases of F/AF chains with \( \alpha \) ranging from \( \alpha_c \) to 2. QMC is not applicable to frustrated interactions. The ground state is a singlet \( (S = 0) \) and is doubly degenerate in the IC phase.

ED up to 24 spins converges to the thermodynamic limit for \( T > T_n(\alpha) \) as seen in Fig. 4 for the HAF. The \( T_n(\alpha) \) in Table III are in units of \( |J_1|/k_B \). They are based on \( S'(T, N) = C(T, N)/T \), whose size dependence is usually stronger than that of \( \chi(T, N) \). The increasing density of states in Fig. 1 with decreasing \( \alpha \) accounts for an order of magnitude variation of \( T_n(\alpha) \). The area per spin under \( S'(T, \alpha, N) \) curves is respectively \( \ln 2 \) for ED and \( (\ln R_c(\alpha, N))/N \) for DMRG, where \( R_c(\alpha, N) \) is the truncated number of states in Eq. 6.

**TABLE III. Reduced temperature \( T_n(\alpha) \) at which the thermodynamic limit of \( S'(T, \alpha) = C(T, \alpha)/T \) is reached for \( N = 24 \) spins in \( J_1 - J_2 \) models with frustration \( \alpha \) in Eq. 3.**

| Model, \( \alpha \) | \( T_n(\alpha) \) | \( S(T_n(\alpha), \alpha) \) | \( S'(T_n(\alpha), \alpha) \) |
|-----------------|-----------------|-----------------|-----------------|
| \( \alpha_c = 1/4 \) | 0.92 | 0.413 | 2.665 |
| 1/3 | 0.06 | 0.481 | 1.838 |
| 1/2 | 0.14 | 0.399 | 1.656 |
| 2/3 | 0.17 | 0.293 | 1.533 |
| HAF | 0.20 | 0.143 | 0.820 |

The singlet quantum phases of spin-1/2 chains are either gapless with a nondegenerate ground state or gapped with a doubly degenerate ground state [31]. The HAF is gapless while the \( J_1 - J_2 \) model has both gapped and gapless singlet phases. The HAF has logarithmic contributions to \( \chi(T) \) and \( C(T) \) at \( T < 5 \times 10^{-3} \) that are followed to several decades lower \( T \) in Ref. 11. The gapped incommensurate (IC) phase runs from the exact quantum critical point [19] \( \alpha_c = 1/4 \) to another critical point [21] around \( \alpha = 0.806 \). The IC gap \( \Delta(\alpha) \) is exponentially small [32], however, and has yet to be evaluated. The ground state degeneracy is followed numerically using DMRG with periodic boundary to compute the static structure factor \( F(q, \alpha) \) at wave vector \( q \) [21]. The \( F(q, \alpha) \) peaks at \( \pm q(\alpha) \) shift in the IC phase from \( q(1/4) = 0 \) to \( q(0.806) = \pi/2 \). The decoupled phase [21] for \( \alpha > 0.806 \) is gapless and commensurate. Its singlet ground state is nondegenerate and has quasi-long-range order with \( q = \pi/2 \).

Neither logarithmic corrections nor IC gap matters for the thermodynamics at \( T > 0.01 \). Returning to Table III, we note that the average value of \( S'(T_n, \alpha) \) up to \( T_n(\alpha) \) is \( S(T_n(\alpha))/T_n \) and does not depend on the actual form of \( S'(T_n, \alpha) \) in the interval. Since the average at \( \alpha = 1/3 \) is more than four times \( S'(T_n, 1/3) \), we infer that \( S'(T, 1/3) \) decreases with \( T \). Although not as strongly, \( S'(T, 1/2) \) and \( S'(T, 2/3) \) also decrease with \( T \) while the HAF has increasing \( S'(T) \) to \( T^* > T_n \).

**A. Critical point, \( \alpha_c = 1/4 \)**

Thermodynamics at the critical point is remarkably different from larger \( \alpha \). ED results in Fig. 5 for \( S'(T, \alpha_c) \) and \( \chi(T, \alpha_c) \) in reduced units are almost power laws over several decades in \( T \). The approximate exponents are \( \gamma = -1.18 \) and \( -0.97 \), respectively. ED to \( N = 24 \) at the critical point indicates that \( T_n(\alpha_c) \sim 0.02 \) and shows the stronger size dependence of \( S'(T, N) \). \( S'(T) \) is a measure of thermal fluctuations while \( \chi(T) \) measures fluctuations of \( M^2 \), where \( -S \leq M \leq S \) are the Zeeman levels of spin-S states.

Sirker et al. [20] studied the \( J_1 - J_2 \) model in zero field on the FM side, \( 0 \leq \alpha \leq \alpha_c = 1/4 \), using field theory and numerical methods. To leading order in \( T \), the exact \( \chi(T, \alpha_c) \) is \( AT^{-4/3} \) with \( A \sim 0.1685 \) according to field
This is a mathematical result. In the present context, 

\[ C = S \]

The steep power-law \( \alpha \) decreases both \( \chi(T, \alpha) \) and \( C(T, \alpha) \). The qualitative changes from \( \alpha \) to the HAF provide a framework for the thermodynamics at intermediate \( \alpha \).

### B. Coupled sublattices, \( \alpha = 2/3 \)

The \( \alpha \to \infty(J_1 = 0) \) limit of Eq. 3 corresponds to HAFs on sublattices of odd and even numbered sites. Finite \( J_1 < 0 \) couples the HAFs and, as shown in Fig. 6 at \( \alpha = 2/3 \), increases both \( \chi(T, \alpha) \) and \( C(T, \alpha) \). The steepness is accommodated by finite size effects and the HAF extrapolations no longer suffice. The reason is that \( S(T, \alpha) \) either decreases monotonically or has a maximum at \( T^* < T_n(\alpha, N) \). We consider an alternative analysis before discussing the \( \alpha = 2/3 \) results.

We suppress the model index \( \alpha \) and recall that the truncated entropy \( S_C(T, N) \) converges to \( S(T, N) \) from below. The approximation that relates finite \( N \) to the thermodynamic limit is

\[
\frac{S_C(T', N)}{\gamma} \leq S(T', N) \leq \frac{S(T')}{\gamma} = \langle S'(T) \rangle_{T'}
\]

where \( T'(N) \) is the maximum defined in Eq. 8. It follows that \( T'(N) \) is less than \( T_n(N) \) but greater than \( T_m(N) \). The maximum of \( S'(T', N) \) in Eq. 10, \( S'(T_{m}, N) > S'(T_n) \). We note that \( S_C(T, N) \) diverges at \( T = 0 \) and \( T'(N) \). Each system size generates a point at \( T'(N) \). It is convenient to define \( T_1 = T'(N_1) \) for the largest system, \( T_2 = T'(N_2) \) for the second largest, and so on.

The mean value theorem can be applied to successive intervals to estimate

\[
S'(T_1/2) \approx \frac{S(T_1)}{T_1}, \quad 0 \leq T \leq T_1
\]

and similarly at \( T = (T_2 + T_3)/2 \). This simple approximation is accurate when the size dependence of \( S'(T, N) \) is weak. The final point at \( S(T_n)/T_n \) is in the thermodynamic limit, where \( S'(T_n) \) is also known. There is one input at each \( T'(N) \) and two at \( T_n \) for estimating \( S'(T) \) up to \( T_n \).

ED and DMRG results for \( \chi(T, N) \) are shown in the upper panel of Fig. 6 for \( H(2/3) \) in Eq. 3. The thermodynamic limit holds for \( T > T_n(2/3) = 0.17 \). The \( \chi(T) \) is less than \( 0.281 \) is lower than 0.6413 for the HAF and \( \chi(T_m) = 0.395 \) is almost three times higher due to F exchange \( J_f \). The bold dashed line that approximates the thermodynamic limit is linear extrapolation of the \( N = 48 \) and 64 maxima. The upturn of \( \chi(T) \) at
low $T$ is consistent with TMRG at $\alpha = 0.6$ in Fig.1 of Ref. 30. So are the magnitude at the peak and the lowest accessible $T$.

The lower panel of Fig. 6 shows $S'(T) = C(T)/T$ and large finite-size peaks. The DMRG curves stop at $T'(N)$, the maximum of $S_C(T, 2/3, N)/T$, which are shown as open circles. The squares are the mean value approximation, Eq. 12, which returns the squares in Fig. 4 (lower panel) when be applied to $S'(T)$ for the HAF. We find $S'(0) \sim 1.88$ at $\alpha = 2/3$, again about three times the HAF value. $S'(T)$ gently decreases with $T$ at $\alpha = 2/3$ instead of gently increasing in the HAF.

C. Incommensurate phase

The $J_1 - J_2$ model at $\alpha \geq 2/3$ can be viewed as HAFs on sublattices with F exchange $J_1 < 0$ reaching $-3J_2/2$ at $\alpha = 2/3$. The singlet ground state persists for more negative $J_1$ down to $\alpha_c = 1/4$ where as seen in Fig. 5 both $C(T)/T$ and $\chi(T)$ decrease sharply with increasing $T$. The $\alpha_c < \alpha < 2/3$ regime is particularly challenging. The thermodynamics is governed by weak AF exchange $J_2 < |J_1|$ at low $T$ and strong F exchange $J_1$ at high $T$.

The Curie law for free spins is $\chi_C = 1/4T$ in reduced units. The $\chi(T, \alpha, 24)/\chi_C$ curves in Fig. 7 deviate from free spins due to competing F and AF exchanges. The “Curie temperatures” $T_C(\alpha)$ at which $\chi(T, \alpha)/\chi_C = 1$ are in the thermodynamic limit, above the $T_n(\alpha)$ in Table III. Offsetting F and AF exchanges lead to free-spin behavior at $T_C(\alpha)$, much as attractive and repulsive interactions in gases cancel at the Boyle temperature. The exact [20] $T^{-1/3}$ divergence at $\alpha_c$ is completely suppressed for $\alpha > \alpha_c$. The $T = 0$ limit of $\chi(T, \alpha)/\chi_C$ is zero for either gapless or gapped chains with singlet ground states.

Finite size gaps typically decrease roughly as $1/N$, but this expectation can fail in frustrated systems. The first (stained) excitation $E_2(N)$ in Table II for $\alpha = 1/2$ is twice as large at $N = 32$ than at $N = 24$. This singlet becomes degenerate with the ground state in the 1C phase. The degeneracy for $N = 4\alpha$ is limited to $n$ points $\alpha_j(N)$. The first is always $\alpha_c = 1/4$ while the last point $\alpha_j(N)$ increases with $N$. The $\alpha_j(N)$ are not distributed uniformly but are densest near the critical point [27]. The gap $E_2(N, \alpha)$ at constant $\alpha$ varies randomly in large systems when $\alpha_j(N) > \alpha$. It vanishes when $\alpha = \alpha_j(N)$, is finite elsewhere, and decreases slowly with $N$ as the number of degenerate points increases. ED indicates [27] that $\alpha_j(24) < 1/2 < \alpha_j(28)$ while DMRG shows [21] that $\alpha_j(192) = 0.66$. Hence $E_2(N)$ is already important at $N = 24$ for $\alpha = 1/2$ but not until much larger $N$ for $\alpha = 2/3$.

Fig. 8 shows $\chi(T)$ and $C(T)/T$ curves at $\alpha = 1/2$. As expected, stronger F exchange compared to $\alpha = 2/3$ increases both and shifts them to lower $T$. The $\chi(T, N)$ peak increases with $N$ and shifts to lower $T$ at large $N$, but $\chi(T, N)$ decreases with $N$ at $T \sim 0.1$. The bold dashed line is linear extrapolation of the $N = 48$ and 64 peaks, shifted up slightly since since the thermodynamic limit is reached from below. It is quite approximate: $\chi(T, 1/2) \sim 0.9$ at $T \sim 0$ and decreases to $\sim 0.7$ at $T \sim 0.06$. The weak maximum of 0.74 at $T = 0.14$ is in the thermodynamic limit.

The $C(T)$ curves in the lower panel have similar $T'(32) \sim T'(48)$ that reflect the approximate nature of Eq. 11. We averaged both $T'(32)$, $T'(48)$ and $S'(T, 32)$, $S'(T, 48)$ to obtain the squares using Eq. 12 for the mean
values in the thermodynamic limit. The dashed line indicates linear 
\( C(T) \sim 4T \) from \( T = 0.01 \) to \( 0.03 \) with downward deviation at \( 0.04 \) for \( \alpha = 0.5 \) in the thermodynamic limit. TMRG [29, 30] for \( C(T) \) at \( \alpha = 0.4 \) was extended [6] down to \( T = 0.01 \). As seen in Fig.5 of Ref. 6, 
\( C(T) \sim 0.05 \) at \( T = 0.01 \). It is almost linear in \( T \) up to \( T = 0.03 \) and deviates downward at \( 0.04 \). The \( T \) dependence is similar and \( C(T) \) is known to increase at low \( T \) with decreasing \( \alpha \) in the singlet phase. 

The degeneracies \( \alpha_j(N) \) are closely spaced at \( \alpha = 1/3 \) and the excitations \( E_j(N) \) are both small and dense.Numerical considerations discussed in Section II limit us to \( N = 32 \). On the other hand, the thermodynamic limit is already reached at \( T_n(1/3) = 0.06 \).

We switch in Fig. 9 to a linear \( T \) scale for \( \chi(T) \)
and \( C(T) \) up to \( T = 0.10 \), the Curie \( T \) for free spins. AF correlations at lower \( T \) lead to slower than \( 1/T \) increase of \( \chi(T) \) and a maximum at \( T \sim 0.04 \). The truncated \( \chi(T, 32) \) peak confirms that \( \chi(T) \) decreases in the thermodynamic limit at least to \( T = 0.02 \). The estimated \( T \sim 0 \) value of \( \sim 1.7 \) is more than 10 times that of the HAF. TMRG [30] at \( \alpha = 0.3 \) indicates a \( \chi(T) \) maximum at \( T \sim 0.02 \). This is consistent with Fig. 9 since the peak shifts to \( T = 0 \) just above \( \alpha_c = 1/4 \).

We have three intervals for \( C(T, N)/T \) based on \( T'(32) = 0.0179, T'(24) = 0.0273 \) and \( T_n = 0.06 \). The mean values using Eq. 12 lead to the squares in the lower panel. The exact \( C(T, 1/3, 24) \) calculation was first reported in Ref. 33. Our results for \( T < T_n \) suggest that the peak in the thermodynamic limit is slightly lower and shifted to higher \( T \). Also shown is the specific heat \( C(T, 1/4) \sim T^{0.03} \) at the critical point. It is almost constant in this interval since the \( C(T)/T \) exponent in Fig. 5 is close to \(-1\).

Spinless fermions [34] can be used to represent spin-1/2 chains; the \( S^z = 0 \) ground state corresponds to a half-filled band. The HAF has two-fermion interactions while the \( J_1 - J_2 \) model, Eq. 3, has up to four-fermion interactions. Both \( C(T)/T = S'(T) \) and \( \chi(T) \) are proportional to the density of states at the Fermi energy as \( T \rightarrow 0 \). The Wilson-Sommerfeld ratio in reduced units is 
\[
R_W(T) = \frac{4\pi^2 \chi(T)}{3S'(T)}
\]

\( R_W(T) = 1 \) for free fermions, independent of \( T \). The HAF result is \( R_W(0) = 2 \) with 10% variations up to \( T = 0.4 \) [11]. The \( J_1 - J_2 \) model has increased \( R_W(0.01) \sim 2.6 \) at \( \alpha = 2/3 \) and \( \alpha = 1/2 \). Much larger \( R_W(0.01) \sim 150 \) is found at \( \alpha_c = 1/4 \). \( R_W(0) \) increases when low-energy excitations have large \( S \) because \( C(T)/T \) contributions go as the \( (2S+1) \), the Zeeman degeneracy, while \( \chi(T) \) contributions go as \( S(S+1)(2S+1)/3 \), the sum over \( M^2 \).

### IV. DISCUSSION

We have presented a hybrid ED/DMRG approach to the thermodynamics of 1D models that never requires the full energy spectrum \( \{E(N)\} \) of large systems and tested it in Section II against the spin-1/2 HAF. The \( 2^N \) states of spin-1/2 chains are found exactly in small systems and suffice for the thermodynamics at high \( T \). DMRG for
larger systems is used to obtain the lowest few thousand excitations $E_j(N)$. Thermodynamics at low $T$ is based on the truncated spectrum $E_j(N) \leq W_C(N)$. The cutoff criterion for convergence to the maximum of $S_C(T,N)/T$ and $\chi_C(T,N)$ with $T$, where $S_C(T,N)$ and $\chi_C(T,N)$ are respectively the truncated zero-field entropy and susceptibility per site. The thermodynamic limit at $T$ is approximated by maximum of $S_C(T,N)/T$ or of $\chi_C(T,N)$ at system size $N$.

Exact diagonalization (ED) of the HAF with $N = 24$ spins becomes quantitative for $T \geq 0.20 J/k_B$ as shown in Fig. 4. DMRG up to $N = 96$ extends the thermodynamic limit for $\chi(T)$ and $S'(T) = C(T)/T$ to an order of magnitude lower $T$, in excellent agreement with exact and numerical results. We are studying the performance of DMRG and truncation in 1D systems such as half-filled Hubbard, extended Hubbard and related models with charge as well as spin degrees of freedom. These models reduce to the HAF in the atomic limit. Charge degrees of freedom limit ED to smaller $N < 20$ with larger finite size gaps. There is greater scope for DMRG and truncation before running into the accuracy issues discussed in Section II A.

The motivation for this work was the thermodynamics of the frustrated $J_1 − J_2$ model, Eq. 3, which is the starting point for the magnetic properties of several compounds with CuO$_2$ chains. $\mathbf{F}$ exchange $− J_1 > J_2$ is inferred [22–26] at high $T$ from Curie-Weiss fits of $\chi(T)$ over a limited interval in which deviations from free spins in Fig. 7 are positive, but different $J_1$, $\alpha$ combinations return [29, 35] similar $\chi(T)$. The net interaction is AF at low $T$ where an applied field can induce the FM state in some system. The $J_1 − J_2$ model specifies the entire range of magnetization and magnetic specific heat. The data set [24] for LiCuSbO$_4$ were successfully modeled [35] by $|J_1| = 28.7$ K and $\alpha = 2/3$ down to $T \sim 5$ K ($T/|J_1| \sim 0.17$) where finite-size gaps limit $N = 24$ results. Data below 5 K require improved thermodynamics as well as taking into account corrections to isotropic exchange and other magnetic interactions.

In an applied magnetic field, the $J_1 − J_2$ model with anisotropic exchange supports a number of exotic quantum phases: IC, multipolar, vector chiral, among others [13, 36, 37]. The nature of the ground states, spin correlations and hidden symmetries are active areas of research, primarily of $T \rightarrow 0$ properties. That limit is beyond our approach. We alluded in the Introduction to mathematical and physical motivations. The CuO$_2$ chains have $− J_1 \sim 10^2$ K and anisotropic $\mathbf{g}$-tensors that indicate $5−10\%$ deviations from isotropic exchange. Direct comparisons of the $J_1 − J_2$ model, Eq. 3, are limited to $T > 1$ K ($T > 0.01$ in reduced units), below which spin-orbit coupling and other magnetic interactions must be included. Considerably lower $T$ is relevant to exact field theory results at $\alpha_c$, for the gap $\Delta(\alpha)$ in the IC phase, or for logarithmic corrections. Quantitative analysis of magnetic data in the $1−10$ K range will be needed extract model parameters.

The hybrid ED/DMRG approach exploits the fact that the thermodynamic limit is reached at high $T$ in small systems that can be treated exactly. DMRG generates the excitations and truncated partition functions of increasingly large systems. We have focused on the spin susceptibility and specific heat of spin-1/2 chains. Other thermodynamic quantities are equally accessible, as indeed are applications to any 1D quantum cell model.

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