

## Efficient Evaluation of Partition Functions of Inhomogeneous Many-Body Spin Systems

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We present a numerical method to evaluate partition functions and associated correlation functions of inhomogeneous 2D classical spin systems and 1D quantum spin systems. The method is scalable and has a controlled error. We illustrate the algorithm by calculating the finite-temperature properties of bosonic particles in 1D optical lattices, as realized in current experiments.

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The study of thermodynamic properties of 2D classical spin systems has a very long and fruitful history. On the one hand, it has provided valuable insights in magnetism and phase transitions. On the other, it has allowed us to describe 1D quantum systems at finite temperature through the Suzuki-Trotter decomposition.

As very few spin models are exactly solvable, many different approximate methods have been proposed to calculate the associated partition functions. Monte Carlo simulations seem to be the method of choice for nonfrustrated systems, but fail in the description of frustrated and fermionic systems due to the notorious sign problem [1]. No such sign problem occurs in the method developed by Nishino [2], where the largest eigenvalue of the transfer matrix of the classical spin model can be approximated by using a variation of the density matrix renormalization group approach [3]. By making use of the Suzuki-Trotter decomposition, this method has also been used to calculate the free energy of translational invariant 1D quantum systems [4]. The main restriction of this method is that it cannot be applied in situations in which the number of particles is finite and/or the system is not homogeneous. The method may also become ill conditioned when the transfer matrix is not Hermitian. Finally, in the case of 1D quantum systems, a recent development [5,6] allows us to overcome these problems by extending the concept of matrix product states [7] to mixed states, e.g., by using the idea of purification of states [5]. This method is, however, specially designed for 1D quantum systems, and cannot be extended to classical 2D models.

Here we take a completely different approach which allows us to overcome the drawbacks of the above mentioned methods in both 2D classical and 1D quantum systems. We achieve this by evaluating the associated partition and correlation functions directly. The main advantages of this method are that the approximations made are very well controlled, that it applies to frustrated, inhomogeneous and finite classical and quantum systems, and that it can be generalized to higher dimensions. We will illustrate its performance with a system of strongly interacting bosonic atoms in optical lattices, a problem

which has attracted a lot of interest in the atomic physics community in the last few years due to the recent experimental achievements [8–10]. In this system, 20–100 atoms are trapped by the combination of a periodic and a harmonic (i.e., inhomogeneous) potential created by lasers in 1D and at a finite temperature. In the so-called Tonks-Girardeau limit [11], the problem can be exactly solved via fermionization [9], and thus this provides us with a reliable benchmark for our method. Outside this limit, we are able to reproduce certain features experimentally observed [8].

Our method relies in reexpressing the partition and correlation functions as a contraction of a collection of 4-index tensors, which are disposed according to a 2D configuration. We will perform this task for both 2D classical and 1D quantum systems. We will then show how the methods introduced in [12] can be used to approximate these contractions in a controlled way, and thus lead to a scalable algorithm for the evaluation of the quantities of interest.

(1) *2D classical systems.*—Let us consider first the partition function of an inhomogeneous classical 2D  $n$ -level spin system on a  $L_1 \times L_2$  lattice. For simplicity we will concentrate on a square and nearest-neighbor interactions, although our method can be easily extended to other short-range situations. We have  $Z = \sum_{\{x^{kl}\}} \exp[-\beta H(x^{11}, \dots, x^{L_1 L_2})]$ , where  $H(\{x^{kl}\}) = \sum_{ij} [H_1^{ij}(x^{ij}, x^{i+1,j}) + H_2^{ij}(x^{ij}, x^{i,j+1})]$  is the Hamiltonian,  $x^{kl} = 1, \dots, n$  and  $\beta$  is the inverse temperature. The singular value decomposition allows us to write

$$\exp[-\beta H_q^{ij}(x, y)] = \sum_{\alpha=1}^n f_{q\alpha}^{ij}(x) g_{q\alpha}^{ij}(y),$$

with  $q \in \{\downarrow, \rightarrow\}$ . Defining the tensors

$$X_{lrud}^{ij} = \sum_{x=1}^n f_{\downarrow d}^{ij}(x) g_{\downarrow u}^{i-1,j}(x) f_{\rightarrow r}^{ij}(x) g_{\rightarrow l}^{i,j-1}(x),$$

the partition function can now be calculated by contracting all 4-index tensors  $X^{ij}$  arranged on a square lattice in such a way that, e.g., the indices  $l, r, u, d$  of  $X^{ij}$  are contracted

with the indices  $r, l, d, u$  of the respective tensors  $X^{i,j-1}$ ,  $X^{i,j+1}$ ,  $X^{i-1,j}$ ,  $X^{i+1,j}$ . In order to determine the expectation value of a general operator of the form  $O(\{x^{kl}\}) = Z \prod_{ij} O^{ij}(x^{ij})$ , one just has to replace each tensor  $X^{ij}$  by

$$X_{lrud}^{ij}(O^{ij}) = \sum_{x=1}^n O^{ij}(x) f_{ld}^{ij}(x) g_{lu}^{i-1,j}(x) f_{lr}^{ij}(x) g_{li}^{i,j-1}.$$

(2) *1D quantum systems.*—We consider the partition function of an inhomogeneous 1D quantum system composed of  $L$   $n$ -level systems,  $Z = \text{Tr} \exp(-\beta H)$ . It is always possible to write the Hamiltonian  $H$  as a sum  $H = \sum_k H_k$  with each part consisting of a sum of commuting terms. Let us, for simplicity, assume that  $H = H_1 + H_2$  and that only local and 2-body nearest-neighbor interactions occur, i.e.,  $H_k = \sum_i O_k^{i,i+1}$  and  $[O_k^{i,i+1}, O_k^{j,j+1}] = 0$ , with  $i, j = 1, \dots, L$ . The more general case can be treated in a similar way. Let us now consider a decomposition

$$\exp\left(-\frac{\beta}{M} O_k^{i,i+1}\right) = \sum_{\alpha=1}^{\kappa} \hat{S}_{k\alpha}^i \otimes \hat{T}_{k\alpha}^{i+1}. \quad (1)$$

The singular value decomposition guarantees the existence of such an expression with  $\kappa \leq n^2$ . As we will see later, a smart choice of  $H = \sum_k H_k$  can typically decrease  $\kappa$  drastically. Making use of the Suzuki-Trotter formula [13],  $Z = \text{Tr}[\prod_k \exp(-\frac{\beta}{M} H_k)]^M + O[\frac{1}{M}]$ , it can be readily seen that the partition function can again be calculated by contracting a collection of 4-index tensors  $X^{ij}$  defined as

$$X_{(l'l')(rr')ud}^{ij} \equiv [\hat{T}_{l'l'}^i \hat{S}_{1r}^j \hat{T}_{2r'}^j \hat{S}_{2r'}^j]_{[ud]},$$

where the indices  $(l, l')$  and  $(r, r')$  are combined to yield a single index that may assume values ranging from 1 to  $\kappa^2$ . Note that now the tensors  $X^{ij}$  and  $X^{i'j}$  coincide, and that the indices  $u$  of the first and  $d$  of the last row have to be contracted with each other as well, which corresponds to a classical spin system with periodic boundary conditions in the vertical direction. A general expectation value of an operator of the form  $O = ZO^1 \otimes \dots \otimes O^N$  can also be reexpressed as a contraction of tensors with the same structure: it is merely required to replace each tensor  $X^{ij}$  in the first row by

$$X_{(l'l')(rr')ud}^{1j}(O^j) = [O^j \hat{T}_{l'l'}^j \hat{S}_{1r}^j \hat{T}_{2r'}^j \hat{S}_{2r'}^j]_{[ud]}.$$

(3) *Tensor contraction.*—In the following, we adapt the algorithm introduced in [14] in order to contract the tensors  $X^{ij}$  introduced above in a controlled way. The main idea is to express the objects resulting from the contraction of tensors along the first and last column in the 2D configuration as matrix product states (MPS) and those obtained along the columns  $2, 3, \dots, L-1$  as matrix product operators (MPO) [5]. More precisely, we define

$$\begin{aligned} \langle \mathbb{X}^1 | &:= \sum_{r_1 \dots r_M=1}^m \text{Tr}(X_{r_1}^{11} \dots X_{r_M}^{M1}) \langle r_1 \dots r_M |, \\ | \mathbb{X}^L \rangle &:= \sum_{l_1 \dots l_M=1}^m \text{Tr}(X_{l_1}^{1L} \dots X_{l_M}^{ML}) | l_1 \dots l_M \rangle, \\ \mathbb{X}^j &:= \sum_{l_1, r_1, \dots=1}^m \text{Tr}(X_{l_1 r_1}^{1j} \dots X_{l_M r_M}^{Mj}) | l_1 \dots \rangle \langle r_1 \dots |, \end{aligned}$$

where  $m = n$  for 2D classical systems and  $m = \kappa^2$  for 1D quantum systems. These MPS and MPO are associated to a chain of  $M$   $m$ -dimensional systems and their virtual dimension amounts to  $D = n$ . Note that for 2D classical systems the first and last matrices under the trace in the MPS and MPO reduce to vectors. The partition function (and similarly other correlation functions) reads  $Z = \langle \mathbb{X}^1 | \mathbb{X}^2 \dots \mathbb{X}^{L-1} | \mathbb{X}^L \rangle$ . Evaluating this expression iteratively by calculating step by step  $\langle \mathbb{X}^j | := \langle \mathbb{X}^{j-1} | \mathbb{X}^j$  for  $j = 2, \dots, L-1$  fails because the virtual dimension of the MPS  $\langle \mathbb{X}^j |$  increases exponentially with  $j$ . A way to circumvent this problem is to replace in each iterative step the MPS  $\langle \mathbb{X}^j |$  by a MPS  $\langle \tilde{\mathbb{X}}^j |$  with a reduced virtual dimension  $\tilde{D}$  that approximates the state  $\langle \mathbb{X}^j |$  best in the sense that the norm  $\delta K := \| \langle \mathbb{X}^j | - \langle \tilde{\mathbb{X}}^j | \|$  is minimized. Because of the fact that this cost function is multiquadratic in the variables of the MPS, this minimization can be carried out very efficiently [5,12,14]; the exponential increase of the virtual dimension can hence be prevented and the iterative evaluation of  $Z$  becomes tractable, such that an approximation to the partition function can be obtained from  $Z \approx \langle \tilde{\mathbb{X}}^{L-1} | \mathbb{X}^L \rangle$ . The accuracy of this approximation

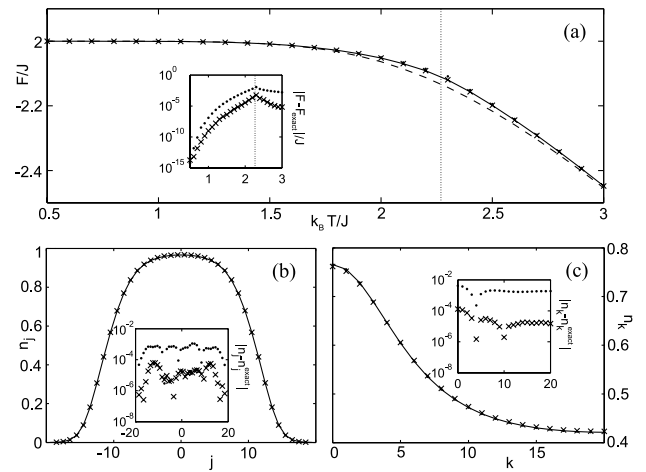


FIG. 1. (a) Free energy of the 2D Ising model ( $J = 1$ ) on a  $50 \times 50$  lattice. (b) and (c) Density and (quasi)-momentum distribution in the Tonks-Girardeau gas limit, plotted for  $\beta J = 1$ ,  $L = 40$ ,  $N = 21$ , and  $V_0/J = 0.034$ . In all parts, the numerical results for  $\tilde{D} = 2$  ( $\tilde{D} = 8$ ) are represented by dots (crosses) and the exact solution is illustrated by the solid line. From the insets, the error of the numerical results can be gathered. For comparison, in (a) the exact solution for the infinite-lattice case is also plotted (dashed line).

depends only on the choice of the reduced dimension  $\tilde{D}$  and the approximation becomes exact for  $\tilde{D} \geq D^L$ . As the norm  $\delta K$  can be calculated at each step,  $\tilde{D}$  can be increased dynamically if the obtained accuracy is not large enough. In the worst case scenario, such as in the NP-complete Ising spin glasses [15],  $\tilde{D}$  will probably have to grow exponentially in  $L$  for a fixed precision of the partition function. But in less pathological cases it seems that  $\tilde{D}$  only has to grow polynomially in  $L$ ; indeed, the success of the methods developed by Nishino [2] in the translational invariant case indicate that even a constant  $\tilde{D}$  will produce very reliable results.

(4.a) *Illustration: 2D Ising model.*—The 2D Ising model on a  $L \times L$  lattice is one of very few nontrivial classical problems that is exactly solvable and shows a phase transition [16]. It is described by the Hamiltonian  $H = J \sum_{\langle i,j \rangle} s_i s_j$ , where  $s_i = \pm 1$ . We have used this model as a first benchmark for our algorithm by comparing the exact solution for the free energy to our numerical results. The outcomes for the special case of a  $50 \times 50$  lattice, antiferromagnetic coupling ( $J = 1$ ) and periodic boundary conditions can be gathered from Fig. 1. In this figure, numerical results for  $\tilde{D} = 2$  and  $\tilde{D} = 8$  are shown. From the inset, it can be gathered that the error of these results is maximal at the critical temperature  $k_B T_c / J \sim 2.2692$  at which the phase transition takes place. At this temperature, the error is of order  $10^{-2}$  for  $\tilde{D} = 2$  and decreases significantly for  $\tilde{D} = 8$ .

(4.b) *Illustration: Bosons in optical lattices.*—A system of trapped bosonic particles in a 1D optical lattice of  $L$  sites is described by the Bose-Hubbard Hamiltonian [17]

$$H = -J \sum_{i=1}^{L-1} (a_i^\dagger a_{i+1} + \text{H.c.}) + \frac{U}{2} \sum_{i=1}^L \hat{n}_i (\hat{n}_i - 1) + \sum_{i=1}^L V_i \hat{n}_i,$$

where  $a_i^\dagger$  and  $a_i$  are the creation and annihilation operators on site  $i$  and  $\hat{n}_i = a_i^\dagger a_i$  is the number operator. This Hamiltonian describes the interplay between the kinetic energy due to the next-neighbor hopping with amplitude  $J$  and the repulsive on-site interaction  $U$  of the particles. The last term in the Hamiltonian models the harmonic confinement of magnitude  $V_i = V_0(i - i_0)^2$ . The variation of the ratio  $U/J$  drives a phase-transition between the Mott-insulating and the superfluid phase, characterized by localized and delocalized particles, respectively [18]. Experimentally, the variation of  $U/J$  can be realized by tuning the depth of the optical lattice [17,19]. On the other hand, one typically measures directly the momentum distribution by letting the atomic gas expand and then measuring the density distribution. Thus, we will be mainly interested here in the (quasi)-momentum distribution  $n_k = \frac{1}{L} \sum_{r,s=1}^L \langle a_r^\dagger a_s \rangle e^{i2\pi k(r-s)/L}$ .

Our goal is now to study with our numerical method the finite-temperature properties of this system for different ratios  $U/J$ . We thereby assume that the system is in a thermal state corresponding to a grand canonical ensemble

with chemical potential  $\mu$ , such that the partition function is obtained as  $Z = \text{Tre}^{-\beta(H-\mu\hat{N})}$ . Here,  $\hat{N} = \sum_{i=1}^L \hat{n}_i$  represents the total number of particles. For the numerical study, we assume a maximal particle number  $q$  per lattice site, such that we can project the Hamiltonian  $H$  on the subspace spanned by Fock states with particle numbers per site ranging from 0 to  $q$ . The projected Hamiltonian  $\tilde{H}$  then describes a chain of  $L$  spins, with each spin acting on a Hilbert space of dimension  $n = q + 1$ . A Trotter decomposition that turns out to be advantageous for this case is  $e^{-\beta(\tilde{H}-\mu\hat{N})} = (\hat{V}^\dagger \hat{V})^M + \mathcal{O}[\frac{1}{M^2}]$ , with  $\tilde{H} = H_R + H_S + H_T$ ,  $H_R = -\frac{J}{2} \sum_{i=1}^{L-1} R^{(i)} R^{(i+1)}$ ,  $H_S = -\frac{J}{2} \sum_{i=1}^{L-1} S^{(i)} S^{(i+1)}$ ,  $H_T = \sum_{i=1}^L T^{(i)}$ ,  $R^{(i)} = \tilde{a}_i^\dagger + \tilde{a}_i$ ,  $S^{(i)} = -i(\tilde{a}_i^\dagger - \tilde{a}_i)$ ,  $T^{(i)} = \frac{1}{2} \tilde{n}_i (\tilde{n}_i - 1) + V_i \tilde{n}_i$ , and  $\hat{V} = e^{-\frac{\beta}{2M} H_R} e^{-\frac{\beta}{2M} H_S} e^{-\frac{\beta}{2M} (H_T - \mu \hat{N})}$ .  $\tilde{a}_i^\dagger$ ,  $\tilde{a}_i$ , and  $\tilde{n}_i$  thereby denote the projections of the creation, the annihilation, and the number operators  $a_i^\dagger$ ,  $a_i$ , and  $n_i$  on the  $q$ -particle subspace. The decomposition (1) of all two-particle operators then straightforwardly leads to a set of 4-index tensors  $X_{lrud}^{ij}$ , with indices  $l$  and  $r$  ranging from 1 to  $(q+1)^3$  and indices  $u$  and  $d$  ranging from 1 to  $q+1$ . Note that the typical second order Trotter decomposition with  $H = H_{\text{even}} + H_{\text{odd}}$  would make the indices  $l$  and  $r$  range from 1 to  $(q+1)^6$ .

Let us start out by considering the limit  $U/J \rightarrow \infty$  in which double occupation of single lattice sites is prevented and the particles in the lattice form a Tonks-Girardeau gas [9]. In this limit, the Bose-Hubbard Hamiltonian maps to the Hamiltonian of the exactly solvable (inhomogeneous) XX model, which allows to benchmark our algorithm. The comparison of our numerical results to the exact results can be gathered from Fig. 1. Here, the density and the (quasi)-momentum distribution are considered for the special case  $\beta J = 1$ ,  $L = 40$ ,  $N = 21$ , and  $V_0/J = 0.034$ . The numerical results shown have been obtained for Trotter-number  $M = 10$  and two different reduced virtual

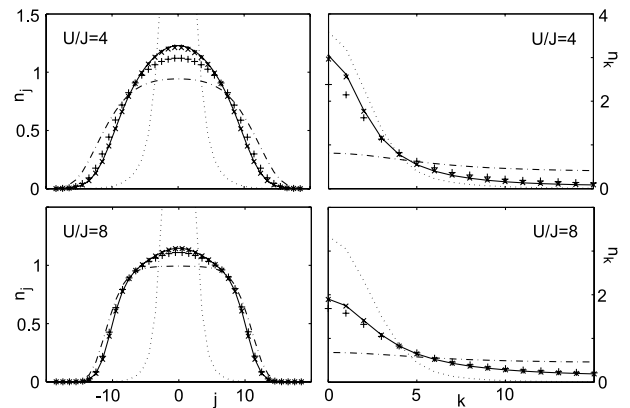


FIG. 2. Density and (quasi)-momentum distributions for interaction strengths  $U/J = 4$  and  $8$ . Here,  $\beta J = 1$ ,  $L = 40$ ,  $N = 21$ , and  $M = 10$ . Numerical results were obtained for  $q = 2$  (pluses),  $q = 3$  (crosses), and  $q = 4$  (solid line). For comparison, the distributions for  $U/J = 0$  (dotted lines) and  $U/J \rightarrow \infty$  (dash-dotted lines) are also included.

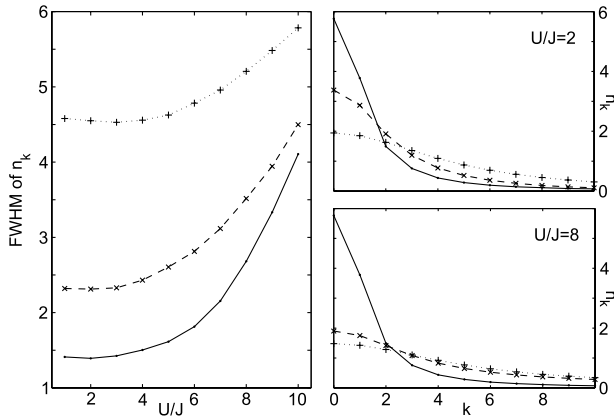


FIG. 3. FWHM of the (quasi)-momentum distribution as a function of  $U/J$ , calculated for temperatures  $\beta J = 0.5$  (plus-sign),  $\beta J = 1$  (crosses), and  $\beta J = 2$  (dots). The corresponding (quasi)-momentum distributions for  $U/J = 2$  and  $U/J = 8$  are illustrated in the plots at the right-hand side.

dimensions  $\tilde{D} = 2$  and  $\tilde{D} = 8$ . From the insets, it can be gathered that the error of the numerical calculations is already very small for  $\tilde{D} = 2$  (of order  $10^{-3}$ ) and decreases significantly for  $\tilde{D} = 8$ .

As the ratio  $U/J$  becomes finite, the system becomes physically more interesting, but lacks an exact mathematical solution. In order to judge the reliability of our numerical solutions in this case, we check the convergence with respect to the free parameters of our algorithm ( $q$ ,  $\tilde{D}$ , and  $M$ ). As an illustration, the convergence with respect to the parameter  $q$  is shown in Fig. 2. In this figure, the density and the (quasi)-momentum distribution are plotted for  $q = 2, 3$ , and  $4$ . We thereby assume that  $\beta J = 1$ ,  $L = 40$ , and  $N = 21$  and consider interaction strengths  $U/J = 4$  and  $8$ . The harmonic potential  $V_0$  is chosen in a way to describe Rb atoms in a harmonic trap of frequency 120 Hz (along the lines of [9]). We note that we have taken into account that changes of the ratio  $U/J$  are obtained from changes in both the on-site interaction  $U$  and the hopping amplitude  $J$  due to variations of the depth of the optical lattice. The numerical calculations have been performed with  $M = 10$  and  $\tilde{D} = q + 1$ . From the figure it can be gathered that convergence with respect to  $q$  is achieved for  $q \geq 3$ .

We now use our numerical algorithm to study a physical property of interacting bosons in an optical lattice, namely, the full width at half maximum (FWHM) of the (quasi)-momentum distribution. It has been predicted that the FWHM shows a kink at zero temperature [20]. This kink is an indication for a Mott-superfluid transition, since the FWHM is directly related to the inverse correlation length. Experiments have also revealed this kink [8,10]; they are, however, performed at finite temperature, something we can study with our algorithm. In Fig. 3, we plot the numerical results for the FWHM as a function of  $U/J$  for three different (inverse) temperatures  $\beta J = 0.5, 1$  and  $2$ . The physical parameters  $L$ ,  $N$ , and  $V_0$  are thereby chosen

as in the previous case. The numerical results have been obtained for  $M = 10$ ,  $q = 4$ , and  $\tilde{D} = q + 1$ . For each temperature, three different regions can be distinguished: the superfluid region with constant FWHM, the Mott-region with linearly increasing FWHM, and an intermediate region in which both phases coexist. The value  $U/J$  at which the Mott region starts increases with increasing temperature, which is consistent with the criteria  $U \gg k_B T, J$  for the appearance of the Mott phase. This behavior could be easily observed in present experiments.

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