Quantum spin chains in a magnetic field

V. A. Kashurnikov1, N. V. Prokof’ev2,3, B. V. Svistunov2, and M. Troyer4

1 Moscow State Engineering Physics Institute, 115409, Moscow, Russia
2 Russian Research Center “Kurchatov Institute”, 123182 Moscow, Russia
3 Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-01, Japan
4 Institute for Solid State Physics, University of Tokyo, Roppongi 7-22-1, Minatoku, Tokyo 106, Japan

We demonstrate that the “worm” algorithm allows very effective and precise quantum Monte Carlo (QMC) simulations of spin systems in a magnetic field, and its autocorrelation time is rather insensitive to the value of H at low temperature. Magnetization curves for the s = 1/2 and s = 1 chains are presented and compared with existing Bethe ansatz and exact diagonalization results. From the Green function analysis we deduce the magnon spectra in the s = 1 system, and directly establish the “relativistic” form \( E(p) = (\Delta^2 + v^2 p^2)^{1/2} \) of the dispersion law.

I. INTRODUCTION

Quantum spin chains have recently been the subject of intensive theoretical, experimental and numerical studies. Many methods were developed and applied first to these systems. In this paper we present precise calculations of the magnetization curves, \( m_z(H) \equiv S_z/L \) (where \( S_z = \sum_{i=1}^{L} s_z(i) \) is the projection of the total spin on the direction of magnetic field, and \( L \) is the number of spins in the system), and excitation spectra in isotropic antiferromagnetic Heisenberg chains.

The magnetization is probably the easiest quantity to measure experimentally, and, on the contrary, the most difficult to calculate numerically, as far as quantum Monte Carlo (QMC) methods are concerned. In canonical ensemble (or \( S_z \)-conserving) schemes, \( m_z \) can be obtained only from the spin and field dependence of the ground state energies \( E(S_z, H) \) with subsequent extrapolation to the thermodynamic limit. Precise QMC calculations of that kind require enormous numerical effort. Also, most of the schemes rely on the Suzuki-Trotter discretization of imaginary time which introduces systematic errors. On the other hand, the loop cluster update (LCU) algorithm is suffering from exponential slowing down in the most interesting cases (see Sec. I). Due to small acceptance rates in a finite magnetic field we are not aware of any large system simulations done using LCU in strong magnetic field. Usually precise calculations of the \( m_z \) curves were done by exact diagonalization (ED) and density matrix renormalization group (DMRG) methods.

With the development of the continuous-time “worm” algorithm (it is called “worm” algorithm because the configuration space of the system is sampled through the worm-like motion of world line discontinuities, or, more generally, source operators) which works with the grand canonical ensemble (i.e., samples all \( S_z \)), the magnetization is calculated as easily as any other “standard” thermodynamic quantity like the energy. Furthermore, in the same calculation one collects statistics for the Green function, \( G(r, \tau) = -T < s^{-0}(0, 0) s^+(r, \tau) > \), where \( T \) stands for the time ordering, and \( s^\pm = s_x \pm is_y \). Thus in a single QMC simulation done at low temperature one can directly measure not just \( E(T, H) \), but also \( m_z(H) \), the single-particle excitation spectrum, critical indices of \( G(i, \tau) \), the susceptibility \( \chi(H) = dm_z(H)/dH \), the spin stiffness \( \Lambda_\chi(H) \), and more. This information may be used for precise calculations of spin gaps and magnon dispersion curves.

In what follows we first verify, in Sec. II, by performing an autocorrelation times analysis that the “worm” algorithm does not suffer strongly from slowing down in finite magnetic field and compare its performance with the continuous-time LCU method for \( s = 1/2 \) chains. In Sec. III we present our data for the magnetization curves in \( s = 1/2 \) and \( s = 1 \) chains and compare them with the results of ED and DMRG studies. In Sec. IV we calculate Haldane gaps and magnon dispersion curves for the \( s = 1 \) system. From our data we confirm the existence of a shallow minimum in \( \chi(H) \) around \( H = 3.2 \) (we use units such that magnetic field, temperature, magnon velocity, and spin gaps are measured in terms of the Heisenberg exchange coupling constant \( J \)), found previously in the ED studies on small systems. We exclude the possibility that this minimum is a finite-size effect, or an artifact of extrapolation procedure used in Ref. I. Our result for the spin gap

\[
\Delta(s = 1) = 0.4105(1) \tag{1}
\]

shows the accuracy to which this quantity may be measured in a single QMC simulation using the “worm” algorithm, and agrees with the ED result \( \Delta(s = 1) = 0.41049(2) \) and the DMRG results \( \Delta(s = 1) = 0.41050(2) \), in Ref. I and \( \Delta(s = 1) = 0.4104892(2) \) in Ref. II. The magnon dispersion curve fits perfectly to the relativistic form \( E^2(p) = \Delta^2 + v^2 p^2 \), where \( v \) is the magnon velocity, and \( p \) is the magnon momentum. We deduced

\[
v(s = 1) = 2.48(1) \tag{2}
\]

from the fit; this result is as accurate as the best known DMRG values deduced from the correlation length \( v(s =
1) $= 2.475(5)$ and magnetization studies $\nu(s = 1) = 2.49(1)$ We also found that for the $s = 1$ chain with $L = 100$ lattice sites even two-magnon states have visible corrections to the hard-core boson picture which is sometimes used in fitting the data.

II. CRITICAL SLOWING DOWN OF THE “WORM” AND LCU ALGORITHMS

The LCU algorithm has been applied successfully to quantum spin systems near phase transitions, without any sign of critical slowing down. As soon as a magnetic field is turned on, however, the LCU updates show a severe, exponential slowing down. The reason is that in the standard LCU method the field cannot be taken into account when building the loop cluster, but is treated as a global weight, modifying the flipping probabilities of the loop clusters.

We illustrate this problem in the simplest case, two spins in a magnetic field

$$H_{\text{dimer}} = JS_1S_2 - H(S_1^z + S_2^z). \quad (3)$$

At $H = J$ the ground state of this dimer system is degenerate, with the $S^z = 1$ triplet and the spin singlet both having energy $-3/4J$. In the world line picture the $S^z = 1$ triplet is represented by two straight world lines with $S_i^z = +1/2$ (Figs. 1a and 2a). Starting from this configuration the LCU method proposes to flip one of the world lines (Fig. 1b). The new configuration however is energetically unfavorable as its energy is $-1/4J$. It will be accepted only with a probability $p = \exp(-\beta J/2)$, which takes an exponential amount of time. Once this configuration has been accepted however it can quickly relax to the energetically favorable singlet state, in which a world line gains exchange energy by jumping between the two sites, as shown in Fig. 1c. Returning from the singlet to the triplet state is again very unlikely, since the LCU first has to create a world line configurations with two straight world lines. Since there is a finite probability density $(2/J)d\tau$ for having the world line jump to the neighboring site if the two spins are antiparallel, removing all the jumps is again exponentially rare. Thus in the LCU for a spin-1/2 dimer at the critical point $J = H$ in a magnetic field the autocorrelation time for the magnetization is exponentially large

$$\tau_{\text{LCU}} \propto \exp(\beta H/2). \quad (4)$$

The dynamic exponent, defined as $\tau \propto \beta^z$ is $z_{\text{LCU}} = \infty$.

We measured the integrated autocorrelation time using a multi cluster loop algorithm and confirmed the exponential slowing down, as shown in Fig. 3. In higher dimensional systems the scaling remains exponential.

The above discussion has pointed out that in going from the triplet to the singlet state we trade potential energy for exchange energy. The LCU method does this in two steps, first paying a huge loss in one, before gaining the other. The worm algorithm on the other hand can make these trades on a local basis, as it allows configurations with broken world lines, as is illustrated in Fig. 2. Starting from the triplet state the worm algorithm...
flips only a short segment of the world line, with a high acceptance rate (Fig. 2b). Once this short segment has been created the world lines can gain exchange energy by jumping between the sites, as shown in Fig. 2c. The worm ends make a random walk along the time direction and need a time proportional to $\beta^2$ to wind once around the time direction and thus change the magnetization. The autocorrelation time is

$$\tau_{\text{worm}}^{\text{dimer}} \propto \frac{\beta^2}{2\beta} \propto \beta,$$  \hspace{1cm} (5)

and the dynamical exponent $z_{\text{worm}}^{\text{dimer}} = 1$. The factor $2\beta$ in the denominator normalizes the time by the minimum time needed in any algorithm, which is proportional to the space-time volume.

We measured $\tau$ in the worm algorithm and confirmed this linear scaling for the dimer. In the worm algorithm we measure the times in units of $N\beta$ proposed local updates of the worm configuration, where $N$ is the number of spins. As shown in Fig. 3 when $\beta H > 5$ the worm algorithm is much faster than the LCU algorithm.

In higher dimensions in an $N$-spin system, the magnetization fluctuates in general by $\sqrt{N/\beta}$. To achieve an independent configuration one has to again spend time

$$\tau_{\text{worm}} \propto \left(\frac{\sqrt{N/\beta}}{\beta}\right)^2 \sim \text{const.}$$  \hspace{1cm} (6)

and thus $z \approx 0$. Close to a critical point the scaling is only slightly worse in one dimension. Modeling the magnons as hard-core bosons and assuming a dispersion $\epsilon(k) \propto k^n$ the number of magnons at low temperatures is $M \propto N \beta^{d/n}$, and the autocorrelation time

$$\tau_{\text{worm}}^{\text{critical}} \propto \max\left(\frac{\sqrt{M/\beta}}{\beta}, 1\right) \propto \max(\beta^{1-d/n}, \text{const})$$  \hspace{1cm} (7)

where $d$ is the dimension. For a one-dimensional spin chain at either critical point, close to the spin gap $H = \Delta$ or close to the fully polarized state $H = 2zJS$ the dispersion is quadratic ($n = 2$) and thus $z = 1/2$. In higher dimensions $z \approx 0$ is predicted from this argument. Measurements of $\tau$ on a chain, also shown in Fig. 3, confirm that $\tau$ indeed increases only very slowly with $\beta h$.

The above discussion assumed that the source operators in the worm algorithm perform a random walk on the lattice. In the simple worm algorithm however they do not perform a pure random walk, but are guided by the Green function. The worm movements can be biased by the inverse of the Green function (or an estimate thereof) though, which makes them a random walk.

Finally we wish to note that work is in progress on improving the scaling of the loop algorithm in a magnetic field. For general couplings in the dimer case and for ferromagnetic couplings on any lattice the exponential slowing down can be removed. However in the most interesting case, discussed here, an antiferromagnet on a chain or higher dimensional lattice, the slowing down remains exponential, although the prefactor can be reduced.

### III. Magnetization Curves

We have seen in the previous Sec. II that the “worm” algorithm is essentially insensitive to the value of $H$. As a testing case we computed the magnetization curve $m_z(H)$ for the $s = 1/2$ chain with $L = 100$ spins and verified that it agrees with the available Bethe ansatz solution.\[3\] Within our error bars the QMC and Bethe ansatz data are in general indistinguishable when calculated at the same value of magnetic field. At $\beta = 80$ and very small fields $H$ one can however see in Fig. 4 the typical finite-size oscillations, which appear when $\beta \sim 2\pi v/L$ and only few magnons are present in the system; at $T = 0$ these oscillations convert into a stair-case curve. These effects can be reduced by going to larger $L$. The whole curve takes about 40 hours of CPU time on an HP-UX 9000/735.

The case of $s = 1$ is more intriguing. A Bethe ansatz solution is not available in this case, and, as mentioned above, one has to rely on ED or DMRG. The magnetization curve for the $s = 1$ chain was calculated in Ref. \[4\]. Some aspects of this study may rise questions. Since the largest system size was only $L = 16$, the expected square-root singularity near $H_{c1} = \Delta(s = 1)$ was hardly seen, although it is possible do recover this singularity using an appropriate finite-size analysis.\[5\]

Also, after extrapolating results for $E(S_z, H)$ to the thermodynamic limit to deduce $m_z(H)$ and subsequent...
FIG. 5. Magnetization curve of the $s = 1$ antiferromagnetic Heisenberg chain.

Differentiation of $m_z(H)$, a very shallow minimum in $\chi(H)$ around $H \approx 3.2$ was predicted. The amplitude of the $\chi(H)$ variation around the minimum was only a few percent, and one might suspect that the procedure of eliminating finite-size effects was simply not accurate enough.

In Fig. 5 we show our data for $m_z(H)$ calculated with high accuracy to ensure reliable values for the field derivative $\chi(H)$. Obviously, there is a wide region in $H$ where $m_z(H)$ is almost perfectly linear. In Fig. 6 we demonstrate that, beyond any doubts, there is a minimum in $\chi(H)$ around $H \approx 3.2$, and that the technique developed in Ref. 1 for eliminating finite-size effects in small clusters is remarkably accurate once the system size is larger than the correlation length ($\xi = 6.03(1)$ for the $s = 1$ chain). The origin of this minimum is not understood theoretically yet. Furthermore, we calculated $\chi(H)$ in the region between $H = 2.8$ and $H = 3.2$, where $d\chi/dH$ is negative, at higher temperature. If the minimum was any kind of finite-size effect due to level quantization, it would have been strongly affected by temperature variation. We see, that higher-temperature points, marked by crosses in Fig. 6, are not affected within error bars, and also give a negative $d\chi/dH$ in this region.

Clearly, for the system with $L = 100$, we already see the square-root singularity $m_z \sim \sqrt{H - \Delta}$ near the spin gap values. It is smeared out very close to the gap due to finite temperature. The physics of $m_z(H)$ behavior near the gap is usually described by a free-fermion model with periodic/antiperiodic boundary conditions depending on the odd/even value of $S_z$. Or a hard-core boson model.

FIG. 6. Derivative of the magnetization with respect to the field $\chi(H)$, for the $s = 1$ antiferromagnetic Heisenberg chain at $\beta = 100/J$. The region around the minimum is shown enlarged in the inset. Higher temperature data (at $\beta = 50/J$) are marked by crosses.

FIG. 7. Magnetization curve of the $s = 1$ antiferromagnetic Heisenberg chain close to the gap $\Delta$ on an $L = 100$ site chain at $\beta = 100$. The solid curve shows the prediction of the hard-core boson theory assuming $\Delta = 0.4105$ and $v = 2.48$. 

which is exact in the dilute limit $m_z \to 0$. It is tempting then to fit the QMC data near $H_{c1}$ to the prediction of the hard-core boson theory at finite, but very low temperature. In Fig. 6 we show the result of such a fit, done using the following ansatz for the magnon spectrum

$$E(p) = \sqrt{\Delta^2 + v^2 p^2},$$

with $\Delta(s = 1) = 0.4105$ and $v(s = 1) = 2.48$. Since finite size corrections in a chain with periodic boundary conditions are exponentially small, we used the known values of $\Delta(s = 1)$ and $v(s = 1)$. Surprisingly, the fit is not good already for $m_z > 0.02$, i.e., when only two magnons are inserted into the system. Also, the theory predicts visible finite-size oscillations in $\chi(H)$ at $\beta = 100$, which are not present in the calculated $m_z(H)$. Although it is possible to get an almost perfect fit of the QMC data to the hard-core boson theory up to $m \sim 0.06$ using $v(s = 1) = 2.25$, we rather suggest that the difference between the theoretical and calculated $m_z$ is due to magnon-magnon interactions other than on-site repulsion. The gap and the magnon velocity were deduced independently with high accuracy from the Green function (see next Section) and exclude the possibility that $v = 2.25$. It means that one must be extremely cautious in extracting spin velocity from multi-magnon states, i.e., states with $S_z \geq 3$, since longer range interactions between the magnons are usually ignored in such studies.[12]

We note, that the magnetization curve itself in Fig. 7 is sufficient to deduce the gap value rather accurately $\Delta(s = 1) = 0.410(2)$ even without the Green function analysis to which we proceed now.

IV. MAGNON SPECTRA

Since the “worm” algorithm collects “by passing” the complete histogram for the system’s Green function, one may use it in a very efficient way to deduce the single-particle (magnon) spectrum. In the present study we demonstrate how well the method works for the case when an analytic continuation of $G(i, \tau)$ to real frequencies is not necessary.

At very low temperature and $|H| < H_{c1}$, the statistics is dominated by the ground-state configurations, and a piece of an extra world line, corresponding to the $S_z = \pm 1$ states. If $H_{c1} - H < H_{c3}$ and $T < H_{c1} - H$, then most of the $G(p, \tau)$ histogram (in momentum representation) is determined by the $S_z = +1$ configurations except for very short $\sim 1$ negative times. (since the typical length in time of an extra worldline is of order $1/(H_{c1} - H)$, we keep $H$ rather close to the critical field in order to make the worldline longer; this allows one more precise determination of the Green function decay in time). In our simulations we used $\beta = 200$ and $H_{c1} - H \sim 10/\beta$.

One then expects that (counting $E(p)$ from $H$)

$$G(p, \tau) \sim e^{-E(p)\tau},$$

i.e., a simple exponential decay from which the magnon spectrum is readily obtained as

$$E(p) = -\frac{\ln[G(p, \tau)/G(p, \tau_0)]}{\tau - \tau_0}.$$ (10)

This definition is normalization free, although normalization is not a problem and is fixed by the condition $-G(i = 0, \tau = 0) = s + 1$.

First of all, we verify that the decay of $G(p, \tau)$ in time is purely exponential for $\tau \gg 1$ until the value of $G$ becomes too small and statistical fluctuations start dominating. We then use Eq. (10) to determine the spectrum. For each momentum state the reference point was set to $\tau_0 = 1/E(p)$, and then the value of $E(p)$ was obtained from the best exponential fit to the data between $\tau_0$ and $\tau_{max}$, where $\tau_{max}(p)$ was close to the onset of statistical fluctuations in $G(p, \tau)$ (typically $E(p)\tau_{max} \sim 4 - 5$). The error bars are estimated from the fluctuations of results of up to twelve independent simulations. Our results for the chain $s = 1$ are shown in Fig. 8. For the $s = 1$ chain we studied a system with $L = 100$ spins. The precision of the data, obtained in only 50 hours of CPU time on an HP-UX 9000/735, is sufficient to determine $\Delta(s = 1) = 0.4105(1)$ — the most accurate QMC result so far. No finite size corrections are necessary since these are exponentially small, given the rather short correlation length for $s = 1$. This value agrees with the ED and DMRG data. The magnon velocity was found to equal $v(s = 1) = 2.48(1)$. This is also the most ac-
curate QMC result and agrees with the DMRG values $v(s = 1) = 2.475(5)$ in Ref. [10] and $v(s = 1) = 2.49(1)$ in Ref. [11].

One note is in order here. From Fig. 3 we see, that the parabolic expansion $E(p) = \Delta + v^2 p^2/2\Delta$ is not accurate for the chain $L = 100$, except maybe for the first nonzero-momentum state, but the data are consistent with the form [6] for all the reliably determined states. This unambiguously confirms the "relativistic" ansatz for the dispersion law. The spin velocity is sometimes determined from the ground-state energies $E(S_z, L)$ for chains of comparable sizes assuming parabolic expansion and ignoring magnon-magnon interactions (other than on-site repulsion) [6]. Since we found that both aspects have noticeable corrections to the data in chains with $L \sim 100$, we suspect that these corrections somehow compensate each other and the net result turns out to come right, e.g., the DMRG result obtained in Ref. [11] is $v = 2.49(1)$.

Our data give the dispersion law directly and do not rely on any assumptions about its form. Also, they are not affected by the magnon-magnon interactions since the parameters $H$ and $T$ are chosen in such a way that only single-magnon virtual states are contributing to the statistics.

V. CONCLUDING REMARKS

In the present study we have shown that "worm" algorithm is very efficient for simulations of spin systems in finite magnetic field. Its autocorrelation time is almost independent of $\beta$ and $H$. For the isotropic antiferromagnetic Heisenberg chains $s = 1/2$ and $s = 1$ the accuracy of our data for the magnetization curves, spin gaps and magnon velocities is comparable with the Bethe ansatz, exact diagonalization and DMRG results. Moreover, from these data we found visible range-longe (apart from onsite hard-core repulsion) magnon-magnon interactions, and unambiguously verify the relativistic form of the magnon dispersion law. Our results for the magnon spectrum are the most straightforward ones, i.e., they are not affected by the finite-size effects ($L/\xi > 10$), spin excitations at the chain ends, or magnon-magnon interactions. Also, the numerical effort is not extreme, since one has to perform only one simulation to get the above results. This is made possible through the evaluation of the Green function of the system.

It was demonstrated recently how to implement the "worm" idea within the framework of the LCU method [21]. Since $\Delta(s = 2)$ is rather small $\sim 0.09$ (see Refs. [22] [23]), one may deduce the gap and the spectrum very accurately from the Green function even at $H = 0$ making use of improved estimators available in LCU algorithm [24].

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