Monte–Carlo Thermodynamic Bethe Ansatz

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ABSTRACT

We introduce a Monte–Carlo simulation approach to thermodynamic Bethe ansatz (TBA). We exemplify the method on one particle integrable models, which include a free boson and a free fermions systems along with the scaling Lee–Yang model (SLYM). It is confirmed that the central charges and energies are correct to a very good precision, typically 0.1% or so. The advantage of the method is that it enables the calculation of all the dimensions and even the particular partition function.
Conformal field theory in two dimensions and its perturbed integrable models have attracted considerable attention, since the work [1]. A great deal of interest stems from the work of Al. Zamolodchikov who considered first the thermalization of integrable systems (see ref. [2] and ref. therein). See also [3], and for further developments see [4]. Here we offer an approach to thermodynamic Bethe ansatz based on a Monte–Carlo simulation.

We consider a collection of particles moving in a box of length $l$. For simplicity we assume only one particle specie in a purely inelastic scattering matrix, $S$, and also assume periodic boundary condition on the box.

We assume that the particles are at the locations $x_1, x_2, \ldots x_n$ and that the distances $x_i - x_j$ are large, so that we can use the scattering matrix to compute the relative phase. We denote the scattering amplitude by $S(\beta)$ where $\beta$ is the relative rapidity, $p = m \sinh \beta$ is the momentum, $E = m \cosh \beta$ is the energy, and where $m$ is the mass of the particle.

The Bethe ansatz assumes that the wave function is

$$\psi(x_1, x_2, \ldots, x_n) = \prod_r e^{i x_r p_r} \theta(x_1 < x_2 < \ldots < x_n) + \ldots, \quad (1)$$

where the theta ensures that $x_1 < x_2 < \ldots < x_n$ and the dots correspond to other arrangements of the coordinates, picking up a factor of $S(\beta_i - \beta_j)$ every time $x_i$ crosses $x_j$. For example for two particles, the wave function is

$$\psi(x_1, x_2) = e^{ix_1 p_1 + ix_2 p_2} \left[ \theta(x_2 - x_1) + S(\beta_1 - \beta_2) \theta(x_1 - x_2) \right]. \quad (2)$$

The amplitude in a unitary theory can be written as,

$$S(\beta) = e^{i \delta(\beta)}, \quad (3)$$

where $\delta(\beta)$ is a real phase.
The basic equation follows from taking a particle all around the box, picking up a phase each time we exchange two particles location and a phase from the wave function factor $e^{ip_i x_i}$. It is

$$e^{ip_i} \prod_{j \neq i} S(\beta_i - \beta_j) = 1. \quad (4)$$

Taking a log of this equation we arrive at the Bethe equation,

$$ml \sinh \beta_i + \sum_{j \neq i} \delta(\beta_i - \beta_j) = 2\pi n_i, \quad (5)$$

where $i$ and $j$ take the values 1 to $n$, and $n$ is the number of particles. $n_i$ are some integers which determine the energy levels.*

The energy of this collection of particles is given by

$$\bar{E} = rE = mr \sum_{i=1}^{n} \cosh \beta_i, \quad (6)$$

where $r$ is the inverse temperature,

$$r = \frac{1}{kT}, \quad (7)$$

where $T$ is the temperature, and $k$ is Boltzmann constant. We redefined the energy by multiplying it by $r$ and denoted by $\bar{E}$.

* Denoting the wave function for these $n_i$’s by $\psi_{n_1, n_2, ..., n_m}(x_i)$, the actual wave function has to take into account that these are identical particles. Thus, the full wave function assumes the form:

$$\tilde{\psi}(x_i) = \sum_{p} h^{s(p)} \psi_{p(n_1), p(n_2), ..., p(n_m)}(x_i),$$

where $p$ is any permutation of $m$ objects, and $s(p)$ is 0 (1) if $p$ is an even (odd) permutation, respectively, and $h = 1$ ($h = -1$) for Bose (Fermi) statistics, respectively. It follows that the wave function is defined for $n_1 \leq n_2 \leq \ldots \leq n_m$ for Bose statistics, and, $n_1 < n_2 < \ldots < n_m$ for Fermi statistics.
We define a grand canonical partition function by summing over all the particle numbers, $m$, without a chemical potential, $\mu = 0$, and summing over the energy levels, $n_i$, taking into account that all the particles are identical. These means that we have to limit the sum on $n_1 \leq n_2 \leq \ldots \leq n_m$. The partition function then becomes,

$$Z(m, r, l) = \sum_{n_1, m} \exp[-\bar{E}(n_i)].$$

(8)

In the case of Fermi statistics, when the $n_i$ are all different we may write the partition function as,

$$Z(m, r, l) = \sum_{n_i, m} \frac{1}{m!} \exp[-\bar{E}(n_i)].$$

(9)

The average energy is given, as usual, by

$$\bar{E}(m, r, l) = \langle \bar{E} \rangle = -r \frac{\partial}{\partial r} \log Z(m, r, l).$$

(10)

The conformal limit is obtained by taking the mass to zero, $m \to 0$. In this limit the partition function becomes only a function of the ratio $\tau = r/l$.

$$\lim_{m \to 0} Z(m, r, l) = Z(r/l),$$

(11)

and we denote by $\bar{E}(r/l) = \lim_{m \to 0} \bar{E}(m, r, l)$ the average energy in this limit. We expect the partition function to be equal to the path integral on the torus with a modulus $i\tau$ of the corresponding conformal field theory. Denote by $\mathcal{H}$ the Hilbert space of this theory. Then the following correspondence emerges,

$$Z(r/l) = \text{Tr} e^{-2\pi r(L_0 + \bar{L}_0)/l},$$

(12)

where $L_0$ and $\bar{L}_0$ are the left and right moments of the stress energy tensor, i.e., the Hamiltonians of the system, whose eigenvalues are the conformal dimensions. The relation, eq. (12), can be used to evaluate all the dimension of the CFT and even the particular modular invariant used, by evaluating the partition function.
We can now use modular invariance [5, 6]. This means that the function,

\[ f(r/l) = Z(r/l) e^{2\pi r c/(12l)}, \]  

where \( c \) is the central charge, is invariant under \( l \) and \( r \) replaced,

\[ f(l/r) = f(r/l). \]  

By deriving the log of this equation with respect to \( r \), we get a relation among energies,

\[ \tilde{E}(r/l) + \tilde{E}(l/r) = \frac{2\pi c}{12} \left( \frac{l}{r} + \frac{r}{l} \right). \]  

This is a very useful relation for evaluating the central charge. An exception to this relation occurs for free bosons where: 1) There is an infinite factor in \( Z \) due to the zero mode, \( n_i = 0 \), which we can ignore (or eliminate by giving a chemical potential \( \mu \)) for the \( n_i = 0 \) mode. 2) \( f \) has to be multiplied by

\[ (l/r)^{1/2} f(r/l), \]  

to make it modular invariant. This changes the relation eq. (15), to be

\[ \tilde{E}(r/l) + \tilde{E}(l/r) + 1 = \frac{2\pi c}{12} \left( \frac{l}{r} + \frac{r}{l} \right), \]  

where the central charge \( c = 1 \) for one free boson.

We start by studying some simple examples, which we take to be systems of one free boson or one free fermion.
For a free boson the different modes are independent and the partition function for the system is readily evaluated to be,

\[
Z(r/l) = \prod_{m=-\infty \atop m \neq 0}^{\infty} \sum_{s_m=0}^{\infty} e^{-2\pi r|m|s_m/l} = \prod_{n=1}^{\infty} (1 - q^n)^{-2},
\]

where \(s_m\) is the number of particles at the \(m\)th energy level and we defined \(q\) to be

\[
q = e^{-2\pi r/l}.
\]

We ignored the zero mode which is a constant (infinite) factor, which can be controlled by adding a chemical potential, as explained above.

We see immediately, that eq. (12) is indeed obeyed, and that \(Z\) is exactly the partition function of one free boson, on a torus with a modulus \(i\tau\). We can also verify that equation (17) holds giving the central charge \(c = 1\) as expected.

Let us consider now a system of one free fermion. We assume that \(\delta(\beta) = 0\) and that the boundary condition is anti-periodic. We take a Fermi statistics, i.e., only one particle is allowed for each energy level. This implies that the Bethe equation, eq. (5), becomes,

\[
ml \sinh \beta_i = 2\pi (n_i + 1/2),
\]

and the partition function becomes,

\[
Z(r/l) = \prod_{m=0}^{\infty} \left(1 + q^{m+\frac{1}{2}}\right)^2,
\]

where \(q\) is again given by eq. (19).

Again, this is precisely the partition function for a free fermion in the Neveu–Schwarz sector, confirming eq. (12). We can verify that eq. (15) holds, giving the correct central charge, \(c = 1/2\).
The Ramond sector is obtained by taking the trivial scattering matrix \( S = 1 \), periodic boundary conditions and Fermi statistics. The partition function can be easily evaluated using eqs. (5,9), and it is

\[
Z(r/l) = 2 \prod_{n=1}^{\infty} (1 + q^n)^2. \tag{22}
\]

We see that, indeed, it is identical to the free fermion CFT partition function, which is

\[
Z_{\text{cft}}(r/l) = 2q^{1/12} \prod_{n=1}^{\infty} (1 + q^n)^2. \tag{23}
\]

We note however, that the overall factor is different. Thus we define

\[
\bar{\chi}_R = q^{-\Delta + c/24} \chi_R, \tag{24}
\]

where \( \Delta \) is the dimension of the primary field corresponding to this block, and \( \chi_R \) is the usual Ramond character. We then see that the correspondence with the CFT is,

\[
Z(r/l) = 2|\bar{\chi}_R|^2. \tag{25}
\]

We conclude that two differences arise, in general, in eq. (12): 1) Each block in the CFT occurs for a different boundary conditions. 2) The overall factor eq. (24) has to be eliminated, making the character into a “q-series”, i.e., only integer non–negative powers of \( q \) are allowed in the character.

Now, for an interacting system it is quite difficult, in general, to compute this partition function. For example, the Lee–Yang theory \( M(2,5) \), which is the perturbed minimal model with \( p = 2 \) and \( q = 5 \) [1]. This theory has only one particle in the spectrum, particle \( A \) with a mass \( m \) and the scattering amplitude
Thus, we resort to a numerical algorithm for evaluating the partition function $Z(m, r, l)$. There are two stages in this algorithm, which are basically, 1) Solving the basic equation (5). 2) Simulating the grand canonical ensemble eq. (8).

To solve the equation we must calculate $\bar{E}(n_i)$ for any set of levels, $n_i$. This we do by taking the initial guess $\beta_i^0 = 0$ and solving eq. (5) by iterations,

$$
\beta_i^s = \sinh^{-1} \left[ \frac{2\pi n_i - \sum_{j \neq i} \delta(\beta_i^{s-1} - \beta_j^{s-1})}{m l} \right],
$$

where $s$ denotes the $s$th iteration. Usually 5 or so iterations are enough to get $\beta_i$ with sufficient precision ($10^{-6}$ or so).

The second stage we use is to make a Monte–Carlo simulation of the system using a Metropolis type algorithm, in order to find the average energy, $\bar{E}(m, r, l)$. We use three types of steps, preserving the detailed balance to get the correct population of particles.

For the first step, we change any of the $n_s$’s for all the $s$ by one $n_s \rightarrow n_s \pm 1$,

$$
n_1, n_2, \ldots, n_m \rightarrow n_1, n_2, \ldots, n_{s-1}, n_s \pm 1, n_{s+1}, \ldots, n_m.
$$

If the energy of the new configuration is less, we accept the new configuration. If the energy is greater, we accept it with the probability

$$
\exp[\bar{E}_{\text{old}} - \bar{E}_{\text{new}}],
$$

which ensures the detailed balance distribution of probability $\exp[-\bar{E}]$. This step allows us to move in momentum space, corresponding to a thermalized random walk in the $n$ lattice, covering all the possible values of $n_s$ (ergodicity).
The second and third steps allow for changing the numbers of particles. i.e.,
we either insert a new level somewhere, \( n_s = 0 \) for some \( s \), or eliminating a level
which is zero \( n_r = 0 \). The adding of a particle corresponds to the step:

\[
 n_1, n_2, \ldots, n_m \rightarrow n_1, n_2, \ldots, n_{s-1}, 0, n_{s+1}, \ldots, n_m
\]  

and the elimination of a particle corresponds to the step

\[
 n_1, n_2, \ldots, n_{s-1}, 0, n_{s+1}, \ldots, n_m \rightarrow n_1, n_2, \ldots, n_m.
\]  

Again we take the new configuration if its energy is lower. If the new con-
figuration is higher in energy, we take the new configuration with the probability
eq. (28). This allows the change of the number of particles and the population of
energy levels is according to the grand canonical distribution eq. (8). The relation
eq. (28) ensures the correct detailed balance. We use configurations of \( n_s = 0 \) as
“gateways” to change the number of particles, deleting or adding only zero energy
levels.

Actually, the algorithm above does not take into account the ordering of the
energy levels, \( n_1 \leq n_2 \leq \ldots \leq n_m \). This we do in a different way for bosons and
fermions. For fermions we add a particle with the probability \( \exp[-\Delta E]/(m + 1) \) if the energy is higher, and 1 if it is lower. We delete a particle with the
energy \( \exp[-\Delta E] \) if the energy is higher and \( 1/(m + 1) \) if it is lower. If the \( n_i \)
already contains some \( n_i = 0 \) we do not add a particle, and leave the configuration
unchanged. Likewise if the configuration does not contain 0 we do not delete a
particle.

For free fermions this algorithm can be simplified since adding a particle always
raises the energy, and deleting it always lowers it. So, we add a particle with the
probability \( \exp[-\Delta E]/(m + 1) \) and remove it with the probability 1.

For bosons we use the same algorithm but allow only the configurations which
are ordered: \( n_1 \leq n_2 \leq \ldots \leq n_m \) discarding any other new configurations. We
change $n_i \rightarrow n_i \pm 1$ at some location. If the new configuration is not ordered, we do not make the change. This guarantees detailed balance.

This allows us to calculate the energies, eq. (10), preserving correctly the detailed balance.

The easiest systems to simulate are, of course, the free fermions and free boson systems. For a free fermion system we took $\delta(\beta) = 0$ along with antiperiodic boundary condition and Fermi statistics. For $r/l \leq 1$ we took 10000000 sweeps for each temperature, and for $r/l \geq 1$ we took 400000000 sweeps. The results are listed in tables (1) and (2). Here $E_{mc}$ and $N_{mc}$ are the average energy and average particle numbers, as found in the simulation. We define the “partial” central charge as:

$$c_{mc}(r/l) = \frac{12E_{mc}(r/l)}{2\pi(l/r + r/l)},$$

and the central charge is given by, using eq. (15),

$$c_{mc}(r/l) + c_{mc}(l/r) = c,$$

where $c$ is the Monte–Carlo value of the central charge of the theory. For example we can calculate, from tables (1-2),

$$c_{mc}(0.5) + c_{mc}(2) = 0.481836 + 0.0178107 = 0.499647,$$

which is impressively close to the actual central charge $c = 0.5$, in accordance with eq. (15).

$E_{calc}$ is the energy calculated from eq. (10). Here the average number of particles $N_{calc}$ is calculated by introducing a chemical potential $\mu$,

$$Z(r/l, \mu) = \sum_{n_1, n_2, \ldots, n_m}^{n_1 \leq n_2 \leq \ldots \leq n_m} \exp[-E(n_i) - \mu m],$$

10
for Bose statistics. For Fermi statistics we have,

\[ Z(r/l, \mu) = \sum_{n_1 < n_2 < \ldots < n_m} \exp[-\bar{E}(n_i) - \mu m] = \sum_{n_1 < n_2 < \ldots < n_m} \frac{1}{m!} \exp[-\bar{E}(n_i) - \mu m]. \tag{35} \]

For a free fermion \( Z \) assumes the form,

\[ Z(r/l, \mu) = \prod_{n=0}^{\infty} (1 + \exp[-2\pi r(n + 1/2)/l - \mu])^2, \tag{36} \]

and for a free boson it is

\[ Z(r/l, \mu) = \prod_{n=1}^{\infty} (1 - \exp[-2\pi rn/l - \mu])^{-2}. \tag{37} \]

The energy is given as in eq. (10),

\[ \bar{E}_{\text{calc}} = -r \frac{\partial}{\partial r} \log Z(r/l, 0), \tag{38} \]

We calculate the derivative with respect to \( \mu \) to get the average number of particles,

\[ N_{\text{calc}} = -\lim_{\mu \to 0} \frac{\partial}{\partial \mu} \log Z(r/l, \mu). \tag{39} \]

From tables (1-2), we see that across the range of temperatures the average energy and average \( N \) are typically only 0.1% off the calculated numbers, which is a very reasonable correspondence. This demonstrates the very agreeable efficacy of the Monte–Carlo approach.

In tables (3–4) we list the results for a free boson system, for \( r/l \leq 1 \) (table (3)) and \( r/l \geq 1 \) (table (4)). We take a chemical potential for the zero modes, \( \mu = 0.5 \). At this value only a few \( n_i = 0 \) are created. Also we make 100000000
sweeps of the Monte–Carlo. Again, the correspondence between the Monte–Carlo results and the calculated ones is very good, around 0.1%. We defined here $c_{mc}$ as

$$c_{mc}(r/l) = \frac{12[E(r/l) + 1/2]}{2\pi(l/r + r/l)}. \tag{40}$$

It follows from eq. (17) that the Monte Carlo value of the central charge is, again,

$$c_{mc}(r/l) + c_{mc}(l/r) = c_{mc}. \tag{41}$$

For example, from tables (3–4),

$$c_{mc}(0.8) + c_{mc}(1.25) = 0.528855 + 0.471513 = 1.000368, \tag{42}$$

which is very close to the theoretical value $c = 1$.

The zero modes of the bosonic system, i.e., for $n_i = 0$ have to be treated carefully, since they have zero energy. First, we introduce a chemical potential, only for the zero modes, in the Monte–Carlo simulation. Second, in calculating $N_{mc}$ we count only the number of the non–zero modes, in order to correspond with eq. (37), the partition function. We see from tables (3–4) that this leads to a very good agreement with the theoretical results.

We now turn our attention to the scaling Lee Yang model, which is the perturbed minimal model $M(2,5)$. We first need to establish some facts about the minimal models, in general [1]. The models are labeled by two integers $p$ and $p'$ assumed to be strange to each other, and labeled by $M(p,p')$. The central charge is

$$c = 1 - \frac{6(p - p')^2}{pp'}. \tag{43}$$

The fields are given by $n = 1, 2, \ldots, p - 1$ and $m = 1, 2, \ldots, p' - 1$, denoted by $\phi_{n,m}$ whose dimensions are

$$\Delta_{n,m} = \frac{(np' - mp)^2 - (p - p')^2}{4pp'}. \tag{44}$$

The field $\phi_{n,m}$ is identical to the field $\phi_{p-n,p'-m}$. These models are unitary only for $p' = p + 1$ [8]. In particular, the model $M(2,5)$ is not unitary. However, it is only
“weakly” non-unitary, since the scattering matrix $S_{AA}$, eq. (26) is unitary and also, as we shall see, the model is modular invariant. This enables us to calculate the partition function as if it was a unitary theory.

The character of the field $\varphi_{m,n}$ is defined by
\[ \chi_{n,m} = \text{Tr} \exp[2\pi i\tau(L_0 - c/24)]. \]  
\[ (45) \]

We define the classical theta functions at the level $p$ by [9],
\[ \Theta_{n,p}(\tau) = \sum_{j=\frac{n}{2p}+\text{integer}} e^{2\pi ipj^2\tau}, \]  
\[ (46) \]
where $n$ is defined modulo $2p$. The theta functions are modular forms, transforming by the modular transformation $\tau \to -1/\tau$ as [9]
\[ \Theta_{n,p}(-1/\tau) = (-i\tau)^{-1/2} \sum_{\tilde{n}} S_{n,\tilde{n}} \Theta_{\tilde{n},p}(\tau), \]  
\[ (47) \]
where the sum is over $\tilde{n}$ modulo $2p$ and the matrix $S$ is given by
\[ S_{n,\tilde{n}} = \frac{1}{\sqrt{2p}} e^{-\pi in\tilde{n}/p}. \]  
\[ (48) \]
The characters of the minimal model, $M(p,p')$ can then be seen to be,
\[ \chi_{n,m}(\tau) = \frac{\Theta_{n_-pp'}(\tau) - \Theta_{n_+pp'}(\tau)}{\eta(\tau)}, \]  
\[ (49) \]
where we defined,
\[ n_\pm = np' \pm mp, \]  
\[ (50) \]
and where the Dedekind eta function is defined by,
\[ \eta(\tau) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n). \]  
\[ (51) \]

It is immediately seen that these characters give the correct central charge and dimensions, eq. (43-44). Moreover, they give the null vector for the field $\phi_{n,m}$ at
the levels $\Delta = \Delta_{n,m} + mn$ and $\Delta = \Delta_{n,m} + (p - n)(p' - m)$, in accordance with [1].

The characters, so defined, are modular functions of a subgroup of the modular group. They are seen to transform according to,

$$\chi_{n,m}(-1/\tau) = \sum_{\bar{n}, \bar{m}} W_{n,m,\bar{n},\bar{m}} \chi_{\bar{n},\bar{m}}(\tau),$$

where the matrix $W$ is can be seen, from eq. (48), to be

$$W_{n,m,\bar{n},\bar{m}} = \sqrt{8} \frac{pp'}{p'} \frac{(-1)^{\bar{n}m + \bar{m}n}}{k + 2} \sin\left(\frac{\pi \bar{n} \bar{m} p}{p'}\right) \sin\left(\frac{\pi n \bar{m} p}{p'}\right).$$

It is immediately seen that the theory $M(p, p')$ is equivalent, at the level of the modular matrix, to $SU(2) \times SU(2)$ at the “pseudo” levels $p/p'$ and $p'/p$ [10, 11],

$$M(p, p') \approx SU(2)_{p/p'} \times SU(2)_{p'/p}.$$  

The factor $(-1)^{\bar{n}m + \bar{m}n}$ in equation (53) can be ignored since the left movers and the right movers differ by an even integer. Here, twice the $SU(2)$ isospin is given by $j = n - 1$, $l = m - 1$, $\bar{j} = \bar{n} - 1$, $\bar{l} = \bar{m} - 1$, and the level is $k = p - 2$, $k' = p' - 2$. In this notation, the modular matrix of $SU(2)_{p'/p}$ is given by [9, 6, 10, 11]

$$S_{j\bar{j}} = \sqrt{\frac{2}{k + 2}} \sin\left(p \frac{\pi (j + 1)(\bar{j} + 1)}{k + 2}\right),$$

and, indeed, eq. (53) is exactly a product of two such factors, for $p/p'$ and for $p'/p$.

For the modular transformation $T$, which is generated by $\tau \rightarrow \tau + 1$, we have

$$T_{n,m} = e^{2\pi i (\Delta_{n,m} - c/24)} = e^{2\pi i n^2 p'/(4p)} e^{2\pi i m^2 p/(4p')} (-1)^{mn} e^{-2\pi i c/24}.$$  

The factor $(-1)^{mn}$ is irrelevant since it cancels between the right and left movers, as they differ by an even number, and so is the factor with the central charge. The
other factors correspond exactly to the dimensions of $SU(2)_{p/p'}$ and $SU(2)_{p'/p}$,

$$\Delta_j = p \frac{j(j + 2)}{4(k + 2)},$$  \quad (57)

and

$$\Delta_l = p \frac{l(l + 2)}{4(k' + 2)}.$$  \quad (58)

We infer that, also, the modular matrix $T$ is a product of two $SU(2)'s$ at the pseudo levels $p$ and $p'$. (At the level of the dimensions, the correspondence with $SU(2) \times SU(2)$ was noted already in [12]).

We conclude that the general modular invariant partition function is given by,

$$Z(\tau) = \frac{1}{2} \sum_{n,m,n',m'} N_{n,m} K_{m,m'} \chi_{n,m}(\tau) \chi_{n',m'}(\tau)^*,$$ \quad (59)

where the factor of $1/2$ accounts for the field identifications, and where $N$ and $K$ are any modular invariants of $SU(2)$ at the levels $k = p - 2$ and $k' = p' - 2$, respectively, which are in relation with the simply laced Lie algebras of types ADE [6, 13]. For a proof see [14]. This solves the problem of classifying the acceptable partition functions.

The modular transformations also imply that the fusion rules of the model $M(p,p')$ are the same as a product of two $SU(2)'s$,

$$\phi_{n,m} \times \phi_{\bar{n},\bar{m}} = \sum_{q,t} f_{n,\bar{n},q} f_{m,m',t}^{p'} \phi_{q,t},$$ \quad (60)

where $f_{n,\bar{n},q}$ is the fusion rule of $SU(2)$ at the level $k = p - 2$ according to the “depth rule” [6]. We have that $f_{n,\bar{n},q}$ is equal to one if:

$$n - \bar{n} + q = 1 \mod 2, \quad q \geq |n - \bar{n}| + 1, \quad q \leq \min(n + \bar{n} - 1, 2p - n - \bar{n} - 1),$$ \quad (61)

and is zero otherwise. These fusion rules can be seen to be in accordance with the Verlinde formula [15]. When we use the $S$ matrix eq. (53) we recover the correct
fusion rules, eqs. (60–61). This implies that these are fully consistent conformal data for a unitary theory, obeying all the axioms of unitary conformal data.

Actually, the model $M(p,p')$, for $p - p'$ odd, has exactly the same conformal data as the unitary model

$$L = SU(2)_1 \times SU(2)_{(p'/p)-1} \times SU(2)_{(p/p')-1},$$

where we include in the chiral algebra the field $\rho = [1] \times [p - 2] \times [p' - 2]$, and where each of the numbers correspond to twice the isospin of $SU(2)$. The central charge of the model is calculated to be,

$$c = 1 + 3(p'/p - 1)(p - 2) + 3(p/p' - 1)(p' - 2) = 1 - \frac{6(p - p')^2}{pp'},$$

i.e., exactly as the central charge of $M(p,p')$, eq. (43). The field $\rho$ has integer dimension, for $p - p'$ odd, and so we can include it in the chiral algebra. Also, the consistency of the pseudo conformal field theory, i.e., at the level $p - p'$ requires that $p - p'$ is odd [10]. The extended field implies: 1) The field identifications, $\phi_{n,m} = \phi_{p-n,p'-m}$, by multiplying any of the fields with this field. 2) The total isospin has to be an integer, for locality with respect to this field: $[s] \times [j] \times [l]$ obeys $s + j + l = 0 \mod 2$. It can be easily verified that the modular properties of the theory $L$, with this extended field, are exactly the same as $M(p,p')$ theory, eqs. (53,56). In particular, this implies the fusion rules, eqs. (60-61), using, for example, the Verlinde formula [15]. For $p' = p + 1$ we recover the conformal data of the coset model $SU(2)_1 \times SU(2)_p/SU(2)_{p+1}$, as is well known [16].

A similar correspondence holds when $p$ and $p'$ are both odd. In this case we define the model

$$M \approx SU(2)_{(p+p')/p}/Z_2 \times SU(2)_{p/p'},$$

where $SU(2)_k/Z_2$ stands for the conformal field theory of integer isospin representations of $SU(2)$, see [10]. It can be immediately verified that the central charge
is correct, giving eq. (43), up to an integer, and that the modular transformations are identical with eqs. (53,56). We conclude that for all the minimal models, their conformal data can be realized by full fledged unitary conformal field theories.

For the model $M(2,5)$, the SLYM, we have two fields $\phi_{1,1} = 1$, which is the unit operator, and $\phi = \phi_{1,2}$ which has the dimension $\Delta_{1,2} = -1/5$. According to eq. (59), only the diagonal modular invariant is allowed in this case.

The fusion rules are easily read from eqs. (60–61) and are given by,

$$\phi^2 = 1 + \phi.$$  \hfill (65)

These are the same fusion rules as $(G_2)_1$ and $SU(2)_3/Z_2$. The later is the conformal theory consisting of the integer isospin representations of $SU(2)_3$, see [10]. However, the modular matrix of $M(2,5)$ is at pseudo level 3 of $SU(2)_3/Z_2$ and so is different from these cases (which are at the pseudo levels $\pm 1$).

It is convenient to define the characters,

$$\bar{\chi}_{m,n}(\tau) = q^{-\Delta_{m,n}+c/24} \chi_{m,n}(\tau),$$ \hfill (66)

so that $\bar{\chi}$ contains only integer powers of $q$ (a “q-series”) starting at 1. The square of this object is what we actually compute in the Monte–Carlo simulation, and with which we want to make the comparison. We have approximately, using eq. (49), the character of the identity,

$$\bar{\chi}_{1,1}(q) = \frac{1 - q - q^4 + q^7 + \ldots}{(1-q)(1-q^2)(1-q^3)\ldots},$$ \hfill (67)

and of the field $\phi$,

$$\bar{\chi}_{1,2}(q) = \frac{1 - q^2 - q^3 + q^9 + \ldots}{(1-q)(1-q^2)(1-q^3)\ldots},$$ \hfill (68)

where we defined, as usual,

$$q = \exp(2\pi i \tau),$$ \hfill (69)

and were, for the comparison, $\tau = ir/l$, following eq. (12). The square of one of
these two quantities, we expect to recover in the Monte–Carlo simulation, according to eq. (12).

Now, in the conformal limit, \( m \to 0 \), we can, actually, solve exactly the Bethe ansatz for the SLYM system, eq. (5). Inspecting the scattering matrix in this case, \( \delta_{AA}(\beta) \), we see from eq. (26) that

\[
S_{AA}(\beta) = e^{i\delta_{AA}(\beta)},
\]

(70)

and that for \( \beta = 0 \), \( \delta_{AA}(\beta) = \pi \) and that for \( \beta \gg 1 \), \( \delta_{AA}(\beta) = 0 \). This means that in eq. (5), since we can assume that if \( \beta_i - \beta_j \) is not zero, it is very big, so if \( n_i \neq n_j \) then the Bethe equation for \( i \) and \( j \) decouples. This implies that we need to solve the partition function only for \( n_i \)'s which are all the same. In this case, we simply need to take \( n_i \to n_i - 1/2 \) if the number of particles is even, and to leave it unchanged, \( n_i \), if the number of particles is odd.

We conclude that the partition function for SLYM is:

\[
Z(r/l) = \prod_{s=1}^{\infty} \left( 1 + q^s + q^{2s-1} + q^{3s} + q^{4s-2} + q^{5s} + q^{6s-3} + \ldots \right)^2.
\]

(71)

(We omitted the zero mode, which gives an infinite factor, and as explained before, it can be controlled by adding a chemical potential for the zero mode.) It is immediately observed that this partition function, eq. (71), is different from the square of the characters, eqs. (67–68). We conclude that the scattering matrix, eq. (26) needs to be modified by a “Z-factor” to make it correct for the SLYM system. We conjecture that it needs to be multiplied by the solution of the Yang Baxter equation based on the Hard Hexagon model, \( IRF((G_2)_1, \phi, \phi) \) [10]. Further work on this is required.

We hope that the Monte–Carlo simulation approach to the thermodynamic Bethe ansatz can be a valuable tool in the investigation of integrable systems, and as demonstrated here it can lead to very precise results.
Table 1.
Free Fermion Results, $r/l \leq 1$.

| $r/l$ | $E_{mc}$   | $N_{mc}$ | $c_{mc}$ | $E_{calc}$ | $N_{calc}$ |
|-------|------------|----------|----------|------------|------------|
| 0.05  | 5.23606    | 4.39815  | 0.49876  | 5.24908    | 4.40616    |
| 0.1   | 2.64036    | 2.19051  | 0.49928  | 2.64417    | 2.19318    |
| 0.15  | 1.78325    | 1.45019  | 0.499623 | 1.7846     | 1.451      |
| 0.2   | 1.36164    | 1.0766   | 0.500103 | 1.36135    | 1.07633    |
| 0.25  | 1.11179    | 0.847974 | 0.499617 | 1.11256    | 0.848415   |
| 0.3   | 0.951349   | 0.694035 | 0.500076 | 0.950611   | 0.693539   |
| 0.35  | 0.838011   | 0.580287 | 0.499037 | 0.837359   | 0.580059   |
| 0.4   | 0.753898   | 0.492667 | 0.496496 | 0.753123   | 0.492233   |
| 0.45  | 0.686255   | 0.421321 | 0.490472 | 0.686626   | 0.421479   |
| 0.5   | 0.630722   | 0.362648 | 0.481836 | 0.631075   | 0.362824   |
| 0.55  | 0.583235   | 0.313676 | 0.470359 | 0.582343   | 0.313237   |
| 0.6   | 0.536727   | 0.270202 | 0.452238 | 0.537975   | 0.270783   |
| 0.65  | 0.496334   | 0.234034 | 0.433148 | 0.496578   | 0.234155   |
| 0.7   | 0.458426   | 0.202888 | 0.411322 | 0.457424   | 0.202418   |
| 0.75  | 0.419849   | 0.174717 | 0.384889 | 0.420183   | 0.174866   |
| 0.8   | 0.385041   | 0.151055 | 0.358719 | 0.384752   | 0.150935   |
| 0.85  | 0.351453   | 0.13026  | 0.331229 | 0.351144   | 0.130158   |
| 0.9   | 0.319961   | 0.112321 | 0.303853 | 0.319412   | 0.112135   |
| 0.95  | 0.289654   | 0.0965256| 0.276236 | 0.289617   | 0.0965201  |
| 1.    | 0.262427   | 0.0832056| 0.250599 | 0.261799   | 0.0830094  |

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Table 2.
Free Fermion Results, $r/l \geq 1$.

| $r/l$ | $\bar{E}_{\text{mc}}$ | $N_{\text{mc}}$ | $c_{\text{mc}}$ | $\bar{E}_{\text{calc}}$ | $N_{\text{calc}}$ |
|-------|-----------------------|----------------|---------------|---------------------|---------------|
| 1.05263 | 0.234377             | 0.0706784       | 0.22352     | 0.234671           | 0.0707662     |
| 1.11111 | 0.206624             | 0.0590791       | 0.196221    | 0.207096           | 0.0592151     |
| 1.17647 | 0.179296             | 0.0484496       | 0.168978    | 0.179385           | 0.0484738     |
| 1.25     | 0.151874             | 0.0386435       | 0.141491    | 0.151936           | 0.0386596     |
| 1.33333 | 0.124918             | 0.0298078       | 0.114516    | 0.125233           | 0.0298832     |
| 1.42857 | 0.100163             | 0.0223123       | 0.089871    | 0.0998352          | 0.0222393     |
| 1.53846 | 0.0764025            | 0.0158057       | 0.0666761   | 0.0763599          | 0.015797      |
| 1.66667 | 0.0555191            | 0.0106026       | 0.0467796   | 0.0554371          | 0.0105871     |
| 1.81818 | 0.0377313            | 0.00660547      | 0.0304291   | 0.0376456          | 0.00659048    |
| 2.00000 | 0.0233141            | 0.0037105       | 0.0178107   | 0.0234235          | 0.00372794    |

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Table 3.
Free Boson Results, \( r/l \leq 1 \).

| \( r/l \) | \( \bar{E}_{\text{mc}} \) | \( N_{\text{mc}} \) | \( c_{\text{mc}} \) | \( \bar{E}_{\text{calc}} \) | \( N_{\text{calc}} \) |
|--------|----------|----------|----------|----------|----------|
| 0.1    | 4.29141  | 3.80843  | 0.906032 | 4.28835  | 3.80781  |
| 0.15   | 2.56987  | 1.83794  | 0.860102 | 2.5692   | 1.8375   |
| 0.2    | 1.72245  | 1.03771  | 0.816261 | 1.72271  | 1.03759  |
| 0.25   | 1.22361  | 0.637259 | 0.774554 | 1.22529  | 0.638052 |
| 0.3    | 0.903667 | 0.414006 | 0.737837 | 0.902409 | 0.41351  |
| 0.35   | 0.67905  | 0.277354 | 0.702127 | 0.679256 | 0.277446 |
| 0.4    | 0.517753 | 0.190424 | 0.670264 | 0.518432 | 0.190651 |
| 0.45   | 0.399507 | 0.1334   | 0.642885 | 0.399148 | 0.133236 |
| 0.5    | 0.308222 | 0.0940281| 0.617436 | 0.308909 | 0.094242 |
| 0.55   | 0.239491 | 0.0671612| 0.596375 | 0.239727 | 0.067244 |
| 0.6    | 0.186348 | 0.0483229| 0.578307 | 0.186231 | 0.048284 |
| 0.65   | 0.144824 | 0.0348669| 0.562735 | 0.14465  | 0.0348313|
| 0.7    | 0.112077 | 0.025171 | 0.549186 | 0.112247 | 0.0252108|
| 0.75   | 0.0866057| 0.0182176| 0.537761 | 0.086975 | 0.0182923|
| 0.8    | 0.0676613| 0.0133725| 0.528855 | 0.0672725| 0.0132962|
| 0.85   | 0.0519823| 0.00968116| 0.520219 | 0.0519312| 0.00967727|
| 0.9    | 0.0398549| 0.00702419| 0.512675 | 0.0400067| 0.00705006|
| 0.95   | 0.0308441| 0.00514874| 0.506253 | 0.0307573| 0.00513968|
| 1.     | 0.0235342| 0.00373636| 0.499938 | 0.0235988| 0.00374886|

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Table 4. 
Free Boson Results, $r/l \geq 1$.

| $r/l$  | $\bar{E}_{mc}$ | $N_{mc}$  | $c_{mc}$  | $\bar{E}_{calc}$ | $N_{calc}$ |
|-------|----------------|----------|-----------|------------------|-----------|
| 1.    | 0.0234887      | 0.00373087 | 0.499895  | 0.0235988       | 0.00374886 |
| 1.05263 | 0.0177955      | 0.00268717 | 0.493809  | 0.0178181       | 0.00269044 |
| 1.11111 | 0.0130254      | 0.00186362 | 0.487197  | 0.0130086       | 0.00186161 |
| 1.17647 | 0.00916301     | 0.00123849 | 0.479864  | 0.00912634      | 0.00123387 |
| 1.25   | 0.00611186     | 0.00077747 | 0.471513  | 0.00610499      | 0.00077701 |
| 1.33333 | 0.00386213     | 0.00046036 | 0.461907  | 0.00385577      | 0.000460143|
| 1.42857 | 0.00225915     | 0.00025103 | 0.450652  | 0.00227017      | 0.000252884|
| 1.53846 | 0.00125341     | 0.00012921 | 0.437441  | 0.00122546      | 0.000126766|
| 1.66667 | 0.000561796    | 0.00005319 | 0.421766  | 0.000593164     | 0.0000566413|
| 1.81818 | 0.000261345    | 0.00002242 | 0.403444  | 0.000249743     | 0.0000218611|
| 2.     | 0.000104389    | 0.00000785 | 0.382052  | 0.0000876474     | 0.00000697 |

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APPENDIX

Calculating the average energy and number of particles.

Enclosed is a Mathematica program which calculates the partition function $ff[a, l, \mu]$, for one free fermion in a box of length $l$, the inverse temperature $a$ and a chemical potential $\mu$, using eq. (21). Then it calculates the average energy $ee[a, l]$ and the average number of particles, $nn[a, l]$. For free bosons we use the function $ff[b[a, l, \mu]$ listed below too, which gives the partition function of one free boson, without the zero mode, and with a chemical potential $\mu$.

```
ff[a_, l_, \mu_] := Product[(1 + Exp[-\mu - 2 Pi a/l (n + 1/2)])^2, {n, 0, 60}]

ee[a_, l_] := -x D[Log[ff[x, l, 0.]], x] /. x -> a

nn[a_, l_] := -D[Log[ff[a, l, \mu]], \mu] /. \mu -> 0.

Print[ee[0.05, 1], " ", nn[0.05, 1]]

5.24908 4.40616

ffb[a_, l_, \mu_] := Product[(1 - Exp[-\mu - 2 Pi a/l n])^2, {n, 1, 60}]
```

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