A Multi-Grid Method for the Resolution of Thermodynamic Bethe Ansatz Equations

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Abstract

We present a multi-grid algorithm in order to solve numerically the thermodynamic Bethe ansatz equations. We specifically adapt the program to compute the data of the conformal field theory reached in the ultraviolet limit.

Program classification: 4.12-11.1
PROGRAM SUMMARY

Title of program: TBA

Catalogue number:

Program available from: CPC Program Library, Queen’s University of Belfast, N. Ireland

Computer: IBM RS6000/560

Operating system: AIX 3.2

Programming language used: FORTRAN 77

Number of lines in program: 1287

Key words: two-dimensional systems away from criticality, conformal field theory, thermodynamic Bethe ansatz, multi-grid methods.

Nature of the physical problem: resolve the thermodynamic Bethe ansatz equations corresponding to a factorized scattering theory and extract the data of the underlying conformal field theory reached in the ultraviolet limit.

Method of solution: non linear multi-grid method with full adaptive scheme.

Typical running time: strongly dependent on the dimension of the system of coupled integral equations, see Table 1.

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2. W. Hackbusch, Multi-grid methods and applications (Springer-Verlag Berlin, Heidelberg, 1985).

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1 Introduction

Massive relativistic field theories can be described on-shell by their scattering matrix. This approach is specially fruitful in two dimensions, where there exists a large class of models which are integrable, and their $S$-matrix can be computed exactly, being factorizable [1]. Unfortunately there is no general direct method in order to compute the $S$-matrix of a theory, but usually it is conjectured from general axioms and the underlying symmetries of the corresponding Hamiltonian.

The thermodynamic Bethe ansatz (TBA) was developed in order to provide a means to link a conjectured scattering theory with the underlying field theory [2]. It describes the finite temperature effects of the factorized relativistic field theory, using the $S$ matrix as an input. If one studies the high temperature limit of the TBA equations, one can identify the conformal field theory (CFT) which governs the ultraviolet behaviour of the underlying field theory. One should though note, that it is not guaranteed that every consistent $S$-matrix describes the scattering in some field theoretical model! Therefore the axiomatic bootstrap approach is only of limited value if not linked to field theory by some means, wherefrom the TBA is one of the most powerful ones.

Given the scattering data one can in most cases extract analytically the central charge of the CFT reached in the conformal limit, and in some cases the dimension of the perturbing operator, if the symmetry of the problem is known. Numerical calculations on the other hand can solve the TBA equations and therefore extract any measurable quantity. In [2, 3] the TBA equations were resolved by an iterative method. We propose here a multi-grid algorithm, which is considerable faster, an important fact if many particles are involved. The heart of the program is the resolution of the coupled integral equations. Around this core we have designed some utility-programs, in order to make the tool easier to use. We specialize our application to the case of diagonal $S$-matrices, see e.g. [2, 3, 5].

As physical quantities we extract the central charge, the dimension of the perturbing field and the perturbation expansion. Note though, that one can easily add subroutines
2 The TBA Equations

Consider an integrable massive scattering theory on a cylinder. This implies factorized scattering, and so one can assume that the wave function of the particles is well described by a free wave function in the intermediate region of two scattering. Take the ansatz

$$\psi(x_1 \ldots x_n) = e^{i \sum p_j x_j} \sum_P A(P) \Theta(x_P) ;$$

$A(P)$ are coefficients of the momenta whose ordering is specified by

$$ \Theta(x_P) = \begin{cases} 1 & \text{if } x_{p_1} < \ldots < x_{p_n} \\ 0 & \text{otherwise} \end{cases} .$$

Let the permutation $P$ differ from $P'$ by the exchange of the indices $k$ and $j$. Then

$$A(P') = S_{kj}(\beta_k - \beta_j)A(P) .$$

(1)

We impose antiperiodic boundary conditions for our wave functions, which provides that two particles cannot have equal momenta, leading to the condition

$$A(k, p_2, \ldots, p_n) = -e^{ip_kL}A(p_2, \ldots, p_n, k) ,$$

(2)

$L$ being the length of the strip on which we consider the theory. Comparing (1) and (2), one realizes

$$e^{iLm_k \sinh \beta_k} \prod_{j \neq k} S_{kj}(\beta_k - \beta_j) = -1 \quad \text{for } k = 1, 2, \ldots, n .$$

(3)

We introduce the phase $\delta_{kj}(\beta_k - \beta_j) \equiv -i \ln S_{kj}(\beta_k - \beta_j)$. In terms of these the equation become

$$Lm_k \sinh \beta_k + \sum_{j \neq k} \delta_{kj}(\beta_k - \beta_j) = 2\pi n_k \quad \text{for } k = 1, 2, \ldots, n ,$$

(4)

$n_k$ being some integers. These coupled transcendental equations for the rapidities are called the Bethe ansatz equations. One tries to solve these equations in the thermodynamic limit introducing densities of rapidities for each particle species and transferring
the equations into integral equations. That is, let \( \rho^{(a)}(\beta) = \frac{n}{\Delta \beta} \), where we assume that there are \( n \) particles in the small interval \( \Delta \beta \), be the particle density and \( \rho^{(a)}(\beta) = \frac{n}{\Delta \beta} \) be the level density corresponding to the particle \( a \), then (4) becomes

\[
m_a L \cosh \beta + \sum_{b=1}^{n} \int_{-\infty}^{\infty} \varphi_{ab}(\beta - \beta') \rho^{(a)}_{1}(\beta') d\beta' = 2\pi \rho^{(a)}.
\] (5)

In order to compute the ground state energy one needs to minimize the free energy

\[
R L f(\rho, \rho_1) = R H_B(\rho_1) + S(\rho, \rho_1),
\] (6)

where \( H_B = \sum_a m_a \int \cosh \beta \rho^{(a)}_{1} d\beta \) and \( S \) denotes the entropy. The extremum condition for a fermionic system\(^1\) takes the form

\[
- r M_a \cosh \beta + \epsilon_a(\beta) = \sum_{b=1}^{n} \int_{-\infty}^{\infty} \varphi_{ab}(\beta - \beta') \log(1 + e^{-\epsilon_b(\beta)}) \frac{d\beta'}{2\pi},
\] (7)

where we introduced the so-called pseudo-density \( e^{-\epsilon_a} \equiv \frac{\rho^{(a)}_{1}}{\rho^{(a)}_{1} - \rho^{(a)}_{2}} \), the scaling length \( r = R m_1 \) and the rescaled masses \( M_a = \frac{m_a}{m_1} \); \( m_1 \) is the lightest particle mass. These coupled integral equations are called the TBA equations. The extremal free energy depends only on the ratios \( \frac{\rho^{(a)}_{1}}{\rho^{(a)}_{2}} \) and is given by

\[
f(r) = -\frac{r}{2\pi} \sum_{a=1}^{n} M_a \int_{-\infty}^{\infty} \cosh \beta \log(1 + e^{-\epsilon_a(\beta)}) d\beta.
\] (8)

One can extract several physical quantities from the solution of the TBA-equations\(^2\). Since very little is known about non-critical systems, one tries to examine the equations in the ultraviolet limit, which corresponds to \( r \to 0 \), where the underlying field theory should become a CFT. The central charge is related to the vacuum bulk energy, and is given by

\[
c(r) = 3r \frac{3r}{\pi^2} \sum_{a=1}^{n} M_a \int_{-\infty}^{\infty} \cosh \beta \log(1 + e^{-\epsilon_a(\beta)}) d\beta.
\] (9)

Having calculated the central charge one would like to extract the conformal dimension of the perturbing operator. For small \( r \), one expects that \( f(r) \) reproduces the behaviour predicted by conformal perturbation theory, which in terms of \( c(r) \) reads as

\[
c(r) = c - \frac{3f_0}{\pi} r^2 + \sum_{k=1}^{\infty} f_k r^{yk},
\] (10)

\(^1\) We use the fermionic TBA equations since in diagonal scattering up to now they turned out to be the relevant ones, see e.g.\(^2\) for the general theory
with possible logarithmic corrections.

The exponent $y$ is related to the perturbing field by $y = 2(1 - \Delta)$ if the theory is unitary and by $y = 4(1 - \Delta)$ if it is non-unitary. The coefficients are related to correlation functions of the CFT \cite{2,3}, and even if one cannot read them off directly, this is an ultimate important check of the theory.

Note that the application chosen is not a limitation of the use of the program. Also non-diagonal S-matrices (see \cite{6}) can be treated, since once one has diagonalized the transfer-matrix also in that case the numerical problem reduces to solving (7). Further quantities to measure can simply be added, and also one can study any range of $r$, being a parameter in the input-data.

3 Description of the Solution Method

Multi-grid (MG) schemes are known to be the most efficient methods for solving elliptic boundary value problems. Actually, the underlying idea of treating the different characteristic length scales of the problem on different grids, applies successfully also to the numerical resolution of various other problems, as the resolution of integral equations \cite{8,11}. The system of non linear Fredholm integral equations (7) has been solved using iterative methods \cite{2,3}. Even if these methods provide a satisfactory solution in terms of accuracy, the number of iterations and corresponding computer process (CPU) time required to reach a specified precision can become excessively large as the number of grid points $N$ increases. Typically a simple one level relaxation would require $O(N^2 \log N)$ operations. With a multi-grid solution technique the computing time for integral equations is reduced to $O(N^2)$ \cite{11}, and in particular cases to $O(N \log N)$ \cite{8}, thus justifying the extra effort in programming.

Now we define our numerical problem and we explain how the multi-grid scheme works for solving it. In discretising the TBA equations (7), we use the trapezoidal rule
on a grid with mesh size $h$ so that our system yields

$$
\epsilon_a(\beta) = r M_a \cosh \beta + \frac{h}{2\pi} \sum_{\beta' \in \Omega_h} w(\beta') \varphi_{ab}(\beta - \beta') \log(1 + e^{-\epsilon_a(\beta')}) \quad , \quad (11)
$$

$a = 1, 2, \ldots, n$, $\beta \in \Omega_h$, where $\Omega_h$ is the set of grid points with grid spacing $h$. The weights are $w(\beta) = 1$ unless on the boundary where $w(\beta) = 1/2$. Now let us introduce a sequence of grids with mesh sizes $h_1 > h_2 > \ldots > h_M$, so that $h_{\ell-1} = 2h_\ell$. The system (11) with discretisation parameter $h_\ell$ will be denoted as

$$
\epsilon_\ell^a = K_\ell^a(\epsilon_b^\ell) + f_\ell^a , \quad a = 1, 2, \ldots, n \quad , \quad (12)
$$

where a summation over $b$ is intended and where

$$
K_\ell^a(\epsilon) = \frac{h_\ell}{2\pi} \sum_{\beta' \in \Omega_{h_\ell}} w(\beta') \varphi_{ab}(\beta - \beta') \log(1 + e^{-\epsilon(\beta')}) \quad . \quad (13)
$$

Following [11] we have applied one (Gauss-Seidel) iteration to (12), and obtained the approximated solutions $\tilde{\epsilon}_a^\ell$, $a = 1, 2, \ldots, n$. We then transfer them onto the next coarser grid, $\tilde{\epsilon}_{\ell-1}^a = \hat{I}_{\ell-1}^{\ell} \epsilon_a^\ell$, where $\hat{I}_{\ell-1}^{\ell}$ is a restriction operator. The coarse grid equations become

$$
\hat{\epsilon}_a^{\ell-1} = K_{\ell-1}^{\ell \times \ell}(\epsilon_a^{\ell-1}) + \hat{f}_a^{\ell-1} , \quad a = 1, 2, \ldots, n \quad , \quad (14)
$$

where

$$
\hat{f}_a^{\ell-1} = I_{\ell-1}^{\ell \times \ell} f_a^{\ell} + \tilde{\epsilon}_a^{\ell-1} - K_{\ell-1}^{\ell \times \ell}(\epsilon_{\ell}^{\ell-1}) - I_{\ell-1}^{\ell \times \ell}(\epsilon_a^{\ell} - K_{\ell}^{\ell \times \ell}(\epsilon_a^{\ell})) \quad , \quad (15)
$$

and with $I_{\ell-1}^{\ell \times \ell}$ another fine-to-coarse grid transfer operator not necessarily equal to $\hat{I}_{\ell-1}^{\ell}$. Having obtained the solution of the coarse grid equation $\hat{\epsilon}_a^{\ell-1}$ the difference $\hat{\epsilon}_a^{\ell-1} - \epsilon_a^{\ell-1}$ is the coarse-grid (CG) correction to the fine-grid solution

$$
\tilde{\epsilon}_a^\ell \leftarrow \epsilon_a^\ell + \hat{I}_{\ell-1}^{\ell} (\hat{\epsilon}_a^{\ell-1} - \epsilon_a^{\ell-1}) \quad , \quad (16)
$$

$a = 1, 2, \ldots, n$, and $\hat{I}_{\ell-1}^{\ell}$ is a coarse-to-fine grid interpolation operator. Finally we perform one relaxation at level $\ell$, in order to smoothen errors coming from the interpolation procedure. To solve the system of equations (12) we employ a coarse-grid correction recursively, i.e. equation (14) is itself solved by iteration sweeps combined with a further CG correction.
4 Numerical Performance

The algorithm used to solve equations (12) is a non-linear multi-grid (NMGM) method (11) with full adaptive scheme (FAS) (9). The program can perform different MG variants: V or W cycle and (non linear) nested iteration, depending on the value of the parameter chosen. In order to reduce the number of parameters as input we have fixed most of them, that is the parameter regarding the multi-grid cycle (in order to optimize it), leaving as an input only the physical ones.

Figure 1: Evolution of residual error norm with CPU time for a 1-particle system at $r = 0.1$ for different HX: solid line for MG, dashed line for iteration only.

For any scaling length $r$ we use an initial approximation which behaves like $r M_a \cosh \beta$, wherefrom the program determines the numerical boundary at which the kernels vanish and verifies that the conditions for the existence of (at least) one solution given by the Schauder’s fixed point theorem are satisfied (12). Having determined the size of the numerical domain for a given $r$ the number of levels $M$ is set such that the finest level has a mesh-size $h_M$ of order of HX, which is one of the input parameters.
We compare the performance of the MG and of a (Gauss-Seidel) iterative scheme in terms of CPU time in Figure 1, where the different initial residual error for MG and iterative scheme is due to the setup of the initial approximated solution in the MG cycle, that is a non-linear nested iteration which uses a MG cycle itself (see [11]). As a norm for the residuals

$$
\tau_a(\beta) = (\epsilon_a - K_{ab}(\epsilon_b) - f_a)(\beta), \quad \beta \in \Omega_{hM},
$$

we define the norm

$$
\| \tau \|_M = \max_{1 \leq a \leq n} \sqrt{\sum_{\beta \in \Omega_{hM}} \tau_a(\beta)^2}.
$$

In order to outline how the multi-grid algorithm becomes important as the number of particles increases we give in Table 1 the CPU time required by the two methods to solve the discretized problem to a value of the residual norm

$$
\| \tau \|_M \leq 1 \cdot 10^{-14}.
$$

| no. equations | CPU time (secs) |
|---------------|----------------|
|               | Relax | Multi-Grid |
| 1             | 4     | 3          |
| 2             | 34    | 22         |
| 3             | 508   | 331        |
| 4             | 1230  | 712        |
| 5             | 2530  | 1320       |

Table 1: A comparison of CPU time required to reach a particular value of the norm (19), for \( r = 0.1, \) \( \text{HX} = 0.1. \)

5 Structure and Use of the Program

As already mentioned in the introduction the program consists of two parts: the core, which resolves the TBA-equations (7) and the periphery, which on the one hand con-
estructs the kernel, and the initial solution, and on the other hand extracts from the solution the central charge, the dimension $y$ and the coefficients $f_i$ of the perturbation expansion (10).

We specifically designed the program for diagonal scattering theories, that is we are concerned with scalar $S$ matrices of the form

$$S_{ab} = \prod_i f(\alpha_{ab}^i), \quad i = 1, \ldots, n_{ab}, \quad a, b = 1, \ldots, n$$

with

$$f(\alpha) = \frac{\sinh \frac{1}{2}(\beta + i\pi\alpha)}{\sinh \frac{1}{2}(\beta - i\pi\alpha)}$$

$n$ being the number of particles in the theory and $n_{ab}$ is the number of factors $f_x$ appearing in the $S$-matrix $S_{ab}$ (for a recent review on this subject and many examples, see [7]). The set of the numbers $\alpha$, and the masses of the theory are sufficient to resolve the TBA-equations.

As input-data we have therefore three data files: TBA.DAT containing general information about the range of $r$, the mesh-size and the number of particles, and the file ALPHA.DAT containing the values of $\alpha$ and MASS.DAT containing the values of the mass of the particles. From the input the program then constructs the kernel, and the initial approximation, which are then used by the multi-grid algorithm. The routine returns the solutions encoded in a matrix array $Q$ which is stored in the output file SOL.DAT. The physical parameters are then calculated in the appropriate following subroutines, see the flow-diagram.

We discuss here specific structure of the algorithm in terms of a simple example. Consider the $S$-matrix

$$S_{11} = f_4 f_\frac{1}{2}, \quad S_{12} = S_{21} = f_\frac{1}{2} f_\frac{3}{2} f_\frac{1}{2} f_\frac{3}{2}, \quad S_{22} = f_\frac{1}{2} f_\frac{3}{2} (f_\frac{1}{2} f_\frac{3}{2})^2;$$

being known to describe the minimal model $\mathcal{M}_{2,7}$, (i.e. $c_{eff} = \frac{4}{7}$) perturbed by the field with dimension $\Delta = -\frac{3}{7}$. The masses of the two particles are

$$M_1 = 1, \quad M_2 = 2 \cos\left(\frac{\pi}{5}\right).$$

Then the input-file ALPHA.DAT should read as
Every factor $f_\alpha$ is characterized by two numbers which are the nominator and denominator of $\alpha$. As a field separator between values $\alpha$ belonging to different $S$-matrix elements one gives a number smaller than $-1$. Since the $S$-matrix is symmetric the program reads only the elements $S_{1,1}, S_{1,2}, \ldots, S_{1,n}; S_{2,2}, \ldots, S_{2,n}; \ldots; S_{n-1,n-1}, S_{n-1,n}; S_{n,n}$.

The file MASS.DAT contains two values:

1.0

1.618033988749895

Finally the file TBA.DAT contains in our example the following data

15,2 I1,I2
1.0d-14,1.0d-2 ZERO,HX
0,1 corresponding to NREL,IWRITE
30,0.01,0.01 MAX,STEP,R0
20.0,7.0,0,0,4 YN,YD,YN,NCEN,MFIT
4.,7. CEXN,CEXD

These parameters are:

I1,I2: corresponding lengths of the files ALPHA.DAT and MASS.DAT (I2 coincides with
the number of equations of our system, NSYS in the program);

ZERO: the order of the value of the residual norm to be reached; HX the finest grid size;

NREL: if NREL= 0 multi-grid algorithm, if NREL= 1 only relaxation is done

MAX: the number of different radii $r$ to be used; $R_0$ is the smallest radius, and STEP give the step-size of the radius in the cycle;

YN, YD: are the numerator and the denominator of the exact exponent if available, otherwise dummy numbers; if NY= 0 the exact exponent is used in the fitting procedure, if NY= 1 the estimated $y$ is used; if MFIT $> 0$ the program calculates the first MFIT coefficients $f_i$ (in this case must be $\text{MAX} \geq \text{MFIT} + 5$). Finally if NCEX= 0, the exact charge ($\text{cexact}=\text{CEXN}/\text{CEXD}$) is used for the fitting procedure.

Some comments: The CPU time is mainly determined from the parameters NSYS, being the dimension of the system, MAX and HX. MAX is chosen corresponding to the physical parameters one wants to compute: in order to get a sensible result for the dimension $y$ it is enough to use $\text{MAX} \sim 5$, whereas if one wants to calculate the coefficients $f_i$ a larger number is required; for example with $\text{MAX} \geq 10$ one can get $f_1$ up to $O(10^{-5})$; the more data is used the better the fit-procedure works and more coefficients can be obtained. HX determines the error of the integration routines calculating $c(r)$. In any case HX=0.01 should be sufficient.

The program produces four files of output. If IWRITE=1 only the physical informations, that is $c$, $y$ and $f_i$ are stored in the file OUTPUT.DAT (see test-run output). When IWRITE=0 the program generates, in addition, the file RES.DAT which contains technical data and the evolution of the value of the residuals during the iterations. Together with RES.DAT other two files are written: TIME.DAT which contains the logarithm of the residual norm and the actual CPU time used, and SOL.DAT (where the solutions for any $r$ are stored).

6 Test-Run Output

The following file was produced using the input files described in the last section:
1. OUTPUT.DAT

| r            | central charge     |
|--------------|--------------------|
| .100000000D-01 | .571403656E+00     |
| .200000000D-01 | .571329513E+00     |
| .300000000D-01 | .571206952E+00     |
| .400000000D-01 | .571036718E+00     |
| .500000000D-01 | .570819520E+00     |
| .600000000D-01 | .570556042E+00     |
| .700000000D-01 | .570246948E+00     |
| .800000000D-01 | .569892886E+00     |
| .900000000D-01 | .569494492E+00     |
| .100000000D+00 | .569052390E+00     |
| .110000000D+00 | .568567192E+00     |
| .120000000D+00 | .568039505E+00     |
| .130000000D+00 | .567469925E+00     |
| .140000000D+00 | .566859042E+00     |
| .150000000D+00 | .566207440E+00     |
| .160000000D+00 | .565515695E+00     |
| .170000000D+00 | .564784379E+00     |
| .180000000D+00 | .564014059E+00     |
| .190000000D+00 | .563205295E+00     |
| .200000000D+00 | .562358645E+00     |
| .210000000D+00 | .561474660E+00     |
| .220000000D+00 | .560553889E+00     |
| .230000000D+00 | .559596875E+00     |
| .240000000D+00 | .558604159E+00     |
| .250000000D+00 | .557576277E+00     |
| .260000000D+00 | .556513761E+00     |
| .270000000D+00 | .555417143E+00     |
| .280000000D+00 | .554286946E+00     |

computed cexact = .57142857D+00
r= .290000000D+00 central charge= .553123695E+00
r= .300000000D+00 central charge= .551927909E+00
error in extrapolation .3365E-09
estimated exponent .285714287D+01
theoretical exponent .285714286D+01
estimated dimension of the corresponding operator
for a unitary theory: DELTA= .285714D+00
for a non-unitary theory: DELTA= -.428571D+00
fitted f_i
f( 1)= .9643967331341316D-01
f( 2)=-.1538311769518447D-02
f( 3)= .6222166295705919D-04
f( 4)=-.3197939259001748D-05
chi-square value of the fitting= .5164E-29
total cpu time (secs) .113E+06

7 Conclusions

We presented a multi-grid scheme for the resolution of the thermodynamic Bethe ansatz equations. The TBA is a means to describe the finite temperature effects of relativistic factorized scattering theories. Our program is specifically designed for theories having a scalar S-matrix. These theories exhibit a unique form, and the only input needed in order to carry out the TBA are the locations of the poles and zeros of the single S-matrix elements.

The program calculates the central charge and in the ultra-violet limit the dimension of the perturbing field and the coefficients of the perturbation expansion. These are the most crucial tests in verifying a conjectured S-matrix. It should not be difficult for the user to add subroutines calculating other physical quantities, as for example for magnetic systems the moments of the total magnetization, or the convergence-region of the perturbation series in [4], [5].
In order to get sensible results for the physical quantities one needs to resolve the integral equations with the highest possible accuracy. This unfortunately renders the calculation extremely time consuming. Therefore the use of an efficient Multi-Grid algorithm gives the possibility to reach high accuracy in the computation together with a sensible reduction of the CPU time, in confrontation with standard iterative techniques.

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