BFKL, MM, Alpert-Rokhlin’s transform, FFTW, ARPACK & all that.

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Abstract
The evolution equation for $q\bar{q}$ production introduced by Marchesini and Mueller posed some intriguing mathematical puzzles, both numerical and analytic. I give a detailed account of the numerical approach which led eventually to the exact solution. While part of the work was in fact along a wrong track, it turns out that some of the techniques involved are interesting in their own and applicable to many other problems, i.e. to the numerical study of Ricci flows.

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1. Introduction

Marchesini and Mueller [1, 2] introduced the following equation for the evolution of $q\bar{q}$ evolution in QCD

$$\frac{\partial u(\tau, \xi)}{\partial \tau} = \int_0^1 \frac{u(\tau, \eta \xi) / \eta - u(\tau, \xi)}{1 - \eta} \, d\eta + \int_0^1 \frac{u(\tau, \xi / \eta) - u(\tau, \xi)}{1 - \eta} \, d\eta$$  (1.1)

where the unknown function $u(\tau, \xi)$ must vanish at $\xi = 0$ to ensure the convergence of the integrals involved. If we put $u(\xi) = \xi \psi(\xi)$ (boundary conditions are then taken into account if $\psi$ is bounded or at least does not grow too rapidly at $\xi \to 0$)

$$\frac{\partial \psi(\tau, \xi)}{\partial \tau} \equiv (K\psi)(\tau, \xi) = \int_0^2 \frac{d\eta}{|\xi - \eta|} \left(\psi(\tau, \eta) - \min(1, \xi / \eta) \psi(\tau, \xi)\right)$$  (1.2)

I shall refer to $K$ as the mm operator. We can easily discretize $K$ on a lattice $\xi_n = na, a = 2/(N + 1)$

$$(K\psi)_i = \sum_{j \neq i} \frac{\psi_j - \min(1, i/j) \psi_i}{|i - j|}.$$  (1.3)

Any trace of $a$ disappears from the discrete equation which is a sign of the scale invariance of the original equation: under $\xi \to \lambda \xi$ only the endpoint changes, hence the result is insensitive to its actual value. The spectrum can be estimated numerically. By Richardson extrapolation from dimension 32, 64, ..., 1024 one gets for the spectrum of $K$

\begin{align*}
E & = \\
2.4990 & \\
1.7993 & \\
0.9604 & \\
0.2179 & \\
-0.3663 & \\
\ldots & \ldots
\end{align*}

$K$ has a negative spectrum except for a few positive eigenvalues, the largest one dominates the evolution (all others are damped away).

Notice that if (accidentally, by mistake!), you ignore the “$\min(1, \xi / \eta)$” factor in Eq.(1.2) the spectrum comes out very simple and, surprisingly enough, independent from $N$ to all available figures:

\begin{align*}
N & = 32 & 64 & 128 & 256 \\
-0.0000 & -0.0000 & -0.0000 & -0.0000 \\
2.0000 & 2.0000 & 2.0000 & 2.0000 \\
3.0000 & 3.0000 & 3.0000 & 3.0000 \\
3.6667 & 3.6667 & 3.6667 & 3.6667 \\
4.1667 & 4.1667 & 4.1667 & 4.1667 \\
4.5667 & 4.5667 & 4.5667 & 4.5667 \\
4.9000 & 4.9000 & 4.9000 & 4.9000 \\
5.1857 & 5.1857 & 5.1857 & 5.1857 \\
5.4357 & 5.4357 & 5.4357 & 5.4357
\end{align*}
What is the secret behind these numbers? Taking the differences we get

\[
\begin{align*}
2.0000 \\
1.0000 \\
0.6667 \\
0.5000 \\
0.4000 \\
0.3333 \\
0.2857 \\
0.2500 \\
\end{align*}
\]

an easily recognizable sequence. Indeed the eigenvalues are given precisely by twice the “harmonic numbers” \( h_n = \sum_{j=1}^{n} j^{-1} \) \( n > 0 \) and \( h_0 \equiv 0 \). This fact is actually an exact property of the modified integral equation, both in its discretized form and on the continuum (a result which goes back to the sixties [3], see Appendix), the eigenvectors being Tchebyshev discrete polynomials [4, 5] which converge to Legendre polynomials in the limit \( N \rightarrow \infty \).

2. Perturbation theory

Following the hint of the previous Section, let us represent \( K \) as the sum of two terms and treat the problem by perturbation theory.

\[
(K \psi)(\xi) = (K_0 \psi)(\xi) - \log(\xi) \psi(\xi) \tag{2.1}
\]

where

\[
(K_0 \psi)(\xi) = \int_{0}^{1} d\eta \frac{\psi(\eta) - \psi(\xi)}{|\xi - \eta|} \tag{2.2}
\]

\( K_0 \) is exactly diagonalizable, with eigenfunctions the Legendre polynomials \( P_n(2\xi - 1) \) and eigenvalues proportional to the harmonic numbers \( h_n = \sum_{j=1}^{n} j^{-1} \) (see Appendix A). Second order perturbation theory gives for the ground state \( E_0 \approx 1.44754 \) hence convergence appears to be rather slow. The usual methods to get high order coefficients are not applicable here, since the matrix \( \langle P_n | \log(\xi) | P_m \rangle \) is full.

One can do better with a purely numerical approach as we discuss in the next section (the coefficients, we shall see, decrease only as \( 1/n \log(n) \), which would require high orders in p.t. to get a meaningful result).

3. Evolution

I recived an old program which was used to study the renormalization group equation of the non–linear sigma model (the “sausage” [6, 7, 8]). The equation is now rather popular in the mathematical literature as the Ricci flow. The idea is to split the evolution of

\[
\frac{\partial \psi(\Delta, \xi)}{\partial \Delta} = K \psi(\Delta, \xi) \tag{3.1}
\]
into two steps

\[ \psi_{\text{tmp}}(\xi) = \psi(\Delta, \xi) + \tau K_0 \psi(\Delta, \xi) \]
\[ \psi(\Delta + \tau, \xi) = \psi_{\text{tmp}}(\xi) - \tau \log(\xi) \psi(\Delta, \xi) \]  

(3.2)

The first step is accomplished by going to the representation in terms of Legendre polynomials (\( \psi = \sum \psi_n P_n(2\xi - 1) \)) where \( K_0 \) is diagonal. Coming back to the \( \xi \)-representation one executes the second step. The program is implemented in \texttt{matlab}.

![Figure 1. Evolution from \( \xi_0 = 1 \)](image)

\textit{En passant} one can study the spectrum of \( K \) within the same program. We get the result of Tab\( ^3 \) where the last line is obtained by extrapolating in the variable \( n^{-1/4} \), which appears at first sight as an approximate scaling law (but see later on). This value should be compared to the approximate saddle point value \( 4 \ln 2 \approx 2.77 \). The strong dependence on the grid size is not surprising, since we have to deal with a singular scale invariant integral operator. The similar operator considered by Tuck [9] is \textit{not} scale invariant and its cutoff dependence is much flatter (i.e. better!).
Due to the very slow convergence toward $N \to \infty$ it is desirable to be able to calculate the spectrum with a high number of collocation points. This is totally unfeasible with the direct method. The calculation with $n = 4096$ required a work space of 1/2 GByte and going further was not possible on available workstations. The way out is to apply some sparse matrix computational tool which should be able to save memory and time. It was shown by Alpert and Rokhlin [10] that it is possible to transform from a Legendre expansion $\sum_{n \leq N} c_n P_n(x)$ to a Tchebyshev expansion $\sum_{n \leq N} \tilde{c}_n T_n(x)$ in $O(N)$ time, even if the amount of memory required may be rather large (at least 200 $N$ words). Since Tchebyshev polynomials of the first kind are just trigonometric functions in disguise, the Legendre transform is reduced to a combination of Alpert-Rokhlin’s transform (ART) and cosine-Fourier-transform. Using Alpert’s implementation of ART combined with FFTW in mode REDFT10/01 (see Ref.[11]) we realized a code essentially equivalent to the previous one but allowing for high dimensional matrix representation of the operator. The ground state has been computed for $N = 2^k, k = 6, 7, \ldots, 18$ giving the result of Tab.2. The difference from the previous calculation is due to a different choice of discretization grid (Gaussian integration points, i.e. the roots of $P_N(x)$, in the former case, Tchebyshev points, uniformly spaced in $\cos(x)$, in the latter). Notice that the results of the fast method anticipate those of the direct method, that is the “fast” result at $N$ is close to the “direct” result at $2N$. In a sense the formal dimension of the real FFTW ($2N$) is the “true” dimension.

For the technically-oriented reader we report the approximate timings of the two algorithms in Appendix B.

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Table 1. $K$ ground state by the direct Legendre transform.

| $N$  | DLT |
|------|-----|
| 32   | 2.030 |
| 64   | 2.144 |
| 128  | 2.235 |
| 256  | 2.308 |
| 512  | 2.368 |
| 1024 | 2.417 |
| 2048 | 2.457 |
| $\infty$ | 2.66 |

4. ALPERT-ROKHLIN’S FAST LEGENDRE TRANSFORM

2B. Alpert very kindly provided us with his Fortran code.

3http://www.fftw.org/#documentation
The extrapolation at $N \to \infty$, assuming a power law scaling as before, seems consistent, giving 2.6733 and 2.6692 (linear and quadratic fit respectively) with the first method, 2.6661 and 2.6704 with the second. We would conclude that the saddle point estimate $4 \log(2)$ is correct within 4%.

| log$_2 N$ | DLT   | ART   |
|-----------|-------|-------|
| 5         | 2.0246| -     |
| 6         | 2.1416| 2.2436|
| 7         | 2.2339| 2.3164|
| 8         | 2.3076| 2.3751|
| 9         | 2.3674| 2.4232|
| 10        | 2.4165| 2.4631|
| 11        | 2.4572| 2.4966|
| 12        | 2.4922| 2.5249|
| 13        | -     | 2.5491|
| 14        | -     | 2.5700|
| 15        | -     | 2.5880|
| 16        | -     | 2.6038|
| 17        | -     | 2.6176|
| 18        | -     | 2.6298|

Table 2. The ground state from Direct Legendre Transform (DLT) and from the fast algorithm (ART+FFTW)

A totally different result is however hiding behind these figures. It must be realized that the crucial point is to identify the correct $N$ dependence, since this is going to make a big difference in the extrapolation at $N \to \infty$. A careful analysis shows that a logarithmic scaling law is much more accurate than a power law. Looking for a fit of the kind $E(N) \approx E(\infty) - C_1/\log(N/\Lambda) - C_2/(\log(N/\Lambda))^2$ we get a very good interpolation (the deviation is uniformly less than 1 part in $10^4$) and the value at $N = \infty$ is compatible with $4\log(2)$ (within the same accuracy). According to this idea we should conclude that, surprisingly enough, the saddle point value is actually exact (see Figg. 3,4). In the case studied by Tuck we find a much steeper scaling law of the kind

$$E(N) = E_1(\infty) + CN^{-2}\log(N)^{-1}$$

as shown in Fig. 5.

It has been realized that the picture is simply due to the different character of the spectrum: continuous for MM and discrete for Tuck’s operators. This fact is made absolutely transparent by adopting a different
representation of the operator $K$:

\[
(K \phi)(x) = (K_0 \phi)(x) + 2 \log(1 + e^{-x/2}) \phi(x) - 4 \log 2 \phi(x)
\]

\[
(K_0 \phi)(x) \equiv \int_0^\infty \frac{\phi(x) - \phi(y)}{2 \sinh \left( \frac{1}{2} (x-y) \right)} \, dy .
\] (4.1)

The integral operator $K_0$ is almost local and it is not very different from a kinetic term. If we consider a wave-function with support in a region far from the origin, the operator reduces to

\[
K_0\phi(x) \approx \int_{-\infty}^{\infty} \frac{\phi(x) - \phi(y)}{2 \sinh \left( \frac{1}{2} (x-y) \right)} \, dy
\] (4.2)

which is diagonal in Fourier space with eigenvalue $-\chi(p)$, the subtracted Lipatov function, explicitly given by $\chi(p) = 2(\psi(1) - \Re(\psi(\frac{1}{2} + ip))) - 4 \log 2$, $\psi$ being the logarithmic derivative of the $\Gamma$ function. $K_0$ is well-known, not necessarily in this form, as the BFKL operator [12].

It has been realized that the representation introduced here is also more convenient to allow a numerical study of the evolution in the case of MM, while this is not the case for Tuck’s equation. Essentially the dominant
Figure 3. Continuum limit with the logarithmic scaling law.

Figure 4. Extrapolation in log-scale shows the emergence of a continuous spectrum

eigenvalue $4 \log 2$ is already built-in, while in the representation of Sec. 3 this value can only be obtained by extrapolating at very large matrix dimensions (see Tab. 4).
To make the difference between MM and BFKL operators more explicit, it would be desirable to be able to apply the method of images (which is usually employed with local differential operators) to get rid of the boundary. However no simple boundary condition seems to be appropriate. Actually by solving the eigenvalue equation by standard linear algorithms (matlab’s eig routine) one finds that the eigenvectors are essentially shifted trigonometric functions, i.e., far from the boundary, $\phi_k(x) \approx \sin(kx + \delta(k))$. By switching $V(x)$ on and off, we can easily check that the behavior at $x = 0$ is strongly influenced by $V(x)$.

The phase shift $\delta(k)$ is particularly interesting. For example, the asymptotic behaviour of $\phi(\Delta, x)$ at large $\Delta$ is strongly influenced by it. This fact is well-known in the theory of potential scattering in quantum mechanics. While the general setup here is quite different, nonetheless there are remarkable analogies which give useful guidelines. For example the vanishing of $\delta$ at $k = 0$ is a signal of the absence of bound states (Levinson’s theorem), were we able to extend the theorem to this context. Details can be found in [2].

The “unbounded” representation helps in understanding what really goes wrong with the initial approach based on the Legendre basis. Introducing
a finite box of side $L$ ($0 \leq x \leq L$) the energy spectrum is discretized and at low energy it is given by $\propto (n\pi/L)^2$. In the Legendre expansion of the previous section all Gaussian points are confined to $x \lesssim L = 2 \log(N)$. This fact explains the logarithmic scaling law depicted in Fig. 3. Also, since a good description of the evolution at large $\tau$ requires $L \gg 100$, this cannot be explored through the Legendre expansion.

5. Further developments

Recent developments pushed our understanding of the problem to a higher level. A precise characterization of the time–dependent solution of MM equation was developed by a perturbative technique which can be pushed to all orders and allows for a full resummation \cite{2}. An exact form for the phase shift and the continuum eigenfunctions has been derived. A rigorous proof on purely algebraic grounds, thus avoiding a delicate problem of resummation, has been later found, thanks to an idea of V. A. Fateev \cite{13}.

There exists another representation of the integral operator which avoids the presence of a boundary. Thanks to the intrinsic scale invariance, the equation can be remapped on the whole of $\mathbb{R}$ by setting $\exp(x) = \exp(x') + 1$, which leaves the kernel invariant and only modifies the potential. In this representation we may apply a spectral algorithm to the evolution equation simply based on Fourier transform, more economic than the combined ART+FFTW. This will be left as a homework.

6. Conclusions and outlook

The integral equation introduced by Marchesini and Mueller is deeply related to another problem in mathematical physics studied by E. Tuck fourty years ago. The connection to Tuck’s equation was used to analyze MM operator’s spectral properties by an efficient (sparse) matrix computation, based on Alpert-Rokhlin transform, FFTW and ARPACK. This analysis suggests that the spectrum is continuous with endpoint $4 \log 2$. A second representation of the integral operator makes the spectral properties more transparent and lends itself to an easier algorithmic implementation which allows to evaluate the evolution at large $\Delta$.

The application of ART to the renormalization group equation for $O(3)$ $\sigma$-model may be useful to achieve greater accuracy than allowed from the direct transform \cite{8}. More generally, the application of a full group theoretical transform without axial symmetry, will make it possible to explore the $O(3)$ Ricci flow in full detail.

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Askey for pointing out to us Tuck’s relevant paper and E. O. Tuck for very valuable correspondence. S. Shaw’s header files, available on the WEB, proved to be very helpful for an ARPACK beginner. This work would have been impossible without the searching capabilities of Google. But, above all, I’m indebted to my dear friends G. Marchesini and V. A. Fateev, for constantly providing new ideas, suggestions and insight.

**Appendix A**

Here is a proof for the discrete form of Tuck’s operator. For the original problem see [3][13].

Let

$$\left( K_0^{(N)} v \right)_i = \sum_{0 \leq j \leq N} \frac{v_j - v_i}{|i - j|}.$$  

(6.1)

Let’s apply the matrix $K_0^{(N)}$ to the vector $v^{(\ell)}_i = i^\ell$. We have

$$\left( K_0^{(N)} v^{(\ell)} \right)_i = \sum_{0 \leq j \leq N} \frac{j^\ell - i^\ell}{|i - j|}$$

$$= \left( - \sum_{j=0}^{i-1} + \sum_{j=i+1}^{N} \right) \sum_{k=0}^{\ell-1} i^{\ell-k-1} j^k$$

$$= \sum_{k=0}^{\ell-1} i^{\ell-k-1} \left( - \frac{2i^{k+1}}{k+1} + O(i^k) \right)$$

$$= -2h_0 v^{(\ell)}_i + \sum_{n<\ell} c_n v^{(n)}_i \hspace{1cm} (6.2)$$

where we used the Euler-MacLaurin summation formula for $\sum j^k$, and the constants $\{c_n\}$ are calculable but unnecessary. This proves that $K^{(N)} v^{(\ell)}$ is contained in the linear span of $[v^{(0)}, v^{(1)}, ..., v^{(\ell)}]$. Since $K_0(N)$ is symmetric, it is diagonalable, its eigenvectors are orthogonal, hence they are given by the orthogonal discrete polynomials with respect to the uniform weight on the set $[0, 1, 2, ..., N]$. The eigenvalues can be read off the coefficient of $v^{(\ell)}$ in the expansion of $K_0^{(N)} v^{(\ell)}$. The explicit form of the eigenvectors is given by Tchebyshev polynomials of a discrete variable [14].

**Appendix B**

We give here some technical details about the algorithms which we have applied in the paper. The direct method consists in building the table of Legendre polynomials $\{P_n(x_j^{[N]})\}, n = 0, 1, \ldots, N-1$ at the Gauss points, i.e. at the roots of $P_N(x)$. The technique, exploiting the recurrence relation of orthogonal polynomials, is due to Golub and Welsch (see Ref. [15]). To find the spectrum of $K$ we simply define $K_0$ to be diagonal in the basis $\{P_n(x)\}$ with eigenvalues $-2h_0$. The matlab routine “eig” is then invoked. The singularity of the logarithm at the boundary is avoided because the zeros of
the polynomials are all internal at the interval \([-1, 1]\). The matrix representation of the free part \(K_0\) is exact, since the Gauss quadrature formula is exact on polynomials of low degree. In finite precision arithmetic \(K_0\) is affected by the accumulation of truncation errors, yielding an error of order \(10^{-13}\) on its spectrum, which is rather irrelevant. The method is presently feasible for dimension less than 4000 and it has the advantage that \(N\) can be any integer, not necessarily a power of 2.

The method based on ART makes use of the expansion on Tchebyshev’s polynomials of the first kind \(T_n(x) = \cos(n \arccos(x))\). Again the Gauss points are interior at the interval and the singularity is avoided. The real DFT of kind \(REDFT10\) precisely makes use of this grid of points. Even if the Gauss-Tchebyshev integration is exact for polynomials of low degree, still a problem arises, namely that \(K_0\) is a symmetric operator with respect to the Lebesgue measure whereas Tchebyshev’s polynomials are orthogonal with respect to a different measure. It turns out that to restore symmetry we have to deal with \(\tilde{K}_0 = (1 - x)^{1/4} K_0 (1 - x)^{-1/4}\), hence we are outside any polynomial subspace and this introduces a systematic error making \(\tilde{K}_0\) only approximately symmetric. This has been checked after realizing that the spectrum of \(K_0\) considered as a symmetric operator contains substantial error, up to 10%. The strategy we adopt is therefore to relax the symmetry condition on \(\tilde{K}_0\) and compute the spectrum with a version of the Arnoldi algorithm which allows to deal with non-symmetric operators provided by ARPACK\cite{16}. The combination ART+FFTW+ARPACK (this latter offers the routine znaupd which applies to general non–symmetric complex matrices) turns out to be again in the game with an accuracy on the spectrum of \(K_0\) comparable if not superior to the direct method. For example at \(N = 64\) we find

\[
E = \begin{bmatrix}
1.00047386511033e-18 \\
2.00000000000000e+00 \\
2.99999999999999e+00 \\
3.66666666666666e+00 \\
4.16666666666666e+00 \\
4.56666666666665e+00 \\
4.90000000001e+00 \\
5.18571428571429e+00 \\
\end{bmatrix};
\]

and the reader can verify by herself that the error is only at the last decimal place. A further (marginal) improvement will be achieved using the real–non-symmetric routine dnaupd; we use the complex version because it was already implemented as a C++ header by Scott Shaw.

Let us now comment upon performance. The first methods grows in time and memory rather quickly \(O(N^2)\) in memory and \(O(N^3)\) in execution time. The fast one is much less memory greedy. Notice that in the largest case
examined, $N = 2^{18}$, the program requires slightly less than half a Gigabyte of memory, half of which simply to allocate ART’s working array ($200N$ words). By contrast the direct method requires $\approx 450$ MB at $N = 4096$ and it would grow to the order of 6 TBytes at $N = 2^{18}$ while the execution would require 50 years at the present cpu speed.

Tables 3,4 report the execution times on a pentium III with clock at 1.13 GHz and on a Xeon with clock at 2.8 GHz, respectively, using Matlab v.6.5. Execution times for the “fast” algorithm are inclusive of the preconditioning (we select the initial vector by executing a number of Trotter steps). As it is rather clear from the table, the execution time grows as expected as $O(N \log(N))$, with some expected deviations when the system switches to virtual memory.

Figure 6. Execution times for the Direct Legendre transform and Alpert-Rokhlin transform.

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Table 3. Timings (sec) (DLT) direct method and for the fast algorithm (ART+FFTW); Pentium-III @ 1.13 GHz

| $\log_2 N$ | DLT | ART |
|------------|-----|-----|
| 5          | 0.01| -   |
| 6          | 0.04| 0.08|
| 7          | 0.29| 0.10|
| 8          | 2.31| 0.15|
| 9          | 33.6| 0.4 |
| 10         | 271.| 0.9 |
| 11         | -   | 2.0 |
| 12         | -   | 4.7 |
| 13         | -   | 9.6 |
| 14         | -   | 22  |
| 15         | -   | 63  |
| 16         | -   | 158 |

Table 4. Timings (sec) (DLT) direct method and for the fast algorithm (ART+FFTW); Xeon @ 2.8 GHz

| $\log_2 N$ | DLT | ART |
|------------|-----|-----|
| 5          | 0.004| -   |
| 6          | 0.02 | 0.02|
| 7          | 0.11 | 0.04|
| 8          | 0.93 | 0.07|
| 9          | 11.44| 0.17|
| 10         | 98.6 | 0.37|
| 11         | 970. | 0.76|
| 12         | -    | 1.75|
| 13         | -    | 3.64|
| 14         | -    | 7.84|
| 15         | -    | 18.4|
| 16         | -    | 43.4|
| 17         | -    | 129.|
| 18         | -    | 219.|

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