A Density Matrix Renormalization Group Approach to an Asymptotically Free Model with Bound States

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We apply the DMRG method to the 2 dimensional delta function potential which is a simple quantum mechanical model with asymptotic freedom and formation of bound states. The system block and the environment block of the DMRG contain the low energy and high energy degrees of freedom, respectively. The ground state energy and the lowest excited states are obtained with an unprecedent accuracy. We compare the DMRG method with the Similarity RG method and propose its generalization to field theoretical models in high energy physics.

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A hallmark of an asymptotically free theory such as QCD is that it contains many degrees of freedom, with very different energy scales, which are coupled by the interaction Hamiltonian. Perturbative methods are valid for short distance physics but they fail for small momentum transfers or for energy scales where the bound states are formed. The existence of multiple energy scales suggests that the Renormalization Group approach is the correct strategy to attack these non perturbative problems. In recent years there has been several proposals to extract effective low energy Hamiltonians using RG methods. Of particular interest is the light-front Hamiltonian approach advocated in references [1,2] which uses a similarity RG method (SRG) [3,4]. In this method the RG flow is given by an unitary transformation which diagonalizes the Hamiltonian by successive elimination of the off-diagonal matrix elements. The SRG-cutoff can be seen as the width of the band which
contains the non vanishing off-diagonal matrix elements of the Hamiltonian. At the end of the SRG flow the width is zero and the corresponding Hamiltonian contains it its diagonal all the eigenvalues of the original one.

In this letter we shall propose an alternative RG approach to study asymptotically free models using the Density Matrix Renormalization Group (DMRG). We shall also show the relations and differences between the DMRG and the SRG methods. The DMRG was proposed by White in 1992 to solve the problems of the old real space RG methods encountered in the 70’s, which led in those days to their abandon in favour of Montecarlo techniques [5]. The DMRG has by now become a standard numerical RG method applied to many body problems in Condensed Matter and other branches of Physics (see references [6,7] for reviews). It is thus challenging to test how the DMRG handles the subtle dynamics of asymptotically free theories. To our knowledge this is the first paper devoted to the subject. For this reason we have choosen as a theoretical lab a simple model possesing the essential properties of asymptotic freedom and formation of bound states, which are shared by realistic theories like QCD.

The natural candidate for such a simple model is provided by a 2d quantum mechanical particle subject to a delta function potential [8]. The solution of the 2d delta function Schrödinger equation requires a regularization and renormalization schemes as in an ordinary quantum field theory. We shall use for our purposes the lattice regularization introduced by Glazek and Wilson in their SRG study of the problem [9,10]. These authors formulated the problem in momentum space where the states are labelled by an integer \( n \) that ranges between an infrared cutoff \( M \) and an ultraviolet cutoff \( N \) (i.e. \( M \leq n \leq N \)). The kinetic energy \( E_n \) of the state \( n \) increases exponentially as \( E_n = b^{2n} \), where \( b \) is an arbitrary constant greater than one. For numerical computations we shall take the value \( b = \sqrt{2} \) as in references [9,10]. The interaction Hamiltonian between the states \( n \) and \( m \) is given by \(-g\sqrt{E_nE_m}\), where \( g \) is the coupling constant of the problem. The discrete lattice Hamiltonian \( H \) is defined by the matrix elements
\[ H_{nm} = \delta_{n,m} b^{2n} - g b^{n+m}, \quad M \leq n, m \leq N \]  

An overall shift of the levels by a constant term, i.e. \( n \to n + n_0 \), implies that \( H_{nm} \) scales with the factor \( b^{2n_0} \). This is a discrete version of scale invariance, which is broken by the infrared and ultraviolet cutoffs \( M \) and \( N \). The latter symmetry implies that all the scales contribute to the observables. As an illustration of this fact let us calculate the energy of the trial wave function \( \phi(n) = cb^{M-n} \), which yields a good approximation to the exact ground state (GS) for large values of \( n \) (\( c \) is a normalization constant). A simple computation yields [9]

\[ \langle H \rangle = c^2 b^{2M} [(N - M + 1) - g(N - M + 1)^2] \]  

This result means that all the scales contribute on equal footing to the GS energy, which makes very hard an accurate determination of its value by methods other than the exact one. The SRG applied to the case \( M = -21, N = 16 \) and \( G = 0.06 \) [9,10] yields a GS energy with an error of 10%, which in any case is a remarkable result taken into account the 10 orders of magnitude between the infrared and ultraviolet cutoffs. For the latter choice of parameters the Hamiltonian (1) has one bound state with energy equal to \(-1\) and 37 “scattering” states with positive energy.

The first step in the DMRG method is the partition of the system in two pieces called the system block and the environment block [5]. The correct choice of these blocks is dictated by the physics of the problem. In our case we shall choose the system block \( B^L_\ell \) to be given by the low energy levels \( n \) which lie between the infrared cutoff \( M \) and the scale \( \ell \) (i.e. \( M \leq n \leq \ell \)), while the environment block \( B^H_\ell \) will contain the high energy levels \( n \) between the ultraviolet cutoff \( N \) and the scale \( \ell \) (i.e. \( \ell \leq n \leq N \)). The whole system, with energy levels ranging from \( M \) to \( N \), is obtained as the “superblock” \( B^L_\ell \bullet \circ B^H_{\ell+3} \), where \( \bullet \) and \( \circ \) are the \( n = \ell + 1 \) and \( n = \ell + 2 \) energy levels respectively (see fig.1).
The parameter $\ell$ varies from $M$ to $N-3$ and it labels the DMRG flow. Let us suppose we want to find the GS of the whole system. We shall choose a trial GS wave function $\psi_\ell(n)$ as follows,

$$\psi_\ell(n) = \begin{cases} 
  a_1 L_\ell(n) & M \leq n \leq \ell \\
  a_2 & n = \ell + 1 \\
  a_3 & n = \ell + 2 \\
  a_4 R_{\ell+3}(n) & \ell + 3 \leq n \leq N
\end{cases}$$

(3)

where $L_\ell$ (resp. $R_{\ell+3}$) is a normalized vector which describes the contribution of the low (resp. high) energy block $B^L_\ell$ (resp. $B^H_{\ell+3}$) to the GS of the superblock $B^L_\ell \circ B^H_{\ell+3}$. The ansatz (3) is the momentum space version of the real space DMRG applied by White to study a free particle in a box [6,7]. Our approach is close in spirit to the momentum space DMRG method proposed by Xiang [11]. The energy of the state (3) can be conveniently written as

$$\langle \psi_\ell | H | \psi_\ell \rangle = \langle a | H_{SB}(\ell) | a \rangle$$

(4)

where $| a \rangle$ is the vector $(a_1, a_2, a_3, a_4)$ and the superblock Hamiltonian $H_{SB}(\ell)$ is the $4 \times 4$ matrix given by

$$H_{SB}(\ell) = \begin{pmatrix}
  h_L & h_{L\bullet} & h_{L\circ} & h_{LH} \\
  h_{L\bullet} & h_\bullet & h_{\bullet\circ} & h_{H\bullet} \\
  h_{L\circ} & h_{\bullet\circ} & h_\circ & h_{H\circ} \\
  h_{LH} & h_{H\bullet} & h_{H\circ} & h_H
\end{pmatrix}$$

(5)

whose entries read
\[ h_L = \langle L_\ell | H | L_\ell \rangle, \quad h_H = \langle R_{\ell+3} | H | R_{\ell+3} \rangle \]

\[ h_\bullet = H_{\ell+1, \ell+1}, \quad h_o = h_{\ell+2, \ell+2} \]

\[ h_{L\bullet} = \sum_{n=M}^\ell H_{n, \ell+1} L_\ell(n), \quad h_{L_o} = \sum_{n=M}^\ell H_{n, \ell+2} L_\ell(n) \]

\[ h_{H\bullet} = \sum_{n=\ell+3}^N H_{n, \ell+1} R_{\ell+3}(n), \quad h_{LH} = \langle L_\ell | H | R_{\ell+3} \rangle \]

\[ h_{H_o} = \sum_{n=\ell+3}^N H_{n, \ell+2} R_{\ell+3}(n) \quad h_{\bullet o} = H_{\ell+2, \ell+3} \]

(6)

where \( H_{n,m} \) are the matrix elements given in eq. (1). Notice that eq.(4) takes the form of an eigenvalue problem in a reduced vector space with only 4 degrees of freedom. The GS of the superblock can be found by looking for the lowest eigenvalue \( E_1(\ell) \) of the \( 4 \times 4 \) matrix \( H_{SB} \).

The variational nature of the construction gives an upper bound of the exact GS energy. If the vectors \( L_\ell \) and \( R_{\ell+3} \) coincide with the low energy and high energy pieces of the exact GS wave function then the DMRG algorithm presented so far would reproduce the exact result. Of course this is not in general the case but nevertheless, one can actually use the DMRG algorithm to improve in successive steps the GS energy. The idea is to apply a continuity argument. Suppose we shift the scale \( \ell \) to the next high energy level, say \( \ell + 1 \). Then the new low energy vector \( L'_{\ell+1} \) will be related to the previous one \( L_\ell \) by the equation

\[ L'_{\ell+1}(n) = \begin{cases} a'_{1} L_\ell(n) & M \leq n \leq \ell \\ a'_{2} & n = \ell + 1 \end{cases} \]

(7)

where \( (a'_{1}, a'_{2}) = (a_{1}, a_{2})/\sqrt{a_{1}^2 + a_{2}^2} \) is the normalized two component vector obtained by the projection of the lowest eigenvalue of \( H_{SB}(\ell) \) into the block \( B^L_\bullet \). Similarly the energy \( h'_{L}(\ell + 1) \) associated to the latter block is given by

\[ h'_{L}(\ell + 1) = (a'_{1}, a'_{2}) \begin{pmatrix} h_{L}(\ell) & h_{L\bullet}(\ell) \\ h_{L\bullet}(\ell) & h_{\bullet}(\ell) \end{pmatrix} \begin{pmatrix} a'_{1} \\ a'_{2} \end{pmatrix} \]

(8)

The data \( L'_{\ell+1} \) and \( h'_{L}(\ell + 1) \) fully characterize the new block \( B^L_{\ell+1} \) which can be regarded as the renormalization of the block \( B^L_\bullet \). The next step is to construct the superblock \( B^L_{\ell+1} \bullet \circ B^H_{\ell+4} \) which by the same techniques leads to the construction of a new block \( B^L_{\ell+2} \) and so on. This procedure is iterated until the scale \( \ell = N - 3 \), where one reverses the
DMRG steps in order to update the high energy blocks $B^H_t$ using the low energy blocks built in the previous steps. After a few sweeps from low to high energy and viceversa the lowest eigenvalue of the superblock Hamiltonian (5) converges to a fix value which gives the DMRG estimation of the GS energy. To start out the process one has to grow up the system to its actual size. This can be done by considering superblocks of the form $B^L_{M+p} \cdot o B^H_{N-p}$ where $p = 0, \ldots, (N - M - 3)/2$. The last value of $p$ yields a system containing all the scales from $M$ to $N$. The low and high energy blocks constructed in the warm up are the starting point for the sweeping procedure explained above (see [6,7] for details). The previous algorithm has been generalized in reference [12] to find out not only the GS but the low lying excitations as well.

Let us now present our DMRG results for the case considered in references [9,10], where $M = -21, N = 16$ and $g = 0.06060600032108866$. The latter value of $g$ is choosen in such a way that the exact ground state energy of (1) is given exactly by $-1$. The DMRG algorithm presented above gives the exact ground state energy with an error of $10^{-14}$ (see table 1). For simple quantum mechanical problems, like a particle in a box or a potential, the DMRG gives GS energies with this order of precision [6,12]. In the latter examples the discrete Hamiltonians are tridiagonal matrices whose entries vary smoothly through the lattice. These features are not shared by the Hamiltonian (1) which indeed varies quite abruptly from entry to entry while having all entries non vanishing. Using the extension of the DMRG proposed in [12] we have also computed the GS and the lowest 3 excited states of the Hamiltonian (1). In table 1 we compare our DMRG results with the exact ones in terms of the relative deviation

$$\delta E_n = \frac{E_n(DMRG) - E_n(exact)}{E_n(exact)}$$

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<td>$\delta E_n$</td>
<td>$7 \times 10^{-15}$</td>
<td>$1.04 \times 10^{-7}$</td>
<td>$3.36 \times 10^{-6}$</td>
<td>$1.41 \times 10^{-6}$</td>
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Table 1. Relative error $\delta E_n$ of the four lowest eigenstates of the Hamiltonian (1).
As shown in table 1 the accuracy of the excited states energies is lower than that of the GS. This feature is peculiar to the delta function Hamiltonian and it does not arise for the quantum mechanical models studied in [12]. There are several reasons for the unprecedent accuracy of the DMRG applied to the Hamiltonian (1). Recall that the SRG method gives the GS energy with a 10% error [9,10]. First of all the DMRG gives a variational upper bound to the exact GS energy which is usually improved in every DMRG step. Secondly all the matrix elements of the whole Hamiltonian are used many times to feedback the superblock so that no information is lost. Finally, the DMRG method focus on the determination of the GS and the low lying states, while the SRG method considers all the eigenstates.

Moreover the DMRG offers the possibility to reconstruct the actual shape of the GS wave function. In fig.2 we plot the wave function in the warm up, which is rather bad, together with the one obtained after the first sweep, which converges to the exact shape. After the third sweep the DMRG wave function is indistinguishable from the exact one. All these results show that the DMRG gives in fact the exact bound state of the discrete delta function potential within the machine precision.

FIG. 2. DMRG v.s. exact wave function.

It is interesting to investigate the nature of the DMRG flow as compared with the one of
the similarity RG method. In the SRG the effective Hamiltonian \( H(s) \) evolves as a function of \( s \) according to the Wegner equation \([4]\),

\[
\frac{dH(s)}{ds} = [[H_d(s), H(s)], H(s)]
\]

(10)

where \( H_d(s) \) is the diagonal part of \( H(s) \). The initial condition of eq.(10) is \( H(0) = H \), where \( H \) is the original Hamiltonian of the problem. The parameter \( s \) ranges from 0 to \( \infty \) and it can be identified with the inverse square of the energy width \( \lambda \), i.e. \( s = 1/\lambda^2 \). Eq. (10) implies that \( H(s) \) is related to \( H \) by an unitary transformation and therefore they share their eigenvalues. When \( s \) increases, the off diagonal matrix elements of \( H(s) \), located at distances greater than the width \( \lambda = 1/\sqrt{s} \), become very small. When \( s = \infty \) the effective Hamiltonian \( H(\infty) \) is diagonal and all its entries coincide with the eigenvalues of \( H \). The numerical integration of eq.(10) requires of course to follow the evolution of all the entries of \( H \). One would like instead to project the effective Hamiltonians to smaller matrices in order to reproduce the bound state eigenvalue. This idea has indeed been pursued in [10] with results within an accuracy of order 10 to 20%. The DMRG method gives a solution to this problem yielding the exact bound state energy. Hence we may wonder if the DMRG gives an exact realization of the SRG ideas. To this end we have studied the RG flow of the eigenvalues \( E_i(\ell)(i = 1, \ldots, 4) \) of the superblock Hamiltonian (5). In fig.3 we plot the lowest eigenvalue \( E_1 \), together with the remaining ones scaled down by a factor \( b^{2\ell} \). We can clearly see from fig.3 that \( E_1 \) stays constant through all the DMRG steps while \( E_i(i = 2, 3, 4) \) vary with the energy scale \( b^{2\ell} \) with some deviations depending on the energy region. The plateaus correspond to low energy regions while the oscillations and bumps occur for intermediate and high energies. To a first order approximation, which is almost exact for the plateaus, the superblock Hamiltonian (5) can be written as

\[
H_{SB}(\ell) = O_\ell \begin{pmatrix}
E_1 & 0 & 0 & 0 \\
0 & E_2'b^{2\ell} & 0 & 0 \\
0 & 0 & E_3'b^{2\ell} & 0 \\
0 & 0 & 0 & E_4'b^{2\ell}
\end{pmatrix} O_\ell^\dagger
\]

(11)
where \( O_\ell \) is a unitary matrix. Using eq.(11) one can show that the superblock Hamiltonians satisfy the following second order recursion relation,

\[
H_{SB}(\ell) = \frac{1}{b+b^{-1}} \left( b^{-1} U_\ell H_{SB}(\ell + 1) U_\ell^\dagger + b U_{\ell-1}^\dagger H_{SB}(\ell - 1) U_{\ell-1} \right)
\]

where \( U_\ell = O_\ell O_{\ell+1}^\dagger \). The continuum limit of eq.(12) gives the flow equations

\[
H_1 \equiv \frac{dH_{SB}}{d\ell} - [\eta, H_{SB}], \quad \frac{dH_1}{d\ell} = [\eta, H_1]
\]

where \( \eta = \frac{dO_\ell}{d\ell} O_\ell^\dagger \). Eq.(13) is a second order differential equation which is to be compared with the first order equation eq.(10). The DMRG flow is a sort of similarity transformation with some eigenvalues running with the scale. Using the standard RG terminology the lowest eigenvalue \( E_1 \) can be associated with a marginal operator while the eigenvalues \( E_i \) for \( i = 2, 3, 4 \) are associated with infrared irrelevant operators which vanish at the fixed point Hamiltonian \( H_{SB}(\ell = M) \). Indeed all the entries of \( H_{SB}(\ell = M) \) are very small except for the entry \( h_H = -0.999 \) whose value is close to the bound state energy. These results suggest that the exactness of the DMRG method is due to a careful treatment of the irrelevants operators, which in other RG methods are difficult to control in general.

From a conceptual point of view the DMRG offers a new way of thinking about cutoffs and RG flows in high energy physics. Traditional cutoffs remove high energy states while the lowering of the cutoff produces effective operators for lower energies [13]. In the Lagrangian formulation this strategy can be implemented perturbatively without much difficulty. However in the Hamiltonian formulation it gives rise to small denominators problems involving energy differences between the states kept and the states truncated in the RG process [14,9]. This latter problems do not arise in the DMRG truncation for it uses a non perturbative self-consistent algorithm to find the best choice of the effective Hilbert spaces and Hamiltonians.

The next step in the application of the DMRG to high energy physics is of course to consider field theoretical models with asymptotic freedom and bound states. The main ideas presented in this letter can in principle be generalized to this type of models.
FIG. 3. Plot of the rescaled superblock eigenvalues $E_i/b^{2\ell}$ ($i = 2, 3, 4$) as a function of the DMRG step L from sweep 2 to 4. We also plot the GS energy $E_1$ which stays constant. The top of the bumps for $i = 2, 3$ occur for $\ell = 13$ while the plateaus appear from $\ell = -21$ to $\ell \sim -5$. The deeps in $i = 4$ occur for $\ell = -21$.

Specifically, the breaking of the system into low energy and high energy blocks which are constantly updated through the DMRG process. On the other hand, the DMRG does not have the sign problems that emerge in the Montecarlo methods used in Lattice Gauge Theories. The remarkable accuracy achieved by the DMRG for the 2d delta function potential is very encouraging.

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