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Entanglement entropy and the simulation of quantum mechanics

José I Latorre

Dept. d'Estructura i Constituents de la Matèria, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain

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Abstract
The relation between entanglement entropy and the computational difficulty of classically simulating quantum mechanics is briefly reviewed. Matrix product states are proven to provide an efficient representation of one-dimensional quantum systems. Further applications of the techniques based on matrix product states, some of their spin-off and their recent generalizations to scale invariant theories and higher dimension systems are also discussed.

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1. Entanglement entropy as a measure of quantum correlations

A common misconception states that, in general, large quantum-mechanical systems cannot be efficiently described by classical means. This prejudice can be illustrated with the simple example of a system composed of n two-level systems or qubits. The Hilbert space of this system corresponds to the direct product $C^{2\otimes n}$ and an arbitrary state can be expressed in the natural (also called computational) basis

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_n=0,1} c^{i_1 i_2,\ldots,i_n} |i_1, i_2, \ldots, i_n\rangle. \tag{1}$$

In order to fully specify an arbitrary state, it seems necessary to provide all the $c^{i_1\cdots i_n}$ coefficients, that is, 2^n complex numbers (minus a global phase and a normalization constraint that we can ignore for the counting of the scaling of needed resources). As n grows, the classical representation of a quantum state requires exponential resources. Furthermore, the processing of the state, e.g. the computation of its time evolution, and the computation of observables also requires exponentially many operations.

The exponential effort needed to deal with quantum mechanics can also be advocated using an argument based on entropy. The precise statement says that an average random state in the Hilbert space is known to carry maximal von Neumann entropy. Let us describe in more

detail this point. Consider a partition of the original state into two parties, A and B. If party A ignores party B, the description of its subsystem is based on the reduced density matrix

$$\rho_A = \mathrm{tr}_B |\psi\rangle\langle\psi|. \tag{2}$$

The description that party A is making of the system ignores quantum correlations between A and B. If A were to suddenly discover that it was correlated to B a surprise would occur. The amount of that surprise is quantified by the von Neumann entropy

$$S(\rho_A) = -\mathrm{tr}(\rho_A \log \rho_A). \tag{3}$$

It is well known that the entropy attached to party A ignoring party B equals the reciprocal one, that is, the entropy attached to party B when ignoring party A. This is a consequence of the Schmidt decomposition

$$|\psi\rangle = \sum_{a=1}^{\chi=\min(\dim H_A, \dim H_B)} \lambda_a |\xi_a\rangle_A |\varphi_a\rangle_B \tag{4}$$

with real $\lambda_a \geqslant 0$, $\sum_a \lambda_a^2 = 1$, and $|\xi_a\rangle_A$ and $|\varphi_a\rangle_B$ being new orthonormal basis for parties A and B. The magic of this decomposition is that it provides a basis such that any state is written with a minimum number of coefficients χ, called the Schmidt number, and the corresponding changes $|\xi_a\rangle = \Gamma_a^i |i\rangle_A$ and $|\varphi_a\rangle = \Gamma_a'^j |j\rangle_B$ to the computational basis. A prominent example is the economical description of a product state since $\chi = 1$ and only the changes of basis are to be retained. By the same token, the Schmidt number χ can be understood as a measure of entanglement. A more sophisticated measure of entanglement is the von Neumann entropy which reads

$$S(\rho_A) = S(\rho_B) = -\sum_{a=1}^{\chi} \lambda_a \log \lambda_a. \tag{5}$$

We can now come back to the alleged misconception on the exponential difficulty to deal with any quantum system. The argument says that the totally random state made with n spins, $n = n_A + n_B$, is such that all the eigenvalues in the reduced density matrix ρ_A are identical and equal to 2^{-n_A}. Thus, $S(\rho_A) = n_A$, which is the maximum possible scaling of the entropy for that subsystem. Thus, the entanglement entropy scales with the volume of the subsystem which corresponds to maximal entropy and quantum correlations pervade the system.

2. Refutation of the need for exponential resources

The argument stating that the representation of any n-body quantum system needs exponential (in n) resources does not apply as a general rule. The reason that invalidates the general argument is a combination of two facts:

- It is not necessary to represent a given state in the original computational basis. This should come as no surprise since we are used to compressing information. Consider a piece of literature. To keep all the information about the text, it is not necessary to write all its characters. We can define a clever conversion table and use shorter characters for frequent words. This procedure can be made close to optimal for arbitrary and long sequences using entropic compression codes (as the Lempel–Ziv based *gzip* [1]). We shall later argue that we already have techniques to represent and manipulate quantum systems which are far better than the naive computational basis. In this sense, we do know compression methods for quantum mechanics.

- In general, typical physical states are not random. Local Hamiltonians produce interactions between neighbouring particles. The quantum correlations that pervade the system are far less than the maximum possible. In other words, typical physical states do not carry maximal entropy.

In recent years, some intense research has addressed the problem of finding an optimal classical representation for relevant quantum systems. Depending on the problem, three main ideas are currently pursued. Whenever possible, exact simulations are carried out. In practice, this is possible only for systems of few particles as shown by the work done on cold gases of few particles. A second avenue of work are Monte Carlo simulations. This is, for instance, the standard technique to investigate quantum field theories regularized on a lattice. The method allows for computations of correlators but it is not appropriate for the detailed simulation of time evolution of quantum systems, neither to get a good grasp on specific wavefunctions as e.g. the ground state. Furthermore, the lattice approach faces the so-called sign problem. A third idea to represent quantum systems looks for a specific basis where correlations are well-represented, which we shall now address.

3. Matrix product sates

Let us consider a n-particle quantum product state

$$\psi = |\xi_1\rangle \otimes \cdots \otimes |\xi_n\rangle = (\alpha_1|0\rangle + \beta_1|0\rangle) \otimes \cdots \otimes (\alpha_n|0\rangle + \beta_n|0\rangle) \tag{6}$$

where α_i can be chosen real and $|\alpha_i|^2 + |\beta_i|^2 = 1$. Note that this state is represented with $2n$ real numbers, far less than the naive exponential counting of 2^n complex numbers. The reason for this saving can be traced to the fact that all bi-partitions of the system carry zero entropy. There is no surprise in adding uncorrelated new particles to any subsystem.

Can this idea be pushed further? Indeed, it is possible to find an economical basis to retain all the correlations in the system. The idea works in an iterative way. We first take the Schmidt decomposition between the first qubit and the rest of the system. Only the change of basis for the first qubit $|\alpha_1\rangle_1 = \Gamma^{[1]i_1}_{\alpha_1}|i_1\rangle_1$ and the χ_1 eigenvalues of this decomposition will be retained. We then proceed to find the Schmidt decomposition between the first two qubits and the rest of the system. Again, we retain χ_2 eigenvalues of the decomposition and find out the change of basis between the basis found in the first decomposition and this second one for the second qubit that amounts to a tensor $|\alpha_1\rangle_2 = \Gamma^{[2]i_2}_{\alpha_1\alpha_2}|\alpha_2\rangle_2$. The procedure is iterated, giving the result [2]

$$|\psi\rangle = \sum_{\alpha_1=1}^{\chi_1} \cdots \sum_{\alpha_{n-1=1}}^{\chi_{n-1}} \Gamma^{[1]i_1}_{\alpha_1}\lambda^{[1]}_{\alpha_1}\Gamma^{[2]i_2}_{\alpha_1\alpha_2}\lambda^{[2]}_{\alpha_2}\ldots\lambda^{[n-1]}_{\alpha_{n-1}}\Gamma^{[n]i_n}_{\alpha_{n-1}}|i_1, i_2, \ldots, i_n\rangle. \tag{7}$$

This construction represents the original coefficients $c^{i_1,\ldots,i_n}$ as a product of matrices, hence the name matrix product state (MPS) [3, 4]. It is an exact representation that is able to adapt to the specific entanglement content of a state. To see this, note that a product state corresponds to a state with $\chi_1 = \cdots = \chi_{n-1} = 1$, that is, any Schmidt decomposition is made with a single term. The more entangled a state the larger the matrices Γ. It is possible to actually find the maximum size of any bi-partition. Let us take a party A made of l qubits versus $n - l$. Then the size of the H_A Hilbert space is 2^l. Thus, $\chi_l \leqslant 2^l$. An arbitrary state will carry maximum entropy and each matrix will reach its maximum possible size. Yet, in most relevant cases, the size of the matrices will be smaller than their maximum.

We may furthermore absorb the eigenvalues λ into the matrices Γ's. We may also decide to extend the original MPS representation and take an extra periodic index and set all the matrices of equal size χ. We then have a periodic boundary representation of the state

$$|\psi\rangle = \sum_{i_1 i_2,\ldots,i_n=0,1} \mathrm{tr}(A^{[1]i_1} A^{[2]i_2} \ldots A^{[n]i_n}) |i_1, i_2, \ldots, i_n\rangle. \tag{8}$$

This expression shows the depth of the idea of matrix product states. All coefficients $c^{i_1 i_2 \ldots i_n}$ are representation as a clever multiplication of matrices. An exact representation will need a different size for the matrices depending on the entanglement present in the state. A simple counting shows that the original 2^n coefficients are now represented with $2n\chi^2$ elements. It is clear that an absolute random state will need $\chi \sim 2^{\frac{n}{2}}$. In general, though, physical states carry less entropy and the MPS representation becomes a powerful tool to represent them.

Let us pause for a moment and give a very simple example that illustrates the idea underlying the compression power of matrix product states. Let us try to communicate a friend the set of numbers 6, 10, 15, 22, 33, 42, 63, 55, 105 and 231. Instead of sending those ten numbers we can as well transmit the instruction of taking all the pair multiplications of 2, 3, 5, 11 and 21. This packing is exponentially economical if we consider multiplications of n numbers. MPS is a sophistication of this multiplicative saving that also handles superpositions, that is entanglement. It is clever compression of entanglement perfectly suited for states which are close to product states.

Let us go one step beyond and see that the size of the matrices involved in the MPS construction is directly related to how much entanglement that state carries. Any partition of the system, say at site a, can be viewed as a Schmidt decomposition

$$\psi = \sum_{\beta=1}^{\chi_a} \lambda_\beta^{[a]} \left(M_{L,\beta}^{i_1 \ldots i_a} \left| i_1 \ldots i_a \right\rangle \right) \left(M_{R,\beta}^{i_{a+1} \ldots i_n} \left| i_{a+1} \ldots i_n \right\rangle \right) \tag{9}$$

where $M_{L,R}$ stand for the product of matrices on the left and on the right of the index a. As a consequence, the entropy for both the left and right parties is

$$S(a) = \mathrm{tr}_{a+1,\ldots,n} |\psi\rangle\langle\psi| = \sum_{\beta=1}^{\chi_a} \lambda_\beta^{[a]} \log \lambda_\beta^{[a]}. \tag{10}$$

The maximum entropy that such a state can carry corresponds to the case where all $\lambda_\beta^{[a]} = 1/\chi_a$. Then,

$$S(a) \leqslant \log \chi_a. \tag{11}$$

This result shows that some amount of quantum correlations can be described with modest values of χ's. It also shows that random states need exponential χ's.

It is also worth noting that an MPS with periodic boundary conditions will always have two indices connecting left and right. One index works as above and a second one wraps around the periodic boundary. The argument gets modified in the sense that $S(a) = 2 \log \chi_a$ for periodic MPS, that is, periodic MPS uses matrices with half the dimension of the ones needed with open boundary conditions.

A final and relevant remark must be emphasized. The typical distributions of the eigenvalues of the reduced density matrix in physical systems are not flat. In some cases, the distribution decays exponentially. This suggests that a truncation in χ may provide a sensible approximation to the system.

4. Entropy and matrix product states for spin chains

We have seen that a certain amount of quantum correlations can be described faithfully with the MPS construction. It remains now to know what is the amount of entanglement present in the ground state of a typical quantum system.

This question can be fully answered for quantum spin chains. It is possible to compute [5–7] the entropy carried by the reduced density matrix of l (out of $n \to \infty$) spins for the ground state of a critical system

$$S_l = \frac{c}{3} \log l, \tag{12}$$

where c is the central charge of the conformal field theory that describes the universality class of the phase transition. This amount of entanglement is far lower than the entropy carried by a random state (which would be $S_l \sim l$). We can now match this result from our previous MPS argument to show that the properties of this l-spin block are faithfully reproduced by a periodic MPS state with size

$$\chi = l^{\frac{c}{6}}. \tag{13}$$

As l grows, only a polynomial increase of computational effort is needed. Thus, quantum phase transitions on spin chains can be efficiently simulated. Indeed, the technique of density matrix renormalization group (DMRG) [8] has been widely applied to one-dimensional systems with hundreds of spins. This would definitely be impossible if the entropy would have grown as a power of l rather than a $\log l$. Yet, even the moderate need of classical resources we have established is commonly considered as a poor representation of critical systems. As we shall shortly see, only non-critical theories can be described with a precision that improves exponentially with χ.

Let us note that the entropy contained in the ground state of a spin chain corresponds to an area law [9, 10]. In higher dimensions, Hamiltonians made with local interactions are expected to deliver ground states with $S_l \sim l^{\frac{d-1}{d}}$, where d stands for the number of spacial dimensions. For $d = 1$ the power law is substituted with a log. The area law growth of entropy must be seen as the quantitative barrier that prevents faithful simulation of higher dimensional quantum systems. Any new technique to handle quantum systems should aim at this problem.

As we just mentioned, it is also possible to compute the entropy content of spin chains away from the quantum phase transition point. There, the entropy saturates to a maximum value dictated by the parameters of the model [6]. An MPS approximation can then be exponentially precise. A large literature on the technique of the above-mentioned DMRG (which is a method to find MPS approximations to ground states of Hamiltonians) shows the power of the entropy calculation.

Further developments on the relation between entropy and renormalization group hint at a decrease of entanglement along renormalization group flows [10, 11]. Moreover, renormalization group transformations can be operated on states and, more specifically, on matrix product states [12]. It would be very nice to obtain further results along these lines for higher dimensional theories.

5. New applications on matrix product sates: continuous variables, Laughlin state, quantum computation

MPS can be used to approximate any computation of a ground state. For instance, it is possible to consider discretizations of quantum field theories and work out the ground state. In [15] it is shown how to deal with a discretized free bosonic theory, that is a set of harmonic oscillators

to get e.g. the entropy present in the ground state or the eigenvalues of the reduced density matrix. The basic idea is to approximate the ground state of the system with local degrees of freedom at positions $x_1, \ldots, x_n$ with

$$\psi(x_1, \ldots, x_n) = \mathrm{tr}(A^{[1]a_1} \ldots A^{[n]a_n}) H_{a_1}(x_1) \ldots H_{a_n}(x_n) \tag{14}$$

where $H_a(x)$ provides a basis for the local continuous Hilbert space (e.g. Hermite polynomials times Gaussians). Entanglement between the basis elements is taken into account by the MPS construction. Furthermore, the MPS method can be extended to an infinite system accepting that all the matrices A are identical. Then the algorithm to compute the ground state can be made to respect translational invariance [15, 16]. This variant produces MPS that right away describe the thermodynamical limit of the system. Further work along these lines is needed to assess the power of this method.

It is also possible to approach other highly entangled systems and represent their ground state as an MPS. Let us consider the Laughlin wavefunction [13]

$$\psi = A_m \prod (z_i - z_j)^m \exp -\frac{1}{2} \sum_i |z_i|^2, \tag{15}$$

where $\nu = 1/m$ is the filling fraction in the system. It is extremely hard to simulate this wavefunction, as shown by the fact that its normalization A_m is unknown in general. If we could find an MPS realization of this wavefunction, we could have a better chance to carry exact computations. Let us see that for $m = 1$ this is indeed possible. Then, the wavefunction corresponds to a fermionic system described by a Vandermonde determinant. The wavefunction can be rewritten as

$$\psi = A' \sum_{a_1, \ldots, a_n = 0}^{n-1} \epsilon^{a_1 \ldots a_n} \phi_{a_1}(z_1) \ldots \phi_{a_n}(z_n), \tag{16}$$

where ϵ is the Levi-Civita fully antisymmetric tensor and $\phi_a(z) = \frac{1}{\sqrt{\pi a!}} z^a \exp -\frac{1}{2}|z|^2$ forms a monoparticular basis. The way to rewrite the coefficients as a product of matrices is simple since this is precisely a property of the Clifford algebra [14]

$$\epsilon^{a_1 \ldots a_n} = \mathrm{tr}(\gamma^{a_1} \ldots \gamma^{a_n} \gamma_5), \qquad \{\gamma^a, \gamma^b\} = 2\delta^{ab} \qquad a, b = 0, \ldots, n-1 \tag{17}$$

where $\gamma_5 \equiv (-i)^{n/2} \gamma^0 \ldots \gamma^{n-1}$ (here, we just consider even dimensions). Note that the original wavefunction for $m = 1$ would carry an apparent number of degrees of freedom n^n because there are n particles that may occupy n states. An exact computation of the entropy for half of the system shows that $S(n/2) = \log \binom{n}{n/2} \sim n$. The periodic MPS state uses matrices whose dimension $\dim \gamma^a = 2^{[n/2]}$ exactly matches the entropy, $\log \chi^2 = n$ in the limit $n \to \infty$. Hence, the MPS construction is optimal. The cases with larger m can be constructed by using a direct product construction of γ matrices. That construction is not optimal since the entropy for an arbitrary m Laughlin wavefunction is known to be bounded by $n \log m$ whereas the direct product construction needs $\mathcal{O}(nm)$ elements.

Let us also mention that some work has pushed the application of MPS to entirely new settings. It is possible, for instance, to simulate the whole evolution of a quantum algorithm using MPS techniques [17]. The initial state is represented as a MPS and then a series of non-local quantum gates are applied as an adiabatic evolution driven by a problem Hamiltonian. It has been possible to solve some NP-complete problem with up to 100 qubits. The one solution, out of 2^{100} possibilities, of a hard problem has been deterministically obtained using an MPS simulation of a quantum algorithm.

6. Spin-off: image compression, differential equations

It is tantalizing to try to develop some spin-off applications of MPS beyond quantum mechanics. Two ideas have already been worked out.

The first one consists of using MPS truncation techniques to compress an image [18]. Let us start by mapping an image into a quantum pure (real) state. Take a telescopic addressing of pixels in quadrants organized as follows. A pixel lying in the first quadrant carries a label $|1\rangle$ (or $|2\rangle$, $|3\rangle$ or $|4\rangle$ for the other options). Each quadrant is subdivided again into fourths. The new labelling for a pixel in quadrant 1, sub quadrant 2, is $|12\rangle$. We can proceed up to n levels, so that the image is made by 4^n pixels. Each pixel carries a grey level that we use as its coefficient. Then

$$4^n \text{ pixel image} \to |\psi\rangle = \sum_{i_1 \ldots i_n = 1}^{4} c^{i_1 \ldots i_n} |i_1 \ldots, i_n\rangle \tag{18}$$

represents a 4^n-pixel grey image where the basis spans over all pixels and the coefficient of each basis element gives the grey level of the corresponding pixel. It is trivial to turn these coefficients into an MPS. A truncation of the size χ of the matrices in the MPS is tantamount to a compression of the picture. Results are remarkably competitive.

A second idea to use MPS outside the domain of quantum mechanics is to solve partial differential equations [15]. A partial differential equation with n variables can be viewed as an operator acting on the variables and coupling them. This is just another form of entanglement. We can take the operator in the differential equation and turn it into a continuous variable problem that can be addressed using the continuous variable techniques presented in the previous section. A minimum distance principle emerges as the error in the solution of the equation. Again, the results obtained are surprisingly good and deserve further attention.

7. Beyond MPS: MERA and PEPs

The shortcoming of MPS is the limited amount of entanglement they can support. Let us take the ground state of a Hamiltonian with local interactions defined on a quantum network in two dimensions. We expect that any geometrical partition of this state will carry an area law entanglement, that is, the entropy will grow linearly as the number of degrees of freedom that define the boundary of the chosen partition. Therefore, there is no good representation of the ground state in terms of MPS as χ should grow exponentially. This is the reason why there are no faithful simulations of higher dimensional quantum systems. In other words, we need a new technique that beats the area law scaling of entanglement.

Two ideas have been launched in recent years to overcome MPS shortcomings. The first one carries the name of multiscale entanglement renormalization ansatz (MERA) [19] and proposes a new way to organize the book-keeping of entanglement using renormalization group ideas to improve on MPS. MERA are built so as to represent quantum systems at a critical point. They combine the block-spin idea with a set of disentangling operations that optimize the way entanglement is retained and manipulated.

A second idea is directly constructed to deal with higher dimensional systems. It extends the matrix product idea to a tensor contraction. This new tensor representation carries the name of projected entangled pairs (PEPs) [20]. PEPs are proven to support area law entanglement. It is also known that the physical construction of PEPs is equivalent to solving NP-complete problems. An algorithm to find the PEPs that describe the ground state of a quantum network is already available.

The conclusion of recent research remains open. We still do not know what is the optimal way to represent quantum systems. Entropy computations are no longer academic results since they establish the amount of entanglement to be represented. MPS are proven efficient on one-dimensional systems. A lot of work is still needed on critical systems and higher dimensions to have fully satisfactory answers to delimit the classical resources necessary to faithfully represent and manipulate quantum-mechanical states.

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