Angular quantization and the density matrix renormalization group

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Abstract

Path integral techniques for the density matrix of a one-dimensional statistical system near a boundary previously employed in black-hole physics are applied to providing a new interpretation of the density matrix renormalization group: its efficacy is due to the concentration of quantum states near the boundary.

There has recently been a revival of interest in the study of statistical properties of quantum field theories in the presence of a boundary. This subject has a long history: it goes back (at least) to the idea of the entropy of black holes. This entropy, associated to Hawking radiation, was studied with quantum field theory in the corresponding curved space-time. It has been proposed that black-hole entropy arises solely from the presence of a horizon and the consequent ignorance of its interior, being an entanglement entropy and having little to do with the curvature of the space-time. Actually, this is indicated by the classical calculation of the density matrix in Rindler space, which will be important in the following.

An interesting connection arose from the study of integrable one-dimensional lattice models, where R. Baxter introduced the corner transfer matrix. In the continuum limit of these models, it is natural to use rapidity variables, in which the integrability conditions adopt a simpler form and, moreover, their symmetry with respect to phase shifts can be understood as a consequence of Lorentz invariance. Substantiating this connection, the type of quantization used in the Euclidean version of Rindler space, namely, angular quantization, has been invoked as a suitable computational formalism in 1+1 integrable quantum field theory.

The corner transfer matrix method is only appropriate for integrable models, but T. Nishino and collaborators realized that it is related to an approximate method to solve quantum systems, namely, the density matrix renormalization group (DMRG).
The DMRG is a numerical renormalization group introduced by S. White [6], which seems to provide unprecedented precision. White intended to tackle the problem of the influence of boundary conditions in the application of the real space RG to finite systems. A first attempt on accounting for the effect of boundary conditions was the combination of boundary conditions approach [7]. It eventually led to the DMRG, by appealing to Feynman’s formulation of the density matrix as the best description of a part of a quantum mechanical system: the DMRG method then reduces the number of states of the subsystem by discarding the smallest eigenvalues of the density matrix. The DMRG is analogous to Wilson’s treatment of the Kondo problem in that, at every step, new states are added at one side of the system and then other states are removed to keep the size of the Hilbert space approximately constant. It seems that, in this process, it is sensible to keep more states near the boundary. This is reminiscent of the concentration of quantum states at a black-hole’s horizon. We shall see that the angular quantization construction of the density matrix shows that the DMRG precisely amounts to an algorithm to keep more states near the boundary in a systematic way.

Before proceeding, it is interesting to mention that there is a well-known condensed matter system whose dynamics can be considered as concentrated on a spatial boundary, namely, the two-dimensional electron system exhibiting the quantum Hall effect. Its connection with the physics of black holes has already been worked out [8].

The type of models to which the DMRG is usually applied consists of those defined on a chain, such as the 1D Hubbard or Heisenberg model, the Ising model in a transverse field, etc. For our purposes, it is convenient to consider simpler models and we shall illustrate the effect of the DMRG on a chain of oscillators. Of course, if it is a harmonic chain, its Hamiltonian can be diagonalized in momentum space, yielding a spectrum of free phonons, and no renormalization group is necessary. Nevertheless, it constitutes a suitable test for the DMRG [9], since this RG acts in real space, where the kinetic term is a coupling in its own right.

The density matrix of half of the harmonic chain is a straightforward generalization of the density matrix of a harmonic oscillator coupled to the environment and can be obtained by the diagonalization of its Hamiltonian, the construction of the ground state, and a subsequent trace over the unobservable variables [2, 10]. However, it is preferable to use path integral methods in the continuum, which are simpler and allow one to obtain more general results [11].

Therefore, we consider a chain of coupled oscillators, which gives rise to phonon-like collective excitations. In the continuum limit, the action for this model is

\[
S[u(x, t)] = \int dt \int dx \left( \frac{\mu}{2} \left[ (\partial_t u)^2 - c^2 (\partial_x u)^2 \right] - V(u) \right),
\]

(1)

where \( u \) is the displacement, \( \mu \) is the mass per unit length, and \( c \) is the speed of sound. The Hamiltonian can be expressed as the integral of the energy density, which is the time-component of the energy-momentum tensor:

\[
H = \int T_{00} \, dx.
\]

(2)
After redefining $t$ and $u$ to have $xt$-symmetry and to remove $\mu$,

$$T_{00} = \frac{1}{2} \left[ (\partial_t u)^2 + (\partial_x u)^2 \right] + V(u). \quad (3)$$

Let us obtain a path integral representation for the density matrix on the half-line of a system that is in its ground state \[11\]. We use the notation corresponding to the oscillator chain but it shall be obvious that the construction is fairly general. In the continuum limit, the half-line density matrix is a functional integral,

$$\rho[\psi^*_0[u_L(x), u_R(x)], \psi_0[u_L(x), u_R(x)]] = \int D u_L(x) \psi_0[u_L(x), u_R(x)] \psi^*_0[u_L(x), u_R(x)], \quad (4)$$

where the subscripts refer to the left or right position of the coordinates with respect to the boundary (the origin). Now, we must express the ground-state wave-functions as a path integral,

$$\psi_0[u_L(x), u_R(x)] = \int D u(x, t) \exp(-S[u(x, t)]), \quad (5)$$

where $t \in (-\infty, 0]$ and with boundary conditions $u(x, 0) = u_L(x)$ if $x < 0$, and $u(x, 0) = u_R(x)$ if $x > 0$. The conjugate wave function is given by the same path integral and boundary conditions but with $t \in [0, \infty)$. Substituting into Eq. (4) and performing the integral over $u_L(x)$, one can express $\rho(u_R, u'_R)$ as a path integral over $u(x, t)$, with $t \in (-\infty, \infty)$, and boundary conditions $u_R(x, 0^+) = u'_R(x)$, $u_R(x, 0^-) = u_R(x)$. In other words, $\rho(u_R, u'_R)$ is represented by a single path integral covering the entire plane with a cut along the positive semiaxis, where the boundary conditions are imposed.

Let us now consider the angular evolution operator $\exp(-2\pi L)$, where $L$ is the generator of rotations around the origin and $2\pi$ is the angle’s range, in analogy with the canonical density matrix $\exp(-\beta H)$. Its matrix element in the Schrödinger representation $\langle u'_R | \exp(-2\pi L) | u_R \rangle$ is given by an angular path integral with boundary conditions $u_R(0) = u'_R$ and $u_R(2\pi) = u_R$, in analogy with the canonical density matrix path integral. Therefore, it precisely coincides with the density matrix path integral.

The DMRG algorithm discards the smallest eigenvalues of the density matrix and is, therefore, equivalent to truncating the spectrum of $L$. Of course, this truncation has the typical variational flavor of real space renormalization groups, and we can say that it selects states adequate to the presence of the boundary.

In Euclidean two-dimensional field theory, the generator of rotations in the $(x, t)$ plane is

$$L = \int dx \left( t T_{11} - x T_{00} \right). \quad (6)$$

To simplify, one can evaluate it at $t = 0$. For the oscillator chain, we must use the value of $T_{00}$ \[3\]. In the Schrödinger representation, we should replace the momentum $\Pi = \partial_t u$ with $\Pi(x) = i \partial u(x)$. However, as in canonical quantization, one rather uses the second-quantization method, which diagonalizes the Hamiltonian by solving the classical equations of motion and quantizing the corresponding normal modes. Let us recall that, in canonical quantization, if we disregard anharmonic terms, the classical equations of motion in the
continuum limit become the Klein-Gordon field equation, giving rise to the usual Fock space. Not surprisingly, the eigenvalue equation for $L$ leads to the Klein-Gordon equation in polar coordinates in the $(x,t)$ plane,

$$(\Delta + m^2)u = \left(\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} + m^2\right)u = 0.$$  

(7)

Separating the angular variable, it becomes a Bessel differential equation in the $r$ coordinate with complex solutions $I_{\pm i \ell}(mr)$ $[12]$, $\ell$ being the angular frequency. We have a continuous spectrum, which becomes discrete on introducing boundary conditions. One of them must be set at a short distance from the origin, to act as an ultraviolet regulator $[2, 11]$, necessary in the continuum limit.

Therefore, the second-quantized field is (on the positive semiaxis $t = 0 \Leftrightarrow \phi = 0, x \equiv r$)

$$u(x) = \int \frac{d\ell}{2\pi} \frac{b_\ell I_{\ell}(mx) + b_\ell^\dagger I_{-\ell}(mx)}{\sqrt{2 \sinh(\pi \ell)}},$$  

(8)

where we have introduced annihilation and creation operators and where the term that appears in the denominator is just for normalization, to ensure that those operators satisfy canonical commutations relations. There is an associated Fock space built by acting with $b_\ell^\dagger$ on the “vacuum state”. These states constitute the spectrum of eigenstates of $L$, which adopts the form $L = \int d\ell \ell b_\ell^\dagger b_\ell$ (where the integral is replaced with a sum for discrete $\ell$).

We proceed to show, by using the eigenfunctions of $L$ instead of free waves, that we have a basis in which the region close to $x = 0$—the boundary point—is more accurately represented than the region far from it when we cut off the higher $\ell$ eigenfunctions. Notice that the functions $I_{\pm i \ell}(mx)$ have wave-lengths that increase with $x$. It is illustrative to represent a real solution,

$$K_{i \ell}(mx) = \frac{i \pi}{2 \sinh(\pi \ell)} [I_{i \ell}(mx) - I_{-i \ell}(mx)].$$

A detailed analysis shows that this solution is oscillatory for $x < \ell/m$, with a wavelength proportional to $x$, and decays exponentially for $x > \ell/m$ (Fig. 1). The other type of real solution, $I_{-i \ell}(mx) + I_{i \ell}(mx)$, has the same behavior for $x < \ell/m$ but for $x > \ell/m$ grows exponentially instead. For unattenuated phonons ($m = 0$), there is no exponential decay or growth. Imposing a maximum value of $\ell$, we restrict the amount of detail that a linear combination of these functions can have but, clearly, the allowed amount of detail is larger for the region close to the origin than for the region far from it. In the second-quantized theory, the $\ell$ cutoff has a similar interpretation: near the origin, a larger range of energy of modes (phonons) is allowed, so representing the influence of the other half of the chain.

Let us see how the numerical DMRG would actually proceed for the chain of coupled harmonic oscillators (see also Ref. [4]). Since the Hilbert space for a single oscillator already has infinite dimension, one must begin by truncating the initial Hilbert space to a finite and rather small number of states per site, $n$ say. Then one obtains the ground state,
Fig. 1. The real solution $K_{8i}(x)$. Its exponential decay is apparent for $x > 8$.

with energy $(1/2) \sum_{k} \omega_k$, $\omega_k$ being the frequencies of the $N$ normal modes $a_k$ (of ordinary canonical quantization). From the ground state, one derives the corresponding density matrix of half of the chain. This can be done numerically, but analytically as well, since the integral for the density matrix is Gaussian [see Eq. (4)]. In White’s original algorithm [6], one begins with only one site, which is reflected on the origin, to compute the two-site ground state and the one-site density matrix. Next, one discards its smallest eigenvalues and iterates: one adds one site at the center with their $n$ new states, reflects, etc. In the present case, the one-site density matrix is Gaussian and therefore equivalent to the thermal matrix of one single oscillator, with a temperature increasing with the coupling strength. Thus it has the form $\exp(-2\pi \mathcal{L})$, where $2\pi \mathcal{L}$ is $\beta \mathcal{H}$ for the “equivalent thermal oscillator” [10].

For even $N \geq 2$, the integral (4) is an ordinary integral in $N/2$ variables. It yields the exponential of a quadratic form, $u_R^T A u_R + u'_R^T A u'_R + u_R^T B u'_R + u'_R^T B u_R$, where $A$ and $B$ are $N/2 \times N/2$ symmetric matrices, the former being positive definite. One can then perform a two-step diagonalization of this quadratic form [13]: If we write $A = M M^T$, with $M$ a $N/2 \times N/2$ nonsingular real matrix (which is always possible [12]), the transformation $v = M^T u$ puts the first part in canonical form, while changing $B \rightarrow M^{-1} B (M^{-1})^T$. This matrix can be diagonalized by an orthogonal transformation $O$, without altering the canonical form of the other part. The result is that the density matrix becomes the product of density matrices of independent modes. Consequently, it adopts the form $\exp(-2\pi \mathcal{L})$, with $2\pi \mathcal{L}$ being the sum of the operators $\beta \mathcal{H}$ for those modes (the equivalent thermal oscillators). Furthermore, the total transformation matrix $O^T M^T$ is the discrete version of the functions $K_{i\ell}(mx)$, such that the first index corresponds to $\ell$ while the second corresponds to $x$. We have plotted in Fig. 2 the second and third file vectors of that matrix, for the case $m = 0.1$ and $N = 24$. It can be seen that they are a discrete version of functions of the type of that in Fig. 1, although with fewer oscillations. The following
file vectors correspond to higher $\ell$, and hence to more rapidly oscillating functions, but the discreteness interferes in such a manner that these oscillations are difficult to perceive.

The inclusion of weak anharmonic terms in the action should not substantially modify the picture above. As mentioned before, in real space the important coupling is actually the kinetic term, which couples neighboring points. As regards to calculation, anharmonic terms prevent us from obtaining analytic expressions for the angular states or performing the functional integrals, which are no longer Gaussian. However, the effect of those terms amounts to a mode-mode coupling, which can be treated perturbatively. Canonical methods for perturbation theory in Rindler space are exposed in Ref. [1]. On the other hand, it is easy to see how to evaluate the functional integral for the density matrix, Eq. (4), in perturbation theory: One must first introduce the coupling to an external current, as usual, and express the interaction term, $V(u) = \lambda u^4$ say, as a derivative with respect to the external current; then, the Gaussian integral can be performed and the perturbation series constructed. At any rate, although these perturbative corrections modify the ground and excited-state energies, the qualitative properties of the spectrum of $\mathcal{L}$ must remain the same.

We must remark that, in quantum field theory in $1 + 1$ dimensions, non-perturbative phenomena may occur and one must have an idea about the type of spectrum of collective excitations before applying a perturbative approach, since these effects can turn a
bosonic spectrum into a fermionic one (or vice versa) [14]. If the collective excitations are bosons, the formulas above would constitute the basis for perturbation theory and the conclusions should not be modified. On the other hand, it should not be difficult to reach analogous conclusions for a fermionic spectrum such as, for example, the spectrum of the Ising model in a transverse field, which has been the subject of many tests for the DMRG. The field-theory forms of $H$ and $L$ given by Eq. (2) and (3), respectively, still hold. Their particular expressions for the free fermion field are easy to obtain. The form of the angular wavefunctions would be similar to the bosonic ones, already studied.

Moreover, regarding the generality of our conclusions, one can argue that the essence of the DMRG, as concerns the effect of boundary conditions, is independent of the type of spectrum or the details of perturbation theory. In a general 1D many-body system that is homogeneous in the continuum limit, such as a system defined on a chain with uniform site-to-site coupling, we can always express the energy by the integral (4) and, therefore, the generator of rotations as $L = \int dx x \epsilon(x)$, where $\epsilon := T_{00}$ does not depend explicitly on $x$. Suppose that we divide the chain into equal-size blocks, with coordinate $x_j$, such that, for sufficiently large blocks, we can approximately write $L = \sum_j x_j \epsilon_j$, except for a small inter-block potential. If we want to discard eigenvalues of the density matrix $\exp(-2\pi L)$ smaller than certain value, then we are to set an upper cutoff for the $L$ eigenvalues, which then implies a cutoff for every $\epsilon_j$, but depending inversely on $j$: for small $j$, that is, close to the boundary, an extensive range of values is included, accounting for the progressive uncertainty in their value as the boundary is approached, whereas for large $j$ only the lowest energy states are allowed. In conclusion, one necessarily has a concentration of quantum states at the boundary, due merely to the existence of this boundary, as in the different physics of black holes.

Finally, let us mention that, for a class of integrable models, one can go beyond perturbation theory and, actually, calculate the correlation functions from the two-body $S$-matrix. Owing to its relation with the corner transfer matrix, the form-factor method to calculate the correlation functions for these models is deeply related with angular quantization [1]. In this context, it would be very interesting to compare the results of the DMRG for these models with those of the form-factor approach.

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