“Entanglement in many-body systems: concepts and algorithms”

Exercise Collection 4 – 19.06.2013

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We said in class that, for any practical purpose, the local Hilbert dimension d_B on each site of a system populated by bosons must be restricted to a maximum occupation number $n_{\max}$, thus giving $d_B = n_{\max} + 1$. Moreover, we noticed that creation/annihilation operators for bosons $\hat{b}^\dagger, \hat{b}$ can be represented as *local, truncated, matrices* $\widetilde{b^\dagger}, \widetilde{b}$ with elements on the sub-/supra-diagonal equal to the proper square roots of population: $\widetilde{b^\dagger}_{mn} = \sqrt{n}\,\delta_{n,m-1}$ $\widetilde{b}_{mn} = \sqrt{m}\,\delta_{n,m+1}$.
These matrices correspond to the raising/lowering operators of a spin $S = n_max$ where the possible states are restricted to projections $S_z = -S, \ldots, 0$, and the population is $\widetilde{n} = S_z + n_{\max}$. The full representation of creators/annihilators reads then $\hat{b}_j^{(\dagger)} = \bigotimes_{i=1}^{j-1} \mathbb{I}_{d_B} \otimes \widetilde{b^{(\dagger)}} \bigotimes_{l=j+1}^{L} \mathbb{I}_{d_B}$.

On the other hand, we also saw that for (polarized) fermions, i.e. with no *internal* degrees of freedom, one should resort to a *non-local* mapping (called Jordan-Wigner transformation), in terms of Pauli matrices $\sigma^0 = \mathbb{I}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\sigma^1 = \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma^2 = \sigma^y = \begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{-i} & 0 \end{pmatrix}$ $\sigma^3 = \sigma^z = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$.
[notice the small shift in notation so that the ordering of the basis is then similar to the bosons above]
Once fixed the local occupation number as $\widetilde{n} = (\sigma^z + \sigma^0)/2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, and defined the raising-lowering spin operators $\widetilde{a}^\dagger = (\sigma^x + i\sigma^y)/2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ $\widetilde{a} = (\sigma^x - i\sigma^y)/2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, the JW mapping prescribes that the creation and annihilation fermionic operators $\hat{c}^\dagger, \hat{c}$ are represented with a parity string attached along a fixed order of the chain sites: $\hat{c}_j^{(\dagger)} = \bigotimes_{i=1}^{j-1}(-\sigma^z) \otimes \widetilde{a}^{(\dagger)} \bigotimes_{l=j+1}^{L} \mathbb{I}_2$. The fermionic nature of the mapping descends from the relation $-\sigma_z = (-1)^{\hat{n}}$. Another important point was that the nearest neighbor nature of hopping terms is preserved by such mapping.

Before tackling the exercises on the next pages, please verify explicitly all the relations stated above.

A. A mixed system of bosons and fermions

Imagine that you have to deal with a system in which interactions constrain some kind of bosonic particles to be at most two per site, and to have as well polarized fermionic particles in the system, living on the same sites. This might be the case in some ultracold atomic setup with optical lattices, where different isotopes of atoms can be trapped and therefore give rise to a mixed statistics tight-binding (Hubbard) model. You are now facing the challenge of formulating the problem in a tensor-network compatible language, i.e. in terms of matrix representations of all operators involved:

i) what local dimension d will you need to describe the Hilbert space of particle configurations?

ii) what form have the matrices for local occupation number, and raising/lowering operators ? Write them explicitly (six $d \times d$ matrices)

iii) what string should be attached to the above matrices, in order to preserve the correct (anti-)commutation relations ? Notice that operators of distinguishable particles fully commute, since they can not give rise to any quantum statistical effect.

B. Two species of fermions

Take now the case of a collection of spinful fermions, for the sake of simplicity spin 1/2 particles like electrons in a solid. Again, you want to formulate the problem in a matrix representation so that it can be tackled via tensor network algorithms:

i) what local dimension d will you need to describe the Hilbert space of particle configurations?

ii) what form have the matrices for local occupation number, spin projection, and raising/lowering operators ? Write them explicitly (six $d \times d$ matrices)

iii) what string(s) should be attached to the above matrices, in order to preserve the correct anti-commutation relations ? Remember that the spin orientation $s = \pm$ is a further quantum number for a set of undistinguishable particles. Imagine that this corresponds to a second coordinate, i.e. that particles sit on a "coupled" chain, and draw a convenient string structure, that minimizes the degree of non-locality of terms that were originally nearest neighbor ones (including spin-flipping ones)

iv) can you see any simplification of the previous result in the case there is no spin-flipping term in the Hamiltonian ruling the system (like it happens in the "elementary" Hubbard model) ? Notice that the supplementary $U(1)$ symmetry (beyond the preservation of particle number) tells you that any observable that does not preserve spin-projection is forbidden, therefore you need to minimize the number of non-trivial string elements only between operators of the same sub-chain.

C. From spins to fermions: exact solution of XY model

Consider now the so-called XY model, consistent of L spins 1/2 arranged on a chain and subject to only nearest neighbor interactions, according to ($S^a \equiv \sigma^a/2$)

$$H_{\gamma,h} = \sum_j (1+\gamma) S_j^x S_{j+1}^x + (1-\gamma) S_j^y S_{j+1}^y + \sum_j h S_j^z \ .$$

The boundary conditions can be either open (i.e. $1 \leq j \leq L-1$ in the first summation) or periodic (i.e. including $j = L$ in the first sum, with the prescription $L+1 \equiv 1$). Such family of models is a cornerstone of exactly solvable models: the key ingredient is the Jordan-Wigner transformation that we saw in class and revisited above, only this time to transform spins into fermions (reasons will be clear below).

i) show that the Hamiltonian can be rewritten, via the raising and lowering operators, as $H_{\gamma,h} = \frac{1}{2}\sum_j \left[\left(a_j^\dagger a_{j+1} + \gamma a_j^\dagger a_{j+1}^\dagger\right) + h.c.\right] + \sum_j h\left(a_j^\dagger a_j - \frac{1}{2}\right)$.

ii) prove that these operators partly resemble Fermi operators in that $\{a_j, a_j^\dagger\} = 1 \quad \left(a_j^{(\dagger)}\right)^2 = 0$ and partly resemble Bose operators in that $[a_j, a_l^\dagger] = [a_j^\dagger, a_l^\dagger] = [a_j, a_l] = 0 \quad j \neq l$

iii) check that the Jordan-Wigner transformation $c_j = \exp\left[i\pi \sum_{l=1}^{j-1} a_l^\dagger a_l\right] \cdot a_j$ is providing fermionic anti-commutation rules to these newly defined operators and is leaving the Hamiltonian of point i) invariant in form (apart from a peculiar boundary term if p.b.c. are adopted $\longrightarrow$ which one ?). [*suggestion:* the local occupation number is limited to to 0 or 1: use it to simplify the expressions].

The Hamiltonian we just found is a nice example of a *quadratic fermionic problem*, of the form

$$H = \begin{pmatrix} \vec{c}^\dagger & \vec{c} \end{pmatrix} \begin{pmatrix} A & B \\ B^\dagger & -A^* \end{pmatrix} \begin{pmatrix} \vec{c} \\ \vec{c}^\dagger \end{pmatrix} \qquad A^\dagger = A \quad B^T = -B \quad \vec{c} = \{c_1 \dots c_L\},$$

like the ones you get across when dealing with BCS theory or Majorana modes (just to mention a few "hot" topics). One could even show that all these problems are exactly solvable and in the end equivalent to a *free fermionic problem* (and therefore fully characterized only by two-operators expectation values . . .). We will focus here on a case in which this is automatically the case, without need of (much) further calculations.

iv) write explicitly the matrices A, B and verify the mentioned relations;

v) consider the special case $\gamma = 0$, where the fermions are already explicitly non-interacting ($B = 0$). As a consequence, one only needs to find the single-particle solutions, i.e. the eigenvalues ϵ_k and the eigenvectors v_k of the matrix A. The correspondent creation/annihilation operators will then be $\psi_k = \sum_j (v_k)_j c_j$ (and *h.c.*), leading to $H = \sum_k \epsilon_k \psi_k^\dagger \psi_k$. Solve the cases of open and periodic boundaries (both with even and odd total population, see above). [*suggestion:* consider the ansatz $(v_k)_j = x\, e^{ikj} + y\, e^{-ikj}$ and work out the quantization for k].

vi) finally, write the many-body ground state by making use of the Fermi-Dirac distribution and compute its total energy. Notice that one could redefine this state as the *vacuum* by performing a particle-hole transformation on the negative part of the spectrum: this is an example of a vacuum which is not empty at all (as we mentioned couple of times in class) :)

vii) **only if you are brave:** can you imagine the way of solving the general problem for $\gamma \neq 0$? [*suggestion:* it has to do with the Bogolubov transformations used in BCS theory, if you already crossed them. Anyway there are purely matrix analysis ways to solve it . . .]