Condensed Matter Review: Homework 2

Due on February 17, 2017

Please submit your solutions to Dropbox in a single ZIP file. Your numerical solutions (for Questions 1c, 1f and 2e) should be within an IJulia notebook.

So far in this course you have learned how to compute the ground state and its entanglement entropy in two types of systems:

- Quantum spin chain: we can compute the ground state of an arbitrary (nearest-neighbor) Hamiltonian H for up to $N \approx 20$ spins (using the Lanczos algorithm).
- System of fermions with a quadratic Hamiltonian H: we can compute the ground state for up to $N \approx 1000$ sites (using either Majorana operators when H only preserves fermionic parity, or fermionic annihilation/creation operators when H preserves particle number).

In this Homework, you will learn to actually take $N \to \infty$ in the fermionic formalism. You will then study the scaling of entanglement entropy in $D = 1$ and $D = 2$ spatial dimensions. For simplicity we will only consider a quadratic H that preserves particle number, although if you want a bit more of a challenge, you can also use a quadratic Hamiltonian that only preserves fermionic parity. You can read more about the scaling of entanglement entropy in 2D systems of fermions in, for example, the paper arXiv:quant-ph/0602094.

1 Free fermions in 1D

Let us consider once more the 1D fermionic quadratic Hamiltonian with PBC, which is given by

$$H = -\sum_{n=1}^{N-1} \left(a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n \right) - \left(a_N^\dagger a_1 + a_1^\dagger a_N \right), \tag{1}$$

or

$$H = \sum A_{mn} a_m^\dagger a_n^\dagger, \qquad A \equiv -1 \times \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & & \vdots & & \ddots & & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}, \tag{2}$$

where the fermionic operators obey the usual anticommutation relations

$$a_n a_m^\dagger + a_m^\dagger a_n = \delta_{m,n}, \qquad a_n a_m + a_m a_n = 0. \tag{3}$$

We consider odd N and we introduce the Fourier modes

$$\hat{a}_k \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^{N} a_n e^{-i\frac{2\pi}{N}kn}, \quad \hat{a}_k^\dagger = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} a_n^\dagger e^{i\frac{2\pi}{N}kn}, \tag{4}$$

or

$$a_n = \frac{1}{\sqrt{N}} \sum_k \hat{a}_k e^{i\frac{2\pi}{N}kn}, \quad a_n^\dagger = \frac{1}{\sqrt{N}} \sum_k \hat{a}_k^\dagger e^{-i\frac{2\pi}{N}kn}, \tag{5}$$

where the sums $\sum_k$ run over the values

$$k \in \left\{ -\frac{N-1}{2}, -\frac{N-1}{2} + 1, \cdots, -1, 0, 1, \cdots, \frac{N-1}{2} - 1, \frac{N-1}{2} \right\}. \tag{6}$$

a) Show that the Hamiltonian can be written as

$$H = \sum_k e_k \hat{a}_k^\dagger \hat{a}_k, \qquad \text{where } e_k = -2\cos\left(\frac{2\pi}{N}k\right). \tag{7}$$

b) Recall that the correlation matrix in momentum space is given by $\widetilde{M}_{kk'} = \delta_{k,k'} \operatorname{sgn}(e_k)$. In this case, the matrix $\widetilde{M}$ is very simple, since

$$\operatorname{sgn}(e_k) = \begin{cases} -1 & \text{for } |k| < N/4 \\ 1 & \text{for } |k| > N/4. \end{cases} \tag{8}$$

(Notice that, for odd N, there is no valid value of k with $|k| = N/4$, for which $e_k = 0$ would not have a well-defined sign.)

From here, we can compute the correlation matrix in real space, to find

$$M_{nn'} = f(n - n') = \frac{1}{N} \sum_k \operatorname{sgn}(e_k) e^{i\frac{2\pi}{N}(n-n')k}. \tag{9}$$

Using $\frac{1}{N}\sum_k e^{i\frac{2\pi}{N}(n-n')k} = \delta_{n,n'}$, show that the function $f(m)$ can be written as

$$f(m) = \delta_{m,0} - \frac{2}{N}\sum_{|k|<N/4} e^{i\frac{2\pi}{N}mk}. \tag{10}$$

c) Recall that $M^\dagger = M$ implies that $f(-x) = f(x)^*$. Notice that, in order to compute the entanglement entropy of an interval of L sites, we just need to know $f(n-n')$ for values of $n-n'$ in the interval $[0, L-1]$ (*i.e.* for L different values of $n-n'$).

For each value of $n-n'$, we need to add $\mathcal{O}(N)$ exponential terms together. As a result, the computational cost of obtaining $f(n-n')$ for $n-n'$ in the interval $[0, L-1]$ grows only as $L \times N$. Diagonalizing the $L \times L$ correlation matrix M has cost $\mathcal{O}(L^3)$. Therefore, if we choose $N = L^2$, the overall cost still scales as L^3. With your laptop you can then afford $L \approx 1000$, which corresponds to $N \approx 10^6$ spins!

For $N = 2^{18} - 1 = (512)^2 - 1 = 262,143$ sites, numerically compute the entanglement entropy for regions of size $L = 2, 4, 8, 16, 32, 64, 128, 256, 512$ sites and plot your results as a function of L. (Make sure that your algorithm scales only as L^3 before you even try such large values of N and L!)

d) Let us now consider the limit $N \to \infty$. This limit will replace the sum over k in Equation (9) with an integral such that

$$M_{nn'} = f(n-n') = \delta_{n,n'} - 2\int_{-\pi/2}^{\pi/2} \frac{dq}{2\pi} e^{i(n-n')q}, \tag{11}$$

where $q = \frac{2\pi}{N}k$ and $dq = \frac{2\pi}{N}$.

Carry out this integral analytically to show that, in the limit $N \to \infty$,

$$f(m) = \begin{cases} 0 & \text{for } m \text{ even,} \\ (-1)^{\frac{m+1}{2}} \frac{2}{m\pi} & \text{for } m \text{ odd.} \end{cases} \tag{12}$$

e) Recall that, for $(1+1)$-dimensional CFTs, the ground state entanglement entropy on a system of size N should scale with L such that

$$S_N(L) = \frac{c}{3}\log_2\left[\frac{N}{\pi}\sin\left(\frac{L\pi}{N}\right)\right] + c_1, \tag{13}$$

where c is a universal number known as the central charge and c_1 is a non-universal constant.

Show that, when L remains finite and $N \to \infty$, we arrive at

$$S(L) \equiv \lim_{N\to\infty} S_N(L) = \frac{c}{3}\log_2(L) + c_1. \tag{14}$$

f) Use the expression in Equation (12) to numerically compute the entanglement entropy $S(L)$ for $L = 2, 4, 8, \ldots, 2^{10} = 1024$ sites. Then, use Equation (14) to extract an accurate estimate of the central charge.

2 Free fermions in 2D

Consider now the same model as in Equation (1), but on a 2D square lattice (with PBC in both directions) such that

$$H = -\sum_{\mathbf{n}} \left(a_{\mathbf{n}}{}^{\dagger} a_{\mathbf{n}+\hat{x}} + a_{\mathbf{n}+\hat{x}}{}^{\dagger} a_{\mathbf{n}} \right) - \sum_{\mathbf{n}} \left(a_{\mathbf{n}}{}^{\dagger} a_{\mathbf{n}+\hat{y}} + a_{\mathbf{n}+\hat{y}}{}^{\dagger} a_{\mathbf{n}} \right), \tag{15}$$

where $\mathbf{n} = (n_x, n_y)$, $n_x \in \{1, 2, \cdots, N_x\}$, $n_y \in \{1, 2, \cdots, N_y\}$, $\hat{x} = (1, 0)$ and $\hat{y} = (0, 1)$. Here, we take $N_x = N_y \equiv N$ and we consider odd N.

In this question, we will use the tricks we have learned from the 1D case to study the scaling of the entanglement entropy in an infinite system ($N \to \infty$) for square regions of $L \times L$ sites.

Let us again introduce the Fourier fermionic modes, which are given in 2D by

$$a_{\mathbf{n}} = \frac{1}{N} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\frac{2\pi}{N}\mathbf{k}\cdot\mathbf{n}}, \quad a_{\mathbf{n}}{}^{\dagger} = \frac{1}{N} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{\dagger} e^{-i\frac{2\pi}{N}\mathbf{k}\cdot\mathbf{n}}, \tag{16}$$

with $k_x, k_y \in \{-\frac{N-1}{2}, \cdots, -1, 0, 1, \cdots, \frac{N-1}{2}\}$.

a) Show that the Hamiltonian can be written as

$$H = \sum_{\mathbf{k}} e_{\mathbf{k}}\, \hat{a}_{\mathbf{k}}^{\dagger}\, \hat{a}_{\mathbf{k}}, \qquad \text{where } e_{\mathbf{k}} = -2\cos\left(\frac{2\pi}{N}k_x\right) - 2\cos\left(\frac{2\pi}{N}k_y\right). \tag{17}$$

b) Show that the correlation matrix in momentum space is given by

$$\widetilde{M}_{\mathbf{k}\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'} f(\mathbf{k}), \qquad \text{with } f(\mathbf{k}) = \begin{cases} -1 & \text{for } \mathbf{k} \in \Omega, \\ 1 & \text{for } \mathbf{k} \notin \Omega, \end{cases} \tag{18}$$

where Ω is the region of momentum space that includes the origin and is bounded by the four lines $k_y = k_x \pm \frac{N}{2}$ and $k_y = -k_x \pm \frac{N}{2}$.

c) Consider now the correlation matrix in real space, which is given by

$$M_{\mathbf{n}\mathbf{n}'} = f(\mathbf{n} - \mathbf{n}') = \frac{1}{N^2} \sum_{\mathbf{k}} f(\mathbf{k}) e^{i\frac{2\pi}{N}(\mathbf{n}-\mathbf{n}')\cdot\mathbf{k}}. \tag{19}$$

Using $\frac{1}{N^2}\sum_{\mathbf{k}} e^{i\frac{2\pi}{N}(\mathbf{n}-\mathbf{n}')\cdot\mathbf{k}} = \delta_{\mathbf{n},\mathbf{n}'}$, show that $f(\mathbf{m})$ can be written as

$$f(\mathbf{m}) = \delta_{\mathbf{m},0} - \frac{2}{N^2} \sum_{\mathbf{k}\in\Omega} e^{i\frac{2\pi}{N}\mathbf{m}\cdot\mathbf{k}}. \tag{20}$$

d) Consider again the limit $N \to \infty$. Replacing the sum in Equation (20) by an integral gives

$$f(\mathbf{m}) = \delta_{\mathbf{m},0} - 2\int_{\mathbf{q}\in\widetilde{\Omega}} \frac{d^2\mathbf{q}}{(2\pi)^2}\, e^{i\mathbf{m}\cdot\mathbf{q}}, \tag{21}$$

where $\mathbf{q} = \frac{2\pi}{N}\mathbf{k}$, $d^2\mathbf{q} \equiv \left(\frac{2\pi}{N}\right)^2$ and the region $\widetilde{\Omega}$ is delimited by the four lines $q_y = q_x \pm \pi$ and $q_y = -q_x \pm \pi$.

Evaluate this integral analytically in order to show that, in the limit $N \to \infty$,

$$f(\mathbf{m}) = \begin{cases} 0 & \text{for } m_x \text{ and } m_y \text{ either both even or both odd,} \\ \frac{4(-1)^{m_x}}{\pi^2(m_x^2 - m_y^2)} & \text{otherwise.} \end{cases} \tag{22}$$

Hint: Use the change of variables $p_1 = q_x + q_y$ and $p_2 = -q_x + q_y$.

e) Use the expression in Equation (22) to numerically compute the entanglement entropy $S(L)$ for square regions of $L \times L$ sites in the limit $N \to \infty$. Plot your results for linear sizes $L = 1, 2, \ldots, 16$. How does the entropy $S(L)$ scale with L?