Finite-size DMRG characterization of the 1D Fermi-Hubbard model phase diagram

University of Pisa, a.y. 2024-2025

Alessandro Gori*

Abstract

The one-dimensional Fermi-Hubbard model at zero temperature is studied, employing finite-size DMRG algorithm to investigate some of its ground state properties. The model contains a hopping term between neighbouring sites, a finite on-site interaction energy, and a chemical potential. [To be continued...]

The entire project heavily relies upon the precedent project carried out by the author together with Marco Pompili, where the 1D Bose-Hubbard model was studied using finite-size DMRG. You may find at this link our previous work.

All of the code can be found at open-access in this repository:
`https://github.com/nepero27178/FermiHubbardDMRG`

Contents

*a.gori23@studenti.unipi.it / nepero27178@github.com

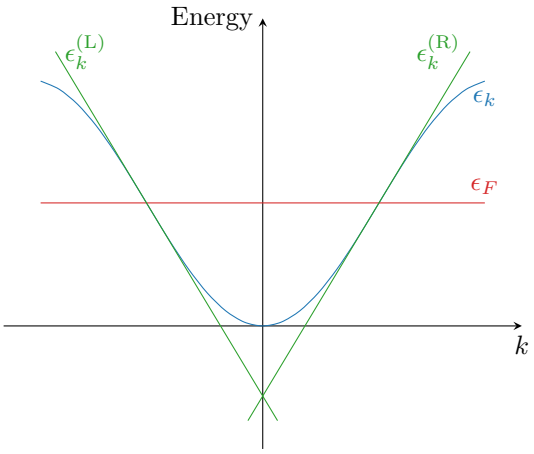


Figure 1: Sketch of the fermionic band ϵ_k, the Fermi level ϵ_F and the two linear bands $\epsilon_k^{(\mathrm{L/R})}$ used to approximate the original bands around the Fermi surface. The double-linear model is often referred to as the Tomonaga-Luttinger model.

1 Theoretical introduction to bosonization

This first, vast section is devoted to the introduction of an extremely powerful technique in one-dimensional fermionic problems, namely, bosonization. It is widely based on the comprehensive work of Giamarchi, [2]. I won't get deep in the calculations neither in refined points about the method, being this last arbitrarily vast. The first part of this section deals with the spinless (a.k.a. polarized) case; the second part introduces the spin degree of freedom.

1.1 Bosonization in a nutshell for spinless fermions

The key idea is simple: start from a conventional fermionic-metallic hamiltonian,

$$\hat{H} = \hat{H}_0 + \hat{V} = \sum_k \xi_k \hat{c}_k^\dagger \hat{c}_k + \hat{V}$$

(we will leave the interaction unspecified, for a moment) where $\xi_k = \epsilon_k - \epsilon_F$ and we are using spinless fermions, for normal bands in ordinary fillings. Consider Fig. 1: the approximation in the above equation is exactly given by making the following assumption: since at low temperature (which, in metals, is a very broad definition) all the relevant Physics takes place at $\xi \sim 0$, and both the deep-down/far-away single-particle states do not contribute either due to Pauli pressure or state depletion, we can as well study the model:

$$\epsilon_k \to \left\{ \epsilon_k^{(\mathrm{L})}, \epsilon_k^{(\mathrm{R})} \right\}$$

Let s be the side index, $s \in \{\mathrm{L}, \mathrm{R}\}$, with

$$\mathrm{sgn}(s) = \begin{cases} +1 & \text{if} \quad s = \mathrm{R} \\ -1 & \text{if} \quad s = \mathrm{L} \end{cases}$$

Then we may approximate around the Fermi surface (in one dimension degenerated in two points)

$$\hat{H}_0 \simeq \hat{K}_0 \equiv \sum_{s \in \{\mathrm{L},\mathrm{R}\}} \sum_k \hbar v_F \left(\mathrm{sgn}(s) k - k_F \right) \left[\hat{c}_k^{(s)} \right]^\dagger \hat{c}_k^{(s)}$$

being $k_F \equiv \sqrt{2m\epsilon_F/\hbar}$ the Fermi wavevector and $v_F \equiv \hbar k_F / m$. $\hat{K}_0$ is the Tomonaga-Luttinger model. In the following, we will set $\hbar = 1$. Now, consider the side-wise density operators,

$$\hat{\rho}_q^{(s)} \equiv \sum_k \left[\hat{c}_{k+q}^{(s)} \right]^\dagger \hat{c}_k^{(s)}$$

Let us use a slightly different, somewhat lighter notation:

$$\hat{\rho}_q^{(s)} \leftrightarrow \hat{\rho}_s(q)$$

From now on, we will proceed only highlighting the important result in the bosonization procedure, since all the detailed derivation is included in [2].

1.1.1 Boson operators

The pivotal result in the bosonization technique is the following:

$$[\hat{\rho}_s(q), \hat{\rho}_{s'}(-q')] = -\delta_{ss'}\delta_{qq'}\mathrm{sgn}(s)\frac{qL}{2\pi} \tag{1}$$

where L is the one-dimensional system length. To get to this point, the very key passage is to employ the identity

$$\hat{A}\hat{B} =: \hat{A}\hat{B} : \; + \langle\Omega|\hat{A}\hat{B}|\Omega\rangle$$

being $\hat{A}$, $\hat{B}$ two operators made of constructions/destructions, $|\Omega\rangle$ the generic many-body vacuum and $: \cdots :$ the normal ordering operation. Eq. (1) only holds if we use this trick, which is, if we make a smart use of the infinite particle populations for the linearized model.

Now, Eq. (1) looks "bosonic". Notice that the left-side density operator vanishes identically for any $q > 0$ on the ground-state Fermi sea $|\Omega\rangle$. This is because it would require to destroy a fermion at any given k and creating one at $k + q$ – but the monotonicity of the linear left band prevents from doing so, because states on the left get deeper and deeper and thus are already occupied. In formulas

$$\hat{\rho}_{\mathrm{L}}(q > 0)\,|\Omega\rangle = 0$$
$$\hat{\rho}_{\mathrm{R}}(q < 0)\,|\Omega\rangle = 0$$

Then, we can define boson operator with finite particle numbers as

$$\hat{b}_q^\dagger \equiv \sqrt{\frac{2\pi}{|q|L}} \sum_{s\in\{\mathrm{L,R}\}} \theta\left(\mathrm{sgn}(s)q\right)\hat{\rho}_s^\dagger(q)$$

$$\hat{b}_q \equiv \sqrt{\frac{2\pi}{|q|L}} \sum_{s\in\{\mathrm{L,R}\}} \theta\left(\mathrm{sgn}(s)q\right)\hat{\rho}_s^\dagger(-q)$$

which of course satisfy

$$\left[\hat{b}_q, \hat{b}_{q'}^\dagger\right] = \delta_{qq'}$$

With a little patience, it can be shown that, taking $q \neq 0$,

$$\left[\hat{b}_q, \hat{K}_0\right] = v_F|q|\hat{b}_q \tag{2}$$

Assuming the (operatorial) basis generated by the bosonic operators to be complete, then this equation completely defines $\hat{K}_0$. It must hold:

$$\hat{K}_0 = \sum_{q\neq 0} v_F|q|\hat{b}_q^\dagger\hat{b}_q + (\text{a term for } q = 0)$$

This is astonishing result of the bosonization method: the kinetic term can be approximated by a quadratic free-bosons hamiltonian. Any quartic fermion interaction term (as are two-body interactions) is density-quadratic and can be cast to an identical form.

Fermionic-bosonic correspondence At the very heart of the bosonization technique, lies a change of basis in operators space: the hamiltonian is mapped from a fermionic representation to a bosonic one, limitedly to the energy regime of our interest. In terms of the boson operators we shall express the fermion field operators,

$$\hat{\psi}_s(x) \equiv \frac{1}{\sqrt{L}} \sum_k e^{ikx} \hat{c}_k^{(s)}$$

To derive the change of basis directly is non-trivial. However, it can be shown:

$$\left[\hat{\rho}_s^\dagger(q), \hat{\psi}_s(x)\right] = -e^{iqx} \hat{\psi}_s(x)$$

The above result is then used to extract the exact field representation in terms of density operators,

$$\hat{\psi}_s(x) = \hat{U}_s \exp\left\{ \mathrm{sgn}(s) \frac{2\pi}{L} \sum_q \frac{e^{iqx}}{q} \hat{\rho}_s(-q) \right\}$$

where $\hat{U}_s$ is a so-called Klein-Haldane factor. The operator $\hat{U}_s$ suppresses a charge uniformly, and is inserted by hand to make the fermion-boson mapping coherent and bijective.

1.1.2 Field-theoretic representation of the free hamiltonian

The final goal is to express the entire hamiltonian in terms of continuous bosonic fields. For now, define:

$$\hat{\phi}(x) \equiv -:\hat{N}: \frac{\pi x}{L} - \frac{i\pi}{L} \sum_{q\neq 0} \frac{e^{-\left(\frac{1}{2}\alpha|q| + iqx\right)}}{q} \sum_{s\in\{\mathrm{L,R}\}} \hat{\rho}_s^\dagger(q) \qquad (\alpha \to 0)$$

$$\hat{\theta}(x) \equiv :\Delta\hat{N}: \frac{\pi x}{L} + \frac{i\pi}{L} \sum_{q\neq 0} \frac{e^{-\left(\frac{1}{2}\alpha|q| + iqx\right)}}{q} \sum_{s\in\{\mathrm{L,R}\}} \mathrm{sgn}(s) \hat{\rho}_s^\dagger(q) \qquad (\alpha \to 0)$$

where $\hat{N} = \hat{N}^{(\mathrm{R})} + \hat{N}^{(\mathrm{L})}$, $\Delta\hat{N} = \hat{N}^{(\mathrm{R})} - \hat{N}^{(\mathrm{L})}$ and α is a convergence cutoff to regularize the theory. Notice that the side-wise number operators appear normal-ordered, thus have finite matrix elements. These field are defined like this for a reason: taking immediately the $\alpha \to 0$ limit and the x derivative, we get

$$\nabla\hat{\phi}(x) = -\pi \left[\hat{\rho}_{\mathrm{R}}(x) + \hat{\rho}_{\mathrm{L}}(x)\right] \qquad \nabla\hat{\theta}(x) = \pi \left[\hat{\rho}_{\mathrm{R}}(x) - \hat{\rho}_{\mathrm{L}}(x)\right] \tag{3}$$

being the spatial density simply given by Fourier-transforming our q-wise density,

$$\hat{\rho}(x) = \frac{1}{L} \sum_q e^{-iqx} \hat{\rho}(q) = \frac{1}{L} \sum_q e^{-iqx} \sum_{s\in\{\mathrm{L,R}\}} \hat{\rho}_s(q)$$

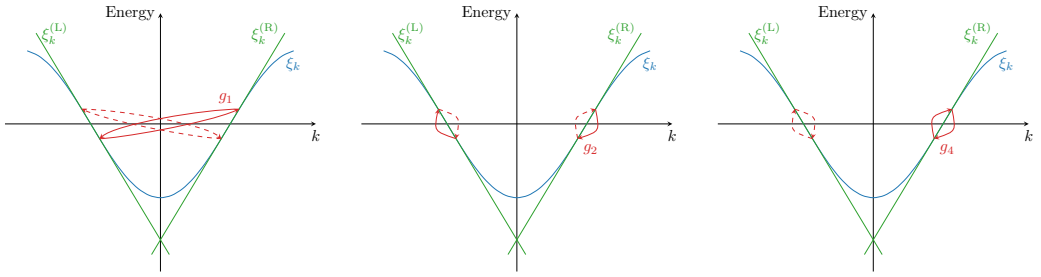
Here, the second "=" sign is the passage where we actively switched to the Tomonaga-Luttinger model of Fig. 1. Then:

$$-\frac{\nabla\hat{\phi}(x)}{\pi} \quad \to \quad \text{particle density, "canonical position"}$$
$$\frac{\nabla\hat{\theta}(x)}{\pi} \quad \to \quad \text{particle RL unbalance, "canonical momentum"}$$

The difference $\hat{\rho}_{\mathrm{R}} - \hat{\rho}_{\mathrm{L}}$ is related to the current operator in one dimension: it just subtracts, point-wise, the left-going density from the right-going density.

Let us go straight to the end: expressing the above fields in terms of boson operators it turns out that

$$\left[\hat{\phi}(x), \frac{\nabla\hat{\theta}(y)}{\pi}\right] = i\delta(x-y)$$



(a) $g_1 = V(q \approx \pm 2k_F)$ process. (b) $g_2 = V(q \approx 0)$ process. (c) $g_4 = V(q \approx 0)$ process.

Figure 2: Diagrammatic sketch of the possible two-fermions interaction in the spinless scenario.

Thus, the fields $\hat{\phi}(x)$ and $\hat{\Pi}(x) \equiv \nabla\hat{\phi}(x)/\pi$ are bosonic and canonically conjugate. Skipping some passages the reader can find in [2], the hamiltonian is represented in field language as:

$$\hat{H}_0 \simeq \hat{K}_0 = \frac{1}{2\pi}\int_0^L dx\, v_F \left[\left(\nabla\hat{\phi}(x)\right)^2 + \left(\nabla\hat{\theta}(x)\right)^2\right] \tag{4}$$

This is the very cornerstone of bosonization. This is the Klein-Gordon bosonic-massless hamiltonian. Apart from pure math, what we obtained is a consequence of the strict one-dimensional topology: in such low dimensionality the Fermi surface reduces to two points ($k = \pm k_F$), thus the only low-energy particle-hole excitations allowed (those collective excitations proper of a system of free fermions) either have a well defined momentum of $q \simeq 0$ or $q \simeq \pm 2k_F$. Low energy spectrum only exists strictly around these points.

Particle-hole excitations are always made of a combined creation and annihilation of fermions, thus intuitively remind of a "bosonic character". In order to interpret such excitations as bosons, however, they must be somewhat stable. This only happens in one dimension: here, particle-hole excitations *are* emergent bosons. We do not enter in deep details here, recalling the main reference of this report [2] and its exceptional cover of the topic. To make the discussion here clearer, however, it must be cited that the reason for insurgence of boson fields is the fact that the use of a linear spectrum ensures independence of the particle-hole spectrum from the starting point on the (degenerated) Fermi surface, and thus lets us make the fermion-to-boson mapping.

1.1.3 Inserting interactions

It is time to let in interactions. As we said, particle-hole excitations exchange a fermion from the Fermi sea with a hole from outside. Due to the strict topology of the Fermi surface, only three processes actually contribute – namely g_1, g_2 and g_4, respectively in Figs. 2a-2b-2c. Note that, for spinless fermions, due to particles indistinguishability, actually g_1 and g_2 are the same process[1].

Now, consider a particle-hole symmetric interaction, *quartic* in the fermionic operators,

$$V \sim c^\dagger c^\dagger c c$$

as is for instance an s-wise spatial density-density interaction,

$$\hat{V} = \sum_{s_1\in\{\mathrm{L,R}\}}\sum_{s_2\in\{\mathrm{L,R}\}}\int_0^L dx_1 \int_0^L dx_2\, V_{s_1 s_2}(x_1 - x_2)\hat{\rho}_{s_1}(x_1)\hat{\rho}_{s_2}(x_2)$$

coupling left-going and right-going fermions. We collect g_4 processes as those terms with $s_1 = s_2$ and g_1, g_2 processes as those terms with $s_1 \neq s_2$,

$$\underbrace{\hat{\rho}_\mathrm{R}(x_1)\hat{\rho}_\mathrm{R}(x_2) \quad \hat{\rho}_\mathrm{L}(x_1)\hat{\rho}_\mathrm{L}(x_2)}_{g_4} \qquad \underbrace{\hat{\rho}_\mathrm{R}(x_1)\hat{\rho}_\mathrm{L}(x_2) \quad \hat{\rho}_\mathrm{L}(x_1)\hat{\rho}_\mathrm{R}(x_2)}_{g_1 = g_2}$$

[1] We here skip an explanation about how we absorb g_1 inside g_2, a detail that will become clear in the spinful case.

At this point, we make an apparently heavy assumption we will heal later. Let us use for now a contact-like interaction,

$$[V(x-y)] = \frac{1}{2}\begin{bmatrix} g_4 & g_2 \\ g_2 & g_4 \end{bmatrix} \delta(x-y) \qquad \text{with } g_2, g_4 \in \mathbb{R}$$

(with a little notation abuse, we used the side indices s_1, s_2 as row-column indices) and let us analyze separately the contributions to the hamiltonian: $\hat{V} = \hat{V}_2 + \hat{V}_4$.

g_4 process. this is the simpler case. The densities vertex contributions to $\hat{K}_0$ is simply

$$\hat{V}_4 = \frac{1}{2} g_4 \int_0^L dx\, [\hat{\rho}_{\mathrm{R}}(x)\hat{\rho}_{\mathrm{R}}(x) + \hat{\rho}_{\mathrm{L}}(x)\hat{\rho}_{\mathrm{L}}(x)]$$

Recalling Eq. (3), we get immediately

$$\begin{aligned}
\hat{V}_4 &= g_4 \int_0^L dx\, \left[\left(\frac{\nabla\hat{\phi}(x) - \nabla\hat{\theta}(x)}{2\pi} \right)^2 + \left(\frac{\nabla\hat{\phi}(x) + \nabla\hat{\theta}(x)}{2\pi} \right)^2 \right] \\
&= \frac{g_4}{2\pi v_F} \times \frac{1}{2\pi} \int_0^L dx\, v_F \left[\left(\nabla\hat{\phi}(x) \right)^2 + \left(\nabla\hat{\theta}(x) \right)^2 \right] \\
&= \frac{g_4}{2\pi v_F} \hat{K}_0
\end{aligned}$$

which is remarkable: considering this process, the hamiltonian looks like:

$$\hat{K}_0 + \hat{V}_4 + \hat{V}_2 = \frac{1}{2\pi} \int_0^L dx\, \underbrace{v_F \left(1 + \frac{g_4}{2\pi v_F} \right)}_{u} \left[\left(\nabla\hat{\phi}(x) \right)^2 + \left(\nabla\hat{\theta}(x) \right)^2 \right] + \hat{V}_2$$

Now, u is the **bosons velocity renormalized by g_4-like interactions**.

g_2 process. In a very similar fashion, it is easy to obtain

$$\begin{aligned}
\hat{V}_2 &= \frac{1}{2} g_2 \int_0^L dx\, \left[2 \left(\frac{\nabla\hat{\phi}(x) - \nabla\hat{\theta}(x)}{2\pi} \right) \left(\frac{\nabla\hat{\phi}(x) + \nabla\hat{\theta}(x)}{2\pi} \right) \right] \\
&= \frac{g_2}{2\pi v_F} \cdot \frac{1}{2\pi} \int_0^L dx\, v_F \left[\left(\nabla\hat{\phi}(x) \right)^2 - \left(\nabla\hat{\theta}(x) \right)^2 \right]
\end{aligned}$$

It is not so immediate to insert this term in the interacting hamiltonian. However, an elegant formulation exists involving two parameters u and K:

$$\hat{K}_0 + \hat{V}_4 + \hat{V}_2 = \frac{1}{2\pi} \int_0^L dx\, \left[\frac{u}{K} \left(\nabla\hat{\phi}(x) \right)^2 + uK \left(\nabla\hat{\theta}(x) \right)^2 \right] \tag{5}$$

trivially defined as

$$\frac{u}{K} \equiv 1 + \frac{g_4}{2\pi v_F} + \frac{g_2}{2\pi v_F} \qquad uK \equiv 1 + \frac{g_4}{2\pi v_F} - \frac{g_2}{2\pi v_F}$$

a condition simultaneously satisfied by

$$u = v_F \sqrt{\left(1 + \frac{y_4}{2} \right)^2 - \left(\frac{y_2}{2} \right)^2} \qquad K = \sqrt{\frac{2 + y_4 - y_2}{2 + y_4 + y_2}} \qquad y_i \equiv \frac{g_i}{\pi v_F}$$

This collection of equation is all we need to completely map a one-dimensional interacting fermionic problem into a renormalized free bosonic problem. Everything we have done hold for spinless fermions and contact interaction, but can be extended.

1.1.4 The euclidean action

We here briefly sketch the derivation of the bosonized euclidean action. Starting from the hamiltonian density,

$$\hat{\mathcal{K}}[\phi,\Pi] = \frac{1}{2\pi}\left[\frac{u}{K}\left(\nabla\hat{\phi}(x)\right)^2 + uK\left(\pi\hat{\Pi}(x)\right)^2\right]$$

the euclidean action is immediately recovered by Legendre-transforming $\hat{\mathcal{K}}$ in imaginary time,

$$\begin{aligned}\mathcal{L}[\phi,\Pi] &= i\Pi\frac{\partial}{\partial\tau}\phi - \mathcal{K}[\phi,\Pi] \\ &= \frac{1}{2\pi}\left[2i\nabla\theta\frac{\partial}{\partial\tau}\phi - \frac{u}{K}\left(\nabla\phi\right)^2 + uK\left(\nabla\theta\right)^2\right]\end{aligned}$$

Now the calculation gets a little intricate, and we will skip it. The key point is to recognize that, being L the lagrangian,

$$S[\phi,\Pi] \equiv \int_0^\beta d\tau\, L[\phi,\Pi] = \int_0^\beta d\tau \int_0^L dx\, \mathcal{L}[\phi,\Pi]$$

and $\mathcal{Z}$ the partition function

$$\mathcal{Z} \equiv \int \mathcal{D}[\phi]\mathcal{D}[\Pi] e^{-S[\phi,\Pi]/\hbar}$$

one is able to complete the square for the $\nabla\theta$ part appearing in $\mathcal{L}$ and reduce the Π part of the above integral to a gaussian form. The same trick holds for any Π-independent observable we may want to average. The final, effective ϕ-action is just

$$S_\phi \equiv \frac{1}{2\pi}\int_0^\beta d\tau \int_0^L dx\, \left[\frac{1}{uK}\left(\partial_\tau\phi(x,\tau)\right)^2 + \frac{u}{K}\left(\nabla\phi(x,\tau)\right)^2\right] \tag{6}$$

which, exponentiated, is the path integral statistical weight.

1.1.5 Spinless fermions observables

The big, heavy (but wondrous) theoretical part is over: let's get operative. Our aim is to estimate the renormalized parameters u and K. First, we need to understand how to get them out of some observables.

Charge compressibility. A very simple observable, capable of letting us estimate easily the ratio u/K, is charge compressibility. Let μ be the chemical potential,

$$\hat{K} \to \hat{K} - \mu\int_0^L dx\, \hat{\rho}(x)$$

Following the convention of Giamarchi, we will define compressibility

$$\kappa \equiv \frac{\partial\rho}{\partial\mu} \qquad \rho = \frac{1}{L}\int_0^L dx\, \langle\hat{\rho}(x)\rangle$$

(notice that usually the definition above is completed by a prefactor ρ^{-2}, we omit). Using Eq. (3)[2],

$$\begin{aligned}\frac{\partial\rho}{\partial\mu} &= \frac{\partial}{\partial\mu}\frac{1}{L}\int_0^L dx\, \langle\hat{\rho}(x)\rangle \\ &= -\frac{1}{\pi L}\frac{\partial}{\partial\mu}\int_0^L dx\, \left\langle\nabla\hat{\phi}(x)\right\rangle\end{aligned}$$

[2]To be complete, we here are hiding a passage. In fact, $\pi\hat{\rho} = \pi\left[\mathrm{RR}+\mathrm{LL}+\mathrm{RL}+\mathrm{LR}\right]$ (here we use the shorthand notation $\mathrm{s_1s_2} = \hat{\psi}^\dagger_{s_1}\hat{\psi}_{s_2}$). Taking the average value, $\pi\langle\hat{\rho}\rangle = \pi\langle\mathrm{RR}+\mathrm{LL}\rangle + \pi\langle\mathrm{RL}+\mathrm{LR}\rangle$, and it's evident by symmetry that $\langle\mathrm{RL}+\mathrm{LR}\rangle = 0$; which justifies our last line, since $\pi\langle\mathrm{RR}+\mathrm{LL}\rangle = -\langle\nabla\hat{\phi}\rangle$.

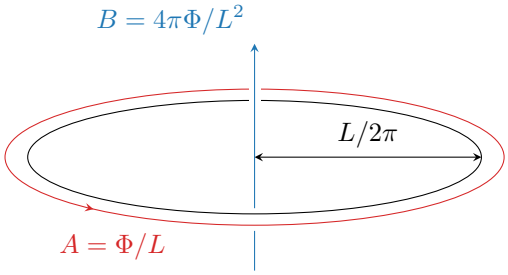


Figure 3: Schematics of a static flux Φ pinning through a ring of circumference L.

Now, consider the term we are adding to the hamiltonian: let us add a pure energy shift term (physically irrelevant) and manipulate the above expression a bit,

$$\begin{aligned} -\mu \int_0^L dx\, \hat{\rho}(x) &= \frac{\mu}{\pi} \int_0^L dx\, \nabla\hat{\phi}(x) + \Delta \\ &= \frac{1}{2\pi} \times 2 \int_0^L dx\, \frac{u}{K} \left(\mu \frac{K}{u}\right) \left(\nabla\hat{\phi}(x)\right) + \underbrace{\frac{1}{2\pi} \int_0^L dx\, \left(\mu \frac{K}{u}\right)^2}_{\Delta} \end{aligned}$$

It is now immediate to see that if we define

$$\hat{\varphi}(x) \equiv \hat{\phi}(x) + \mu \frac{K}{u} x$$

we have:

$$\hat{K} - \mu \int_0^L dx\, \hat{\rho}(x) = \frac{1}{2\pi} \int_0^L dx\, \left[\frac{u}{K} \left(\nabla\hat{\varphi}(x)\right)^2 + uK \left(\nabla\hat{\theta}(x)\right)^2\right]$$

an expression canonically equivalent to Eq. (5). Now, for this new system the term $\nabla\hat{\varphi}$ represents charge density fluctuations. This implies that $\langle\nabla\hat{\varphi}\rangle = 0$ at any point. Then,

$$-\left\langle \nabla\hat{\phi}(x) \right\rangle = \mu \frac{K}{u}$$

Finally:

$$\begin{aligned} \frac{\partial\rho}{\partial\mu} &= -\frac{1}{\pi L} \frac{\partial}{\partial\mu} \int_0^L dx\, \left\langle \nabla\hat{\phi}(x) \right\rangle \\ &= \frac{\partial}{\partial\mu} \mu \frac{K}{\pi u} \times \frac{1}{L} \int_0^L dx = \frac{K}{\pi u} \end{aligned}$$

Then, to measure the ratio u/K we need to measure the quantity $(\pi\Delta\rho/\Delta\mu)^{-1}$ (times $\hbar$, to be dimensionally correct). This most certainly is a simple quantity to be measured by the means of a DMRG simulation.

Charge stiffness Another observable rather easy to compute numerically is the charge stiffness; which is basically the tendency of the system to respond to an external charge-coupling field. Now, assuming a closed-chain topology (as in Fig. 3), we see that a flux Φ threading the ring accounts for a static vector potential

$$A = \frac{\Phi}{L}$$

We define the unit flux as: $\Phi_0 \equiv h/e$. The overall effect on the fermionic system is an overall momentum shift originated by the covariant derivative formulation,

$$k \to k - \frac{e}{\hbar} A = k - \frac{2\pi}{L} \frac{\Phi}{\Phi_0}$$

Let us define the shift angle:

$$\eta \equiv 2\pi \frac{\Phi}{\Phi_0}$$

Finally, absorbing the latter as a gauge transformation, this translates in the presence of twisted boundary conditions by an angle $2\pi\Phi/\Phi_0$ in the wavefunction. Now, given the band $\xi_k[\Phi]$, the current density is simply

$$\begin{aligned} J &= \frac{1}{L} \sum_{k\colon \xi_k \leq 0} \frac{1}{\hbar} \frac{\partial}{\partial k} \xi_k[\Phi] \Big|_\Phi \\ &= J_0 + \frac{1}{L\hbar} \sum_{k\colon \xi_k \leq 0} L \frac{\partial}{\partial \eta} \xi_k[\Phi] \Big|_\Phi \\ &= \frac{1}{\hbar} \frac{\partial}{\partial \eta} E[\Phi] \end{aligned}$$

In the second passage we have isolated the contribution to the derivative given from the free system J_0, null by symmetry, and in the last the ground-state energy $E[\Phi]$ was recognized as the sum of all single-particle occupied states.

Now, charge stiffness is simply the zero-flux current response:

$$\mathcal{D} = \frac{\partial J}{\partial \Phi} \Big|_{\Phi=0}$$

As for the compressibility, we adopt a slightly different (and charge-neutral) definition,

$$\mathcal{D} \equiv \frac{\pi L}{e} \frac{\partial J}{\partial \Phi} \Big|_{\Phi=0} \tag{7}$$

Inserting our previous result,

$$\mathcal{D} = \frac{\pi L}{e} \frac{\Phi_0}{2\pi} \frac{\partial J}{\partial \eta} \Big|_{\Phi=0} = \pi L \frac{\partial^2}{\partial \eta^2} E[\Phi] \Big|_{\Phi=0}$$

The second derivative of the ground-state energy, taken with respect to the twisting angle, is – apart from some factors – the charge stiffness.

We now need to link all of this with the bosonization scheme. The procedure is identical to the one carried out for the charge compressibility in last paragraph:

1. Include the minimally coupled interaction in the euclidean effective action of Eq. (6),

$$S_\phi \to S_\phi - \int dx\, J(x) A(x) = S_\phi - \frac{\Phi}{L} \int dx\, J(x)$$

2. The charge density current is one dimension is obtained easily from the continuity equation:

$$\partial_t \rho + \nabla j = 0 \qquad \Longrightarrow \qquad j = \frac{1}{\pi} \partial_t \phi$$

   having used $\rho = -\nabla\phi/\pi$ and ignored boundary terms.

3. A constant added to the action does not change its variational properties. Thus, defining

$$\varphi \equiv \phi - uK \frac{\Phi}{L} \tau$$

   neither the time nor the spatial part get affected by the transformation, and we recover the action for a flux-free system.

4. Since for the flux-free system the induced current is zero, we have

$$J = \frac{1}{\pi} \langle \partial_\tau \phi \rangle = uK \frac{\Phi}{\pi L}$$

Recalling the definition of $\mathcal{D}$ of Eq. (7), we finally conclude

$$\mathcal{D} = uK \tag{8}$$

which is the second relation we needed in order to determine u and K. The entirety of this derivation could have been worked out analogously by expressing the current in terms of the conjugate momentum field Π and completing the square directly in the hamiltonian.

Equal-time Green's function. The single-particle Green's function is defined in imaginary time, and for s-side fermions, as:

$$\mathcal{G}_s(x,\tau) \equiv -\left\langle \mathrm{T}_\tau \left\{ \hat{\psi}_s(x,\tau)\hat{\psi}_s^\dagger(0,0) \right\} \right\rangle$$

having we assumed in definition spacetime translational invariance, and being $\mathcal{T}_\tau$ the time-ordering operator. Let us take $\tau = 0^-$, thus keeping the order $\hat{\psi}\hat{\psi}^\dagger$ inside the expectation value. We follow here the lead of [2, 4]: the occupation factor $n(k)$,

$$n(k) \equiv \left\langle \hat{c}_k^\dagger \hat{c}_k \right\rangle$$

is given by the Fourier transform of the equal time Green's function:

$$n(k) = \int_0^L dx\, e^{-ikx} \mathcal{G}_s(x, 0^-)$$

both for $s = \mathrm{R}, \mathrm{L}$ due to inversion symmetry. At zero temperature, we have the following algebraic dependence:

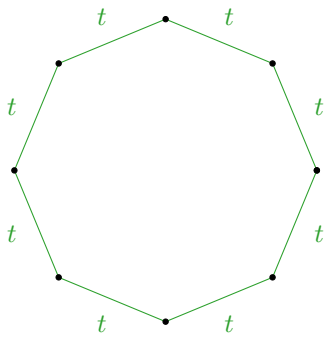
$$n(k) = n(k_F) - A \times \mathrm{sgn}(k - k_F)|k - k_F|^\zeta \qquad \zeta \equiv \frac{1}{4}\left(K + \frac{1}{K} - 2\right)$$

with $A \in \mathbb{R}$. Then, a suitable way to extract the K parameter on a lattice model simulation would be to perform the following computation:

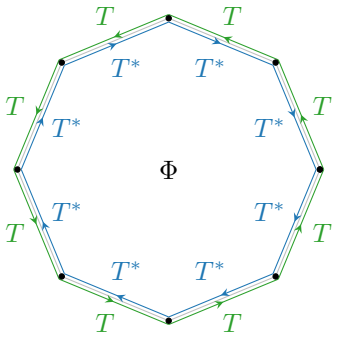
$$n(k) \simeq \left\langle \mathrm{FT}\left\{ \hat{c}_j^\dagger \hat{c}_j \right\} \right\rangle = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} \left\langle \hat{c}_j^\dagger \hat{c}_j \right\rangle e^{ikj}$$

From this measure ζ can be extracted for $k < k_F$ and $k > k_F$, and from the latter K.

Density-density fluctuations. [To be continued...]



(a) Lattice with null flux.



(b) Lattice with finite flux Φ.

Figure 4: In Fig. 4a a schematics of a $1D$ closed lattice is portrayed. The hopping amplitude t is purely real, $t = \mathrm{sgn}(t)|t|$. In Fig. 4b the same lattice is represented, but coupled to a finite threading flux Φ which can be absorbed via the pseudo-gauge transformation in Eq. [To be continued...]. As a consequence, the hopping amplitude acquires a chirality which manifests in a non-null imaginary part, $T = te^{i\Phi/L}$.

2 The Fermi-Hubbard model

In this project we limit ourselves to a polarized (spinless fermions) system. Extension to a spinful system is possible and introduces some refinements in the general bosonization scheme, the most notable being the famous spin-charge separation. Let us take it easy: consider the following interacting hamiltonian:

$$\hat{H} \equiv -t \sum_{\langle j,k \rangle} \left[\hat{c}_j^\dagger \hat{c}_k + \hat{c}_k^\dagger \hat{c}_j \right] + V \sum_{\langle j,k \rangle} \hat{n}_j \hat{n}_k - \mu \sum_{j=1}^{L} \hat{n}_j \tag{9}$$

defined on a closed $1D$ lattice ring, as in Fig. 4a. This is a simple nearest-neighbors (NN) interacting lattice hamiltonian with NN interaction V, chemical potential μ and hopping amplitude t,

$$t, V, \mu \in \mathbb{R}$$

We will also be considering a magnetic flux Φ threading the ring and coupling to the charge degree of freedom. On a ring this pinned flux acts as a tangential vector potential, which is, a momentum offset; thus the correct way to absorb into our lattice framework this interaction is via the pseudo-gauge transformation

$$\hat{c}_j \to e^{-ij\phi} \hat{c}_j \qquad \hat{c}_j^\dagger \to e^{ij\phi} \hat{c}_j^\dagger \qquad \phi \equiv \frac{\Phi}{L}$$

Incorporate the latter in the above hamiltonian: the hopping amplitude becomes complex (which is, chiral) $t \to T \equiv te^{i\phi}$, with $t, \phi \in \mathbb{R}$. We have, as in Fig. 4b

$$\hat{H} \equiv -t \sum_{j=1}^{L} \left[e^{-i\phi} \hat{c}_j^\dagger \hat{c}_{j+1} + e^{i\phi} \hat{c}_{j+1}^\dagger \hat{c}_j \right] + V \sum_{j=1}^{L} \hat{n}_j \hat{n}_{j+1} - \mu \sum_{j=1}^{L} \hat{n}_j \tag{10}$$

where a $\mod L$ operation is intended: $L+1 \leftrightarrow 1$. We want to indagate its ground-state properties. The relevant parameters will be the reduced interaction V/t and chemical potential μ/t.

$V/t > 0$	Repulsive interaction
$V/t < 0$	Attractive interaction

Intuitively, if the interaction becomes dominant with respect to the hopping dynamics, the combined effect of attraction/repulsion and Pauli exclusion principle should lead to two different forms

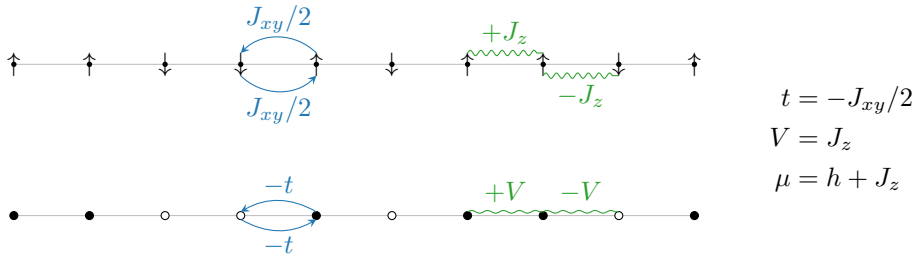


Figure 5: Schematics of the Jordan-Wigner mapping. The above chain represents the XXZ model, while the chain below represents the spinless Fermi-Hubbard model. Hollow circles represent holes, filled circles represents on-site particles. In both chain the two competing processes are represented: the NN interaction and the swapping interaction.

of localization. On one hand, if the interaction is strong and attractive, the ground state should be uniformly filled, because fermions save energy both by closed packing and by increasing density due to the negative chemical potential contribution ($\mu > 0$). On the other hand, a strong repulsive interaction could lead to an half-filled chain, which sacrifices the chemical potential energy gain lost by reducing the particle number by not paying the energy cost of having nearby fermions. In both cases hopping is suppressed, thus fermions are localized; now it is a matter of seeing if these states are actually realized.

2.1 Jordan-Wigner mapping of the Heisenberg XXZ model

The model presented above can be obtained rather easily through a Jordan-Wigner of the Heisenberg XXZ model in transverse field,

$$\hat{H}_{\mathrm{XXZ}} \equiv \sum_{\langle j,k \rangle} \left[J_{xy} \left(\hat{S}_j^x \hat{S}_k^x + \hat{S}_k^y \hat{S}_j^y \right) + J_z \hat{S}_j^z \hat{S}_k^z \right] - h \sum_{j=1}^{L} \hat{S}_j^z \tag{11}$$

The Jordan-Wigner mapping, only feasible in one dimension due to sites ordering, is given by:

$$\hat{S}_j^+ \to \hat{c}_j^\dagger e^{i\pi \sum_{k<j} \hat{c}_k^\dagger \hat{c}_k} \qquad \hat{S}_j^- \to \hat{c}_j e^{-i\pi \sum_{k<j} \hat{c}_k^\dagger \hat{c}_k} \qquad \hat{S}_j^z \to \hat{n}_j - \frac{\mathbb{I}}{2}$$

Notice the appearance of the Jordan string,

$$e^{i\pi \sum_{k<j} \hat{c}_k^\dagger \hat{c}_k} = (-1)^{\zeta_j} \qquad \zeta_j \equiv \sum_{k<j} \hat{n}_k$$

Essentially, the above string counts the fermions *before* the site in question and gives back a factor $+1$ for even number, -1 for odd number. This works for open-end chains, where the concept of *before* is actually well-defined. It is straightforward to see:

$$\begin{aligned} S_j^+ \hat{S}_{j+1}^- &\to (-1)^{\zeta_j + \zeta_{j+1}} \hat{c}_j^\dagger \hat{c}_{j+1} = (-1)^{n_j} \hat{c}_j^\dagger \hat{c}_{j+1} = c_j^\dagger \hat{c}_{j+1} \\ S_j^- \hat{S}_{j+1}^+ &\to (-1)^{\zeta_j + \zeta_{j+1}} \hat{c}_j \hat{c}_{j+1}^\dagger = (-1)^{n_j + 1} \hat{c}_{j+1}^\dagger \hat{c}_j = c_{j+1}^\dagger \hat{c}_j \end{aligned}$$

having we used $\zeta_j + \zeta_{j+1} = 2\zeta_j + n_j$. Let us take a 1D spin chain with open boundary conditions (OBC). The transformation gives

$$\begin{aligned} \hat{H}_{\mathrm{XXZ}} &\equiv \sum_{j=1}^{L-1} \left[\frac{J_{xy}}{2} \left(\hat{S}_j^+ \hat{S}_{j+1}^- + \hat{S}_j^- \hat{S}_{j+1}^+ \right) + J_z \hat{S}_j^z \hat{S}_{j+1}^z \right] - h \sum_{j=1}^{L} \hat{S}_j^z \\ &= \sum_{j=1}^{L-1} \left[\frac{J_{xy}}{2} \left(\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \right) + J_z \left(\hat{n}_j - \frac{\mathbb{I}}{2} \right) \left(\hat{n}_{j+1} - \frac{\mathbb{I}}{2} \right) \right] - h \sum_{j=1}^{L} \left(\hat{n}_j - \frac{\mathbb{I}}{2} \right) \\ &= \sum_{j=1}^{L-1} \left[\frac{J_{xy}}{2} \left(\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j \right) + J_z \hat{n}_j \hat{n}_{j+1} \right] - \sum_{j=1}^{L} h_j \hat{n}_j + \frac{hL}{2} + \frac{J_z (L-1)}{2} \end{aligned}$$

Figure 6: Schematics for the XXZ model phase diagram. We are here considering a zero-field model, $h = 0$ (which is mapped by the maps (12) to a $\mu = J_z$ model). H indicates Heisenberg, I indicates Ising; F stands for Ferromagnet, AF for Anti-Ferromagnet; XY stands for pure XY model. The color of each label recalls the dominant interaction of Fig. 5.

where we defined:

$$h_j = \begin{cases} h + J_z/2 & \text{if} \quad j = 1, L \\ h + J_z & \text{if} \quad 1 < j < L \end{cases}$$

Apart from a constant energy shift, in the bulk ($1 < j < L$) this is our spinless fermions hamiltonian in Eq. (9) with the following maps:

$$t = -\frac{J_{xy}}{2} \qquad V = J_z \qquad \mu = h + J_z \tag{12}$$

A schematics of the mapping is given in Fig. 5.

Now, add another site. This amounts for extra terms in the hamiltonian,

$$\hat{H}_{\text{XXZ}} \to \hat{H}_{\text{XXZ}} + \frac{J_{xy}}{2}\left(\hat{S}^+_L \hat{S}^-_{L+1} + \hat{S}^-_L \hat{S}^+_{L+1}\right) + J_z \hat{S}^z_L \hat{S}^z_{L+1}$$

If we now aim to identify the open ends, which is, close the chain onto itself, the condition is

$$\hat{S}^\alpha_{L+1} = \hat{S}^\alpha_1$$

The first-site Jordan-Wigner string is trivial, $\zeta_1 = 0$. The implementation of periodic boundary conditions requires in operator space then $\zeta_{L+1} \to \zeta_1 = 0$. Finally, it is trivial to see

$$(-1)^{\zeta_L}\hat{c}^\dagger_L = (-1)^{\#_F}\hat{c}^\dagger_L \qquad (-1)^{\zeta_L+1}\hat{c}_L = (-1)^{\#_F}\hat{c}_L$$

with $\#_F$ the total number of fermions on the chain. Putting all together, we see that as long as $\#_F$ is **even** [Check: I have the suspect it should be odd, actually...], we can impose periodic boundary conditions,

$$\hat{S}^+_L \hat{S}^-_1 = \hat{c}^\dagger_L \hat{c}_1 \qquad \hat{S}^-_L \hat{S}^+_1 = \hat{c}^\dagger_1 \hat{c}_L$$

Simpler reasoning holds for the z terms. Putting all together, we see that the PBC-XXZ model is mapped onto a spinless fermionic system on a ring with even number of particles, with the rules of Eq. (12). Since the PBC-XXZ admits for an exact Bethe-Ansatz solution, we can link the phase transitions of the two models.

Phase diagrams

The phase diagram of the XXZ model is readily obtained by the means of exact methods like Bethe Ansatz. Of course, the dominant parameter is the ratio J_z/J_{xy} which measures the dominant contribution to energy given by spin-spin NN interaction (z term) and spin diffusion (xy term). Whenever $|J_z| = |J_{xy}|$, the model is of the Heisenberg class.

The basic, field free phase diagram is represented schematically in Fig. 6.

1. The system tends to an Ising Ferromagnet for $J_z/J_{xy} < -1$, with dominant behavior the complete alignment of spins (which maps onto the spinless Fermi-Hubbard model as a completely filled chain).

2. Moving across the first Heisenberg boundary, $J_z = -J_{xy}$, the dominant behavior is spin diffusion up to a perfect local fields free situation of $J_z = 0$. This phase maps onto the spinless Fermi-Hubbard model as a superconducting phase.

3. Crossing the second Heisenberg boundary, $J_z = J_{xy}$, the system tends to an Ising Anti-Ferromagnet, dominated by the Néel state configuration. The latter maps onto an half-filling and Mott-localized fermionic chain.

For a fixed number system, this is the expected phase dynamics. [Check the correctness of all the claims.]

2.2 Bosonization of the model

[To be continued...]

3 Algorithms and simulations

This section is devoted to delineate the system properties we aim to simulate. The algorithm used is finite-size DMRG, implemented in the `Julia language` via the well supported `ITensors.jl` `ITensorsMPS.jl` packages.

3.1 General strategy and target(s)

Our final aim is to extract the Bosonization parameters u and K for the spinless Fermi-Hubbard model of Eq. (9). Following the lead the XXZ mapping, we expect the model to exhibit [To be continued...]

3.2 Finite-size DMRG

[To be continued...]

4 Data analysis and results

4.1 Ground-state phase physical properties

As a first analysis, I considered two specific parametric configurations, whose Jordan-Wigner mapped ground-states are expected to lie respectively in the XY and Ising Ferromagnet phases,

$$[s_{\mathrm{XY}}]\colon \left(\frac{h}{J_{xy}}, \frac{J_z}{J_{xy}}\right) = \left(-\frac{1}{2}, -\frac{1}{4}\right) \quad \to \quad \left(\frac{V}{t}, \frac{\mu}{t}\right) = \left(1, \frac{3}{2}\right)$$
$$[s_{\mathrm{IF}}]\colon \left(\frac{h}{J_{xy}}, \frac{J_z}{J_{xy}}\right) = \left(-1, \frac{1}{2}\right) \quad \to \quad \left(\frac{V}{t}, \frac{\mu}{t}\right) = (2, 1)$$

I shall indicate these configurations as indicated between square brackets.

PER NON DIMENTICARMI DOVE SONO ARRIVATO Continua con l'analisi degli stati qua sopra. Con potenziale chimico positivo dati i mappings pare che si possa solo vedere la transizione XY-FE. Fatta l'analisi di singoli stati, mappare i bordi di fase dal modello XXZ e fare una sweep orizzontale di compressibilità per vedere la fase gapless. Poi vedere se il calcolo del gap di carica produce dei boundareis sensati.
[To be continued...]

References

[1] Jan von Delft and Herbert Schoeller. "Bosonization for beginners — refermionization for experts". In: *Annalen der Physik* 510.4 (1998), pp. 225–305. DOI: https://doi.org/10.1002/andp.19985100401. eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/andp.19985100401. URL: https://onlinelibrary.wiley.com/doi/abs/10.1002/andp.19985100401.

[2] Thierry Giamarchi. *Quantum Physics in One Dimension*. Oxford University Press, Dec. 2003. ISBN: 9780198525004. DOI: 10.1093/acprof:oso/9780198525004.001.0001. URL: https://doi.org/10.1093/acprof:oso/9780198525004.001.0001.

[3] Mykhailo V. Rakov, Michael Weyrauch, and Briiissuurs Braiorr-Orrs. "Symmetries and entanglement in the one-dimensional spin-$\frac{1}{2}$ XXZ model". In: *Phys. Rev. B* 93 (5 Feb. 2016), p. 054417. DOI: 10.1103/PhysRevB.93.054417. URL: https://link.aps.org/doi/10.1103/PhysRevB.93.054417.

[4] David Senechal. "An Introduction to bosonization". In: *CRM Workshop on Theoretical Methods for Strongly Correlated Fermions*. Aug. 1999. arXiv: cond-mat/9908262.