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

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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

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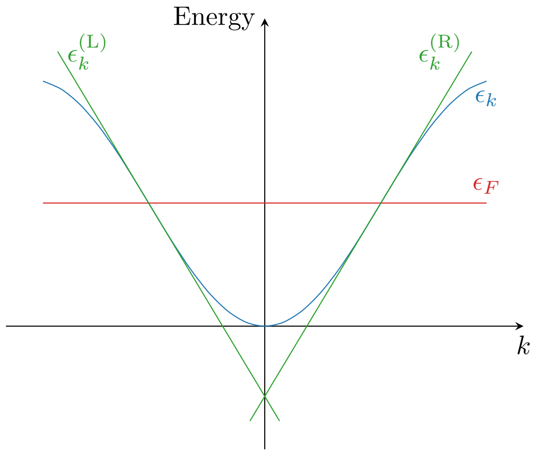


Figure 1: Sketch of the fermionic band ϵ_k, the Fermi level ϵ_F and the two linear bands $\epsilon_k^{(\mathrm{L/R})}$ used to approximate the original bands around the Fermi surface. The double-linear model is often referred to as the Tomonaga-Luttinger model.

1 Theoretical introduction

[To be continued...]

1.1 Bosonization in a nutshell

This sections is intended as a brief sketch and discussion of the powerful **bosonization** method in one dimension. This section is widely based on the comprehensive work of Giamarchi, [2]. 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)

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

being $k_F \equiv \sqrt{2m\epsilon_F}$ the Fermi wavevector and $v_F \equiv k_F/m$. $\hat{K}_0$ is the Tomonaga-Luttinger model. 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].

Boson operators

The pivotal result in the bosonization technique is the following:

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

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

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

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.

Field-theoretic representation of the 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

$$\nabla\hat{\phi}(x) = -\pi\hat{\rho}(x) \qquad \nabla\hat{\theta}(x) = \pi\Delta\hat{\rho}(x) \tag{3}$$

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.

We have $\hat{\rho} \equiv \sum_s \hat{\rho}_s = \hat{\rho}_\mathrm{R} + \hat{\rho}_\mathrm{L}$ and $\Delta\hat{\rho} \equiv \sum_s \mathrm{sgn}(s)\hat{\rho}_s = \hat{\rho}_\mathrm{R} - \hat{\rho}_\mathrm{L}$. Then:

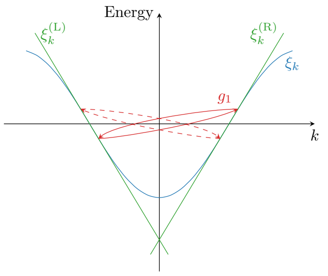
$$-\frac{\nabla\hat{\phi}(x)}{\pi} \quad \rightarrow \quad \text{particle density}$$

$$\frac{\nabla\hat{\theta}(x)}{\pi} \quad \rightarrow \quad \text{particle current}$$

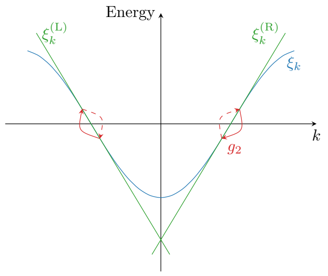
Clearly $\Delta\hat{\rho}$ is the current operator: it just subtracts, point-wise, the left-going density from the right-going density. The remaining unbalance is the current by definition.

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

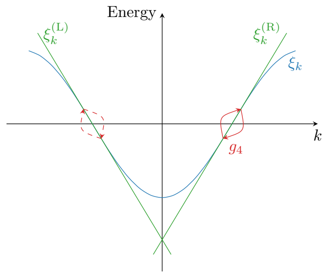
$$\left[\hat{\phi}(x), \frac{\nabla\hat{\theta}(y)}{\pi}\right] = i\delta(x-y)$$



(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:

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

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.

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.

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,

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

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 $s_1 \neq s_2$,

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

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

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

Recalling Eq. (3), we get immediately

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

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

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

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

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

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

$$\hat{K}_0 + \hat{V}_4 + \hat{V}_2 = \frac{1}{2\pi} \int_{\mathbb{R}} dx \; \left[\frac{u}{K} \left(\nabla\hat{\phi}(x)\right)^2 + uK \left(\nabla\hat{\theta}(x)\right)^2 \right]$$

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.

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.

Charge stiffness.

Using a more realistic two-body interaction

1.2 The Fermi-Hubbard model

[To be continued…]

1.3 Adding one effective interaction

[To be continued…]

2 Algorithms and simulations

[To be continued…]

2.1 Finite-size DMRG

[To be continued…]

3 Data analysis and results

[To be continued…]

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