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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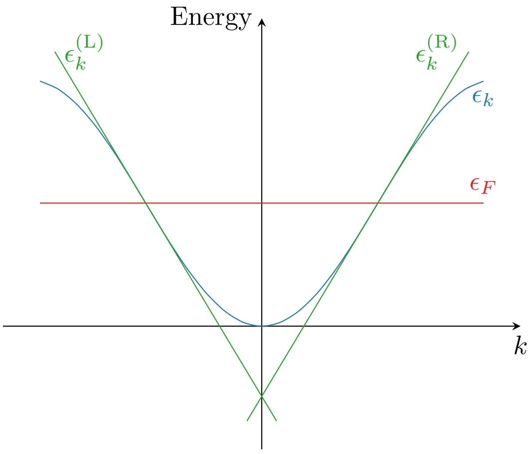


Figure 1: Sketch of the fermionic band ϵ_k, the Fermi level ϵ_F and the two linear bands $\epsilon_k^{(\mathrm{L/R})}$ used to approximate the original bands around the Fermi surface.

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, [1]. 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 $v_F \equiv k_F/m$. 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 [1].

Boson operators

The pivotal result in the bosonization technique is the following:

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

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

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

which of course satisfy

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

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:

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

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,

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

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 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:

$$\begin{aligned}
\hat{\phi}(x) &\equiv -:\hat{N}:\frac{\pi x}{L} - \frac{i\pi}{L}\sum_{q\neq 0}\frac{e^{-\left(\frac{1}{2}\alpha|q|+iqx\right)}}{q}\sum_{s\in\{\mathrm{L},\mathrm{R}\}}\hat{\rho}_s^\dagger(q)\Bigg|_{\alpha\to 0} \\
&= -:\hat{N}:\frac{\pi x}{L} - \frac{i\pi}{L}\sum_{q\neq 0}\sqrt{\frac{|q|L}{2\pi}}\frac{e^{-\left(\frac{1}{2}\alpha|q|+iqx\right)}}{q}\left(\hat{b}_q^\dagger + \hat{b}_{-q}\right)\Bigg|_{\alpha\to 0} \\
\hat{\theta}(x) &\equiv :\Delta\hat{N}:\frac{\pi x}{L} + \frac{i\pi}{L}\sum_{q\neq 0}\frac{e^{-\left(\frac{1}{2}\alpha|q|+iqx\right)}}{q}\sum_{s\in\{\mathrm{L},\mathrm{R}\}}\mathrm{sgn}(s)\hat{\rho}_s^\dagger(q)\Bigg|_{\alpha\to 0} \\
&= :\Delta\hat{N}:\frac{\pi x}{L} + \frac{i\pi}{L}\sum_{q\neq 0}\sqrt{\frac{|q|L}{2\pi}}\frac{e^{-\left(\frac{1}{2}\alpha|q|+iqx\right)}}{|q|}\left(\hat{b}_q^\dagger - \hat{b}_{-q}\right)\Bigg|_{\alpha\to 0}
\end{aligned}$$

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.

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

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

Thus, the fields $\hat{\phi}(x)$ and $\hat{\Pi}(x) \equiv \boldsymbol{\nabla}\hat{\phi}(x)/\pi$ are bosonic and canonically conjugate. Skipping some passages the reader can find in [1], the hamiltonian is represented in field language as:

$$\hat{H}_0 \simeq \hat{K}_0 = \frac{1}{2\pi}\int_{\mathbb{R}} dx\, v_F\left[\left(\boldsymbol{\nabla}\hat{\phi}(x)\right)^2 + \left(\boldsymbol{\nabla}\hat{\theta}(x)\right)^2\right] \tag{3}$$

This is the very cornerstone of bosonization.

Inserting interactions

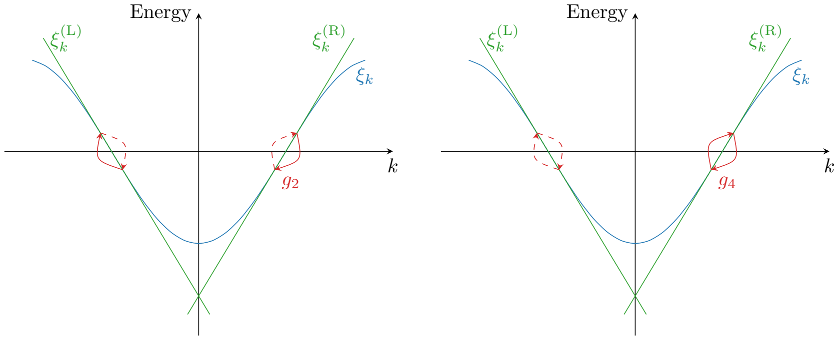
Renormalization interpretation

1.2 The Fermi-Hubbard model

[To be continued...]

1.3 Adding one effective interaction

[To be continued...]



(a) $g_2 = V(q \approx 0)$ process.

(b) $g_4 = V(q \approx 0)$ process.

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

2 Algorithms and simulations

[To be continued. . .]

2.1 Finite-size DMRG

[To be continued. . .]

3 Data analysis and results

[To be continued. . .]

References

[1] 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.