On Non-interacting Spinless Fermions in One Dimension

Jeff Leiberton

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Abstract

We consider a generic Hamiltonian of identical spinless fermions hopping on a 1D lattice with on-site interactions:

$$\hat{\mathcal{H}} = -t \sum_i \left(\hat{c}_i^\dagger \hat{c}_{i+1} + h.c. \right) + \sum_i v_i \hat{c}_i^\dagger \hat{c}_i. \tag{1}$$

We assume that there are L sites with either open boundary conditions (OBC) or periodic boundary conditions (PBC). The lattice constant is a. Equal-time, one-particle pure-state and mixed-state correlations are computed in and out of equilibrium.

Contents

1 Introduction

We begin these notes with a (very) brief introduction to the one-band Hubbard model from which the Hamiltonian 1 is a limit. We then

1.1 One-band Fermi-Hubbard Model

The following is largely inspired by Ref. It is well-known that particles moving under the influence of periodic potentials, that is, one-body potentials $V(x)$ such that $\left[\hat{T}, \hat{V}\right] = 0$ where $\hat{T}$ is the *discrete* lattice translation operator, are described by Bloch wavefunctions $\psi(x) = u(x) e^{ikx}$. We assume here for simplicity a simple one-band model in one-dimension, as this is the most relevant case for the object of interest to us here. Here, $k = 2\pi n/La$ where $n \in \mathbb{Z}$ and $|n| \leq L/2$ is the lattice quasi-momentum and $u(x)$ is the Bloch function. Bloch wavefunctions serve as simple basis states for non-interacting particles moving in crystal potentials, being orthogonal energy eigenstates. However, they are spatially delocalized, and, as such, are hard to interpret as single-particle states. To this end, we consider instead the following linear superpositions of Bloch states:

$$w(x - x_i) = \frac{1}{2N} \sum_{\nu=-N}^{N-1} e^{ik_\nu (x - x_i)} u_{k_\nu}(x) . \tag{2}$$

If we assume here that $u_{k_\nu}(x) \equiv u(x)$ for all k_ν (which we will do for simplicity), then the $w(x - x_i)$ are called Wannier functions, and the set of all such functions (for each lattice site) forms an orthonormal basis. With this orthonormal Wannier basis, we can construct a set of fermionic second-quantized operators $\left\{\hat{c}_i^\dagger\right\}$ and $\{\hat{c}_i\}$ whose action on the vacuum $|0\rangle$ is such that, in the real space, a Wannier orbital is created/annihilated (respectively) at the site i. That is,

$$\left\langle x \middle| \hat{c}_i^\dagger \middle| 0 \right\rangle \doteq w(x - x_i) \tag{3}$$

where $\left\{\hat{c}_i, \hat{c}_j^\dagger\right\} = \delta_{ij}$ and $\left\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\right\} = \{\hat{c}_i, \hat{c}_j\} = 0$. Here and in what follows, we refer to the $\hat{c}_i, \hat{c}_j^\dagger$ as lattice-site operators.

A simple Hamiltonian describing, e.g., electrons moving in a crystal potential with on-site re-

pulsive interactions was proposed by Hubbard in 1967 and takes the form

$$\hat{\mathcal{H}} = \sum_{\langle i,j\rangle,\sigma} \left(t_{ij} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + h.c. \right) + \sum_{i,\sigma} v_i \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma} + \sum_i U_i \hat{c}^\dagger_{i\uparrow} \hat{c}_{i\uparrow} \hat{c}^\dagger_{i,\downarrow} \hat{c}_{i,\downarrow} \tag{4}$$

where $\langle \cdots \rangle$ denotes nearest-neighbor hopping and $\sigma \in \{\uparrow, \downarrow\}$ denotes the m_z quantum number. Here, $t_{ij} = -\int dx w^* (x - x_i) H_I (x) w (x - x_j)$ is the hopping integral where $H_I (x)$ is the effective first-quantized one-body Hamiltonian and is assumed to be local, v_i is some external on-site potential, and U_i is the Coulomb repulsion between doubly occupied sites (note that this term obeys the exclusion principle). This model is, in general, difficult to solve (even in $d = 1$). It can be greatly simplified by ample use of its many admitted symmetries, which we discuss briefly in the next section.

For the present purposes, we consider the case in which the system is subjected to a strong, static external magnetic field. In this way, it far more energetically favorable to add, e.g., $\sigma =\uparrow$ fermions to the system, so that $N = N_\uparrow$. As a result, double occupancy is not allowed, and the effective Hamiltonian reads

$$\hat{\mathcal{H}} = \sum_{\langle i,j\rangle} \left(t_{ij} \hat{c}^\dagger_{i\uparrow} \hat{c}_{j\uparrow} + h.c. \right) + \sum_i v_i \hat{c}^\dagger_{i\uparrow} \hat{c}_{i\uparrow}. \tag{5}$$

In other words, the spin degrees of freedom are no longer relevant, and we might as well just write

$$\hat{\mathcal{H}} = -t \sum_i \left(\hat{c}^\dagger_i \hat{c}_{i+1} + h.c. \right) + \sum_i v_i \hat{c}^\dagger_i \hat{c}_i \tag{6}$$

where it is understood that $\hat{c}^\dagger_i, \hat{c}_i$ creates,destroys a fermion with $\sigma =\uparrow$, respectively, and we take the hopping integral to be independent of the sites i and j, i.e. $t_{ij} = -t$ where the minus sign is conventional. This latter result is, of course, just the Hamiltonian 1. Hence, in summary, we understand the Hamiltonian for non-interacting spinless fermions to be the spin-polarized limit of the Fermi-Hubbard model.

1.2 Symmetries and Conserved Quantities

We limit our considerations here to so-called bipartite lattices, which, loosely speaking, are lattices which can be broken into two identical sublattices (examples include the simple hypercubic lattice and the honeycomb lattice).

1.2.1 Symmetries

Given the goals of this section are no more than to motivate the Hamiltonian 1 and briefly discuss its properties, we do not dwell on the many rich and otherwise remarkable symmetries admitted by the Fermi-Hubbard model, opting instead to point to some references: [11]. We shall, however, at least illustrate some of the most important symmetries. First, a number of discrete symmetries owing to the lattice upon with the system is defined are, in general, embodied by the Hamiltonian 4 (and also 1). One can summarize this behavior as the statement that any transformation of the lattice which preserves the nearest-neighbors should be a symmetry of the Hamiltonian. This includes, for example, "lattice flips" $\mathbb{Z}/2\mathbb{Z}$ wherein the lattice is rotated (e.g.) by π. Second, the Hamiltonian 4 (and also 1) admits a $U(1)$ gauge symmetry in the sense that $\hat{c}^\dagger_{i\sigma} \mapsto e^{-i\theta}\hat{c}^\dagger_{i\sigma}$ and $\hat{c}_{i\sigma} \mapsto e^{i\theta}\hat{c}_{i\sigma}$ does not change its spectrum *nor* the local number density $n_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$. This latter fact means that the Fermi-Hubbard (and spinless fermion) Hamiltonian is particle number conserving. Finally, we point out that the Hamiltonian 4 (and also 1) is particle-hole symmetric.

1.2.2 Conserved Quantities

2 Spectrum and Eigenstates

In this section, we compute the spectrum and eigenstates of equation 1 for various v_i.

2.1 Translationally Invariant Case ($v_i = v$)

Let us begin by treating the translationally invariant case in which $v_i \equiv v$ for every $1 \leq i \leq L$. The above Hamiltonian takes the form

$$\hat{\mathcal{H}} = -t \sum_{i=1}^{L} \left(\hat{c}_i^\dagger \hat{c}_{i+1} + h.c. \right) + v \sum_{i=1}^{L} \hat{c}_i^\dagger \hat{c}_i. \tag{7}$$

Presently, we consider periodic boundary conditions (PBC), whereby we identify $\hat{c}_{L+1} \equiv \hat{c}_1$. We wish to be very precise about the nature of this Hamiltonian. The Fock space is assumed to be spanned by the states $|\{n_i\}\rangle = |n_1, n_2, \ldots, n_L\rangle$ where $n_i \in \{0, 1\}$ corresponds to the occupation of a lattice site by a spinless fermion. The basis states over which the Fock space is defined can be thought of as generalizations to L sites of the $|L\rangle$ and $|R\rangle$ states considered in the symmetric double well potential (Wannier functions). The action of the operator $\hat{c}_i^\dagger$ on the vacuum state $|0\rangle = |n_1 = 0, n_2 = 0, \ldots, n_i = 0, \ldots, n_L = 0\rangle$ is such that a fermion is created at the i^{th} lattice site. Due to the Pauli exclusion principle, the action of the operator $\left(c_i^\dagger\right)^2$ is nilpotent. Likewise, $\hat{c}_i$ annihilates a fermion on the i^{th} site and yields the null state when acting on the vacuum. These operators are taken to follow the usual fermion algebra: $\left\{\hat{c}_i, \hat{c}_j^\dagger\right\} = \delta_{ij}, \{\hat{c}_i, \hat{c}_j\} = 0$, and $\left\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\right\} = 0$.

Because of the translational invariance of equation 7, a translation by na for any $n \in \mathbb{Z}$ does not change the Hamiltonian (this is best seen in the first quantization). This suggests that we introduce the operators

$$\hat{c}_k = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{ikx_j} \hat{c}_j \tag{8}$$

and

$$\hat{c}_k^\dagger = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} e^{-ikx_j} \hat{c}_j^\dagger \tag{9}$$

which are defined on the Fock space generated by $|0\rangle_k = |n_{k_1} = 0, \ldots, n_{k_L} = 0\rangle$. These operators are of course just discrete Fourier transforms of the lattice-site operators $\hat{c}_i, \hat{c}_j^\dagger$. Before continuing, let us verify that the operators defined by equations 8 and 9 are properly defined fermion operators– i.e. they abide by the correct algebra. It is easy to see that $(\hat{c}_k)^2$ and $\left(\hat{c}_k^\dagger\right)^2$ are nilpotent operators (use the binomial theorem). Likewise,

$$\begin{aligned}
\left\{c_k, c_{k'}^\dagger\right\} &= \frac{1}{L} \sum_{j,l} e^{ikx_j} e^{-ik'x_l} \left\{\hat{c_j}, \hat{c}_l^\dagger\right\} \\
&= \frac{1}{L} \sum_{j,l} \delta_{jl} e^{ikx_j} e^{-ik'x_l} \\
&= \frac{1}{L} \sum_{j} e^{i\left(k-k'\right)x_j} \\
&= \delta_{kk'}
\end{aligned} \tag{10}$$

where in the last line we used the definition of the Kronecker delta. By the same procedure, it is easy to see that $\{c_k, c_{k'}\} = \left\{c_k^\dagger, c_{k'}^\dagger\right\} = 0$, as required.

Using equation 8 we write

$$\begin{aligned}
\frac{1}{\sqrt{L}} \sum_k e^{-ikx_l} \hat{c}_k &= \frac{1}{L} \sum_{k'} e^{-ik'x_l} \sum_{j=1}^{L} e^{ikx_j} \hat{c}_j \\
&= \frac{1}{L} \sum_{j,k} e^{-ik(x_l - x_j)} \hat{c}_j \\
&= \sum_j \delta_{jl} \hat{c}_j \\
&= \hat{c}_l
\end{aligned} \tag{11}$$

where in the second to last line we used the fact that $\sum_k e^{-ik(x_l - x_j)} = L\delta_{lj}$. Likewise, we may

conclude that

$$\hat{c}_j^\dagger = \frac{1}{\sqrt{L}} \sum_k e^{ikx_j} \hat{c}_k. \tag{12}$$

From equations 11 and 12, along with the condition that $\hat{c}_j = \hat{c}_{j+L}$ (PBC), we have $\sum_k e^{ikx_{j+L}} \hat{c}_k = \sum_k e^{ikx_j} \hat{c}_k$. Because this holds independently of k and j, we may conclude that

$$e^{ikx_{j+L}} = e^{ikx_j} \tag{13}$$

for every k and j. Using the fact that $x_j = ja$, we arrive at a quantization condition for k: $e^{ikLa} = 1$, implying that

$$k = \frac{2n\pi}{La} \tag{14}$$

where $n \in \mathbb{Z}$ and $|n| \leq L/2$ (assuming $L \in 2\mathbb{N}$). In the limit of large L, the spacing between adjacent k's tends to zero, i.e. $\Delta k = 2\pi/La \to dk$, and the Fourier spectrum becomes continuous. Because of the translational invariance of the Hamiltonian, the values of k are unique only up to mod $2\pi/a$, and it suffices to consider only the region in momentum space defined by $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right)$ (or equivalently $k \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$) known as the first Brillouin zone (in 1D). It is important that only one of the end-points is closed, as will be made apparent shortly.

Inserting equations 11 and 12 into the original Hamiltonian, we find that

$$\begin{aligned}
\hat{\mathcal{H}} &= -t \sum_{j,k,k'} \left(e^{ikx_j} e^{-ik'x_{j+1}} \hat{c}_k^\dagger \hat{c}_{k'} + h.c. \right) + v \sum_{j,k,k'} e^{ikx_j} e^{-ik'x_j} \hat{c}_k^\dagger \hat{c}_{k'} \\
&= -t \sum_{j,k,k'} \left(e^{i(k-k')x_j} e^{-ik'a} \hat{c}_k^\dagger \hat{c}_{k'} + h.c. \right) + v \sum_{j,k,k'} e^{i(k-k')x_j} \hat{c}_k^\dagger \hat{c}_{k'} \\
&= -t \sum_{k,k'} \left(\delta_{kk'} e^{-ik'a} \hat{c}_k^\dagger \hat{c}_{k'} + h.c. \right) + v \sum_{k,k'} \delta_{kk'} \hat{c}_k^\dagger \hat{c}_{k'} \\
&= -t \sum_k e^{-ika} \hat{c}_k^\dagger \hat{c}_k + h.c. + v \sum_k \hat{c}_k^\dagger \hat{c}_k
\end{aligned} \tag{15}$$

where we again used the fact that $\sum_j e^{i\left(k-k'\right)x_j} = \delta_{kk'}$. Now, we recognize that

$$\begin{aligned} e^{-ika}\hat{c}_k^\dagger \hat{c}_k + h.c. &= \left(e^{-ika} + e^{ika}\right)\hat{c}_k^\dagger \hat{c}_k \\ &= 2\cos\left(ka\right)\hat{c}_k^\dagger \hat{c}_k, \end{aligned} \tag{16}$$

so that we can write the above Hamiltonian as

$$\hat{\mathcal{H}} = \sum_k \hbar\omega_k \hat{c}_k^\dagger \hat{c}_k. \tag{17}$$

From this, we conclude that the energy of the system goes like

$$E = \sum_k \hbar\omega_k n_k \tag{18}$$

where

$$\hbar\omega_k = v - 2t\cos ka \tag{19}$$

is the single-particle dispersion and $n_k \in \{0, 1\}$ for each k. Let the total number of fermions be $N = \sum_k n_k$. It follows that the N particle eigenstate is just $|\{n_k\}\rangle = \prod_k^{k_L} \left(\hat{c}_k^\dagger\right)^{n_k} |0\rangle$, which is identified as a Slater determinant of N single particle eigenstates. As written in the previous line, the product is taken over *all* possible k values where it is known *a priori* what the total particle number N is. See that it is equivalent to write the N particle eigenstate as $|\{n_k\}\rangle = \prod_k^N \left(\hat{c}_k^\dagger\right)|0\rangle$. In this way, it is clear how many particles there are from the state alone. Note that the dispersion equation 19 depends on two parameters, the ratio of the amplitude of the on-site potential and the hopping integral t/v and the lattice spacing a. We plot the dispersion for the parameter values (relative to some arbitrary scale) $v = 0.1, t = 1$, and $a = 1$ in Figure 1.

Included in figure 1 is the probability density $|\phi|^2$ of the single particle eigenstates corresponding to the (two-fold degenerate) first excited state. The meaning of ϕ will be made clear in ensuing sections, but it is important to note that what is depicted here is misleading–it is not entirely

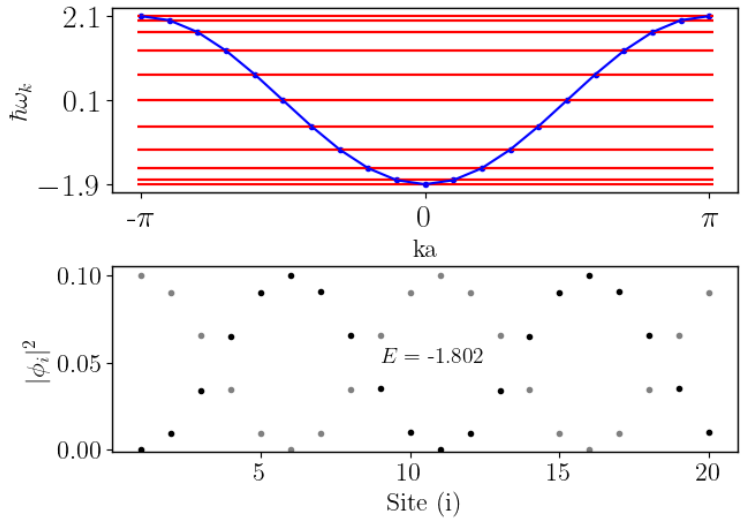

Figure 1: **Top:** Analytic and numeric single particle dispersion (eq. 19) for 1D free fermions on a lattice. The ground state energy of the N particle eigenstate is given by equation 12 with the lowest unoccupied k values filled. Note that if L and N are both even, the ground state is two-fold degenerate. The red lines show the exact single particle spectrum obtained from diagonalizing numerically equation 1 in the lattice site basis. **Bottom**: probability density of single particle eigenkets as a function of site index. The eigenket corresponds to the first single-particle excited state and is hence doubly degenerate. The exact eigenvalue (rounded to 3 decimal places) is shown in the figure.

correct, nor is it wrong. Indeed, ϕ_i^k is given by the overlap of the basis states on which the $\hat{c}_i$ are defined and those on which the $\hat{c}_k$ are defined, i.e. $\phi_i^k = \langle x_i | k \rangle$. What is being shown is $\left|\phi_i^k\right|^2$ plotted as a function of i for a fixed k (which is near zero). It is easy to show (one can do this numerically) that $\sum_i |\phi_i|^2 = 1$ as it necessarily should.

The reason it is claimed that this figure is misleading is that in equation 8 we have that $\phi_i^k = L^{-1/2} e^{ikx_i}$ which would imply that $\left|\phi_i^k\right|^2$ is constant for all i. In the figure, however, this is certainly not the case. The reason for this latter fact, it turns out, is owed to the time-translation symmetry of the Hamiltonian.

Now, I claim that what is shown in the figure is misleading. This is because, as we can see by, e.g., equation 8, $\phi_i^k = L^{-1/2} e^{ikx_i}$ which implies that $\left|\phi_i^k\right|^2$ is constant for all i. Instead, what is being shown in the above figure is $\frac{1}{2}\left|\phi_i^k \pm \phi_i^{-k}\right|^2$. I owe this result to the fact that, (i) the single-

particle dispersion is two-fold degenerate for all non-zero $|k| \neq \pi/a$ and (ii) I did not resolve the translational symmetry of the exact single-particle Hamiltonian before numerically diagonalizing it. One can show that this problem is resolved when the translational symmetry of the Hamiltonian is broken, for example by considering open boundary conditions (OBC), or, as below, a generic non-translationally invariant on-site potential.

There is another subtlety with regard to the two-fold degeneracy of the spectrum. Namely, when L and N are both even, the Fermi energy is two-fold degenerate. For example, consider the case of $L = 4$ and $N = 2$. In the ground state, one particle will of course take the $k = 0$ mode, and the other will be made to choose between $k = \pm\pi/2a$. Regardless of the sign of k, the energy will be $E = 2v - 2t\ \left(\cos\frac{\pm\pi}{2} = 0\right)$. Indeed, for $L, N \in 2\mathbb{N}$, the ground state is two-fold degenerate.

2.1.1 Comparison with Real Space in $L = 2$

For the sake of completeness, let us consider the $L = 2$ case. This case is essentially identical to the deep double well potential considered in section 1.

In the site-occupancy space, there are four possible states corresponding to three different particle number sectors:

Number of Particles	$N = 0$	$N = 1$	$N = 2$
States	$\|n_1 = 0, n_2 = 0\rangle$	$\|1,0\rangle$,$\|0,1\rangle$	$\|1,1\rangle$

likewise, in the momentum space:

Number of Particles	$N = 0$	$N = 1$	$N = 2$
States	$\|n_{k_1} = 0, n_{k_2} = 0\rangle_k$	$\|1,0\rangle_k$,$\|0,1\rangle_k$	$\|1,1\rangle_k$

where we use the subscript k to make apparent the fact that the two sets of states live in different spaces. Presently, k can only admits the values $k = 0, \pi/a$. Note in particular our exclusion of $k = -\pi/a$. As hinted earlier, only one of the endpoints of the Brillouin zone (BZ) is included. One can understand this by envisioning the ends of the BZ "glued" together in the geometrical sense. In other words, the translational symmetry of the system is such that the points $k = \pm\pi/a$ are identical, and so only one is considered.

The real space Hamiltonian reads:

$$\begin{aligned}\hat{\mathcal{H}} &= -t\left(\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_3 + h.c.\right) + v\left(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2\right) \\ &= -2t\left(\hat{c}_1^\dagger \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1\right) + v\left(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2\right)\end{aligned} \tag{20}$$

where in the second line the factor of 2 comes from the fact that $\hat{c}_3 = \hat{c}_1$ due to PBC. Now, the vacuum state is obviously an eigenstate of this Hamiltonian with eigenvalue 0. Likewise, hopping cannot occur in the fully filled ($N = 2$) sector owing to the Pauli exclusion principle (PEP). Hence, only the onsite terms contribute and we conclude that $|1,1\rangle$ is an eigenstate with eigenvalue $2v$. Note that in the case $v = 0$, the fully filled state and the vacuum state are degenerate. It remains to consider the $N = 1$ sector. It is easy to see that in the $N = 1$ basis the Hamiltonian can be represented as

$$\hat{\mathcal{H}} \doteq \begin{pmatrix} v & -2t \\ -2t & v \end{pmatrix} \tag{21}$$

where we order our basis as $\begin{pmatrix} |1,0\rangle & |0,1\rangle \end{pmatrix}^{\mathrm{T}}$. This Hamiltonian is simple enough to diagonalize, the result being the eigenvalues

$$\lambda_\pm = v \pm 2t \tag{22}$$

and the (normalized) eigenvectors

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(|1,0\rangle \mp |0,1\rangle\right). \tag{23}$$

Let us now compare these results with what we determined above. The vacuum state is of course the same, and we can identify $|0,0\rangle \equiv |0,0\rangle_k$. For $N = 1$, we again have two states, $|1,0\rangle_k = \hat{c}_0^\dagger |0\rangle_k$ and $|0,1\rangle_k = \hat{c}_{\pi/a}^\dagger |0\rangle_k$, which admit eigenenergies $v - 2t$ and $v + 2t$, respectively. We can map the

eigenstates to the real space by means of eq. 3:

$$\begin{aligned}\hat{c}_0^\dagger |0\rangle_k &= \frac{1}{\sqrt{2}} \left(\hat{c}_1^\dagger + \hat{c}_2^\dagger\right) |0\rangle \\ &= \frac{1}{\sqrt{2}} \left(|1,0\rangle + |0,1\rangle\right)\end{aligned} \tag{24}$$

and

$$\begin{aligned}\hat{c}_{\pi/a}^\dagger |0\rangle_k &= \frac{1}{\sqrt{2}} \left(\hat{c}_1^\dagger + e^{-i\pi}\hat{c}_2^\dagger\right) |0\rangle \\ &= \frac{1}{\sqrt{2}} \left(|1,0\rangle - |0,1\rangle\right)\end{aligned} \tag{25}$$

where we note that due to translational invariance we may choose $x_1 = 0$. As an aside, recognize that the above states are nothing more than the symmetric/anti-symmetric single particle states we determined for the deep double well potential. For $N = 2$, we see that

$$E = v - 2t + v + 2t = 2v \tag{26}$$

and

$$\begin{aligned}\hat{c}_0^\dagger \hat{c}_{\pi/a}^\dagger |0\rangle_k &= \frac{1}{2} \left(\hat{c}_1^\dagger + \hat{c}_2^\dagger\right) \left(\hat{c}_1^\dagger + e^{-i\pi}\hat{c}_2^\dagger\right) |0\rangle \\ &= \frac{1}{2} \left(\hat{c}_2^\dagger \hat{c}_1^\dagger - \hat{c}_1^\dagger \hat{c}_2^\dagger\right) |0\rangle \\ &= -|1,1\rangle\end{aligned} \tag{27}$$

which differs from our above result only by an overall phase factor. This comes down to a matter of ordering, as an overall phase factor does not change the anti-symmetry of the state $|1,1\rangle$. One could therefore choose the ordering to be $\hat{c}_{\pi/a}^\dagger \hat{c}_0^\dagger$ so that the momentum space and real space results are in complete agreement.

2.1.2 Slater Determinants

Let us here show in detail that the state $\prod_k^N \left(\hat{c}_k^\dagger\right)|0\rangle$ is in the lattice-space a Slater determinant. For simplicity and concreteness, we take $L = 4$ and $N = 2$ such that an arbitrary single particle state can be written in lattice-space as

$$|\psi_k\rangle = \hat{c}_k^\dagger|0\rangle = \frac{1}{2}\left(e^{ikx_1}\hat{c}_1^\dagger + e^{ikx_2}\hat{c}_2^\dagger + e^{ikx_3}\hat{c}_3^\dagger + e^{ikx_4}\hat{c}_4^\dagger\right)|0\rangle\,. \tag{28}$$

Suppose that the initial state is given by $\hat{c}_{k_1}^\dagger\hat{c}_{k_2}^\dagger|0\rangle$. We know from previous considerations that should this state be a Slater determinant it will take the form

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_{k_1}(x_1) & \psi_{k_1}(x_2) \\ \psi_{k_2}(x_1) & \psi_{k_2}(x_2) \end{vmatrix} = \frac{1}{\sqrt{2}}\left[\psi_{k_1}(x_1)\psi_{k_2}(x_2) - \psi_{k_2}(x_1)\psi_{k_1}(x_2)\right] \tag{29}$$

where x_1 and x_2 denote the position of the particle 1 and 2, respectively, and $\psi_{k_i}(x_j) = e^{ik_i x^{(j)}}/\sqrt{L}$ is a single-particle state.

2.1.3 Summary

In summary, we found that non-relativistic free fermions on a 1D lattice with constant on-site energy v admit the spectrum

$$E = \sum_k \hbar\omega_k n_k \tag{30}$$

where $\sum_k n_k = N$ is the total number of particles and $\hbar\omega_k = v - 2t\cos ka$, where a is the lattice spacing. The momentum k takes quantized values $k = 2\pi n/La$ where $n \in \mathbb{Z}$ and $|n| \leq L/2$ with only one end point included. The eigenstates are given by products of single-particle states

$$|\{n_k\}\rangle = \prod_k^N \left(\hat{c}_k^\dagger\right)|0\rangle \tag{31}$$

where $|0\rangle$ denotes the vacuum state. The N particle ground state is a Fermi sea with the N lowest k states filled, and is a Slater determinant of the single particle eigenstates.

2.2 General Case ($v_i \neq v$)

We now consider the case where v_i is not a constant for every i. One can imagine two cases: (i) v_i respects the translational invariance of the lattice Hamiltonian and therefore admits a Fourier spectrum defined on the same BZ as above or (ii) v_i does not respect the translational invariance of the system. Case (i) occurs provided $v_i(x) = v_i(x + a)$ for every i, and the result is an additional k dependent term in the dispersion $\hbar\omega_k$ which depends on the particulars of $v_i(x)$. We do not focus on such a case here. Instead, we consider case (ii), and in particular we take v_i to be of the form $v + g\epsilon_i$ where $\epsilon_i \in [0, 1]$ is a random variable and g is the overall "strength" of the perturbation. In figure 2, we show the single-particle energy spectrum, ground, first, and second excited states for equation 7 with $v_i = v + g\epsilon_i$ for various values of g (defined with respect to the strength of v). Interestingly, as the strength g is increased, the single particle eigenstates become increasingly localized about particular lattice points.

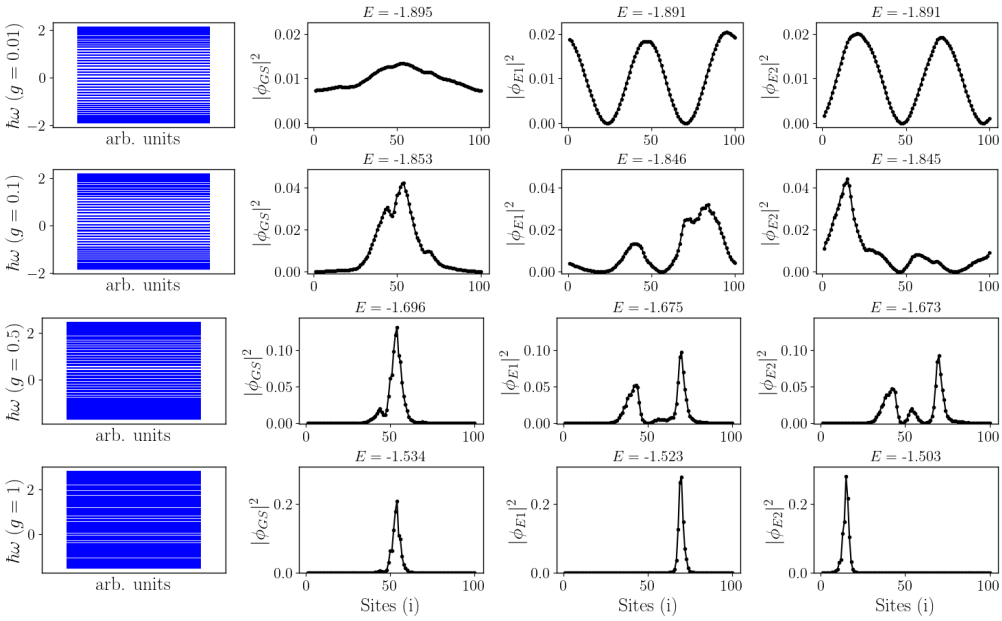

Figure 2: Single particle spectrum (first column) and ground, first excited, and second excited states (second, third, and fourth column, respectively) for 1D free fermions on a lattice with variable on-site potential $v_i = v\,(1 + g\epsilon)$. Here, $\epsilon \in [0, 1]$ is a random variable and g is a dimensionless "strength."

3 Pure State Correlations

In this section, we compute equal-time one-particle correlation functions of the form $\left\langle \hat{c}_j^\dagger \hat{c}_i \right\rangle$ where the expectation value is taken with respect to pure eigenstates of the free fermion Hamiltonian diagonalized in section 2.

3.1 Exact Case

Let us begin by first considering the exact case. We write the eigenstates explicitly as

$$|\{n_k\}\rangle = \prod_k^L \left(\hat{c}_k^\dagger\right)^{n_k} |0\rangle = \hat{c}_{k_1}^\dagger \hat{c}_{k_2}^\dagger \cdots \hat{c}_{k_N}^\dagger |0\rangle \tag{32}$$

where we identify the ordering $k_1 \leq k_2 \leq \ldots \leq k_L$. The dual conjugate $\langle\{n_k\}|$ is obtained by taking the adjoint of the above expression and is given by

$$\langle\{n_k\}| = \langle 0|\, \hat{c}_{k_N} \cdots \hat{c}_{k_1} = (-1)^{N-1} \langle 0| \prod_k^L (\hat{c}_k)^{n_k} \tag{33}$$

where in the last line we adopted the ordering defined in equation 32 (and hence the sign). The equal-time one-particle correlation function for a pure state follows as

$$\begin{aligned} C(i,j) &= \left\langle \hat{c}_j^\dagger \hat{c}_i \right\rangle \\ &= (-1)^{N-1} \left\langle 0 \middle| \prod_k^L (\hat{c}_k)^{n_k} \hat{c}_j^\dagger \hat{c}_i \prod_k^L \left(\hat{c}_k^\dagger\right)^{n_k} \middle| 0 \right\rangle \end{aligned} \tag{34}$$

Using equations 11 and 12, we expand the real space fermion operators in the momentum space so that we may write

$$\begin{aligned} C(i,j) &= \frac{1}{L} (-1)^{N-1} \left\langle 0 \middle| \prod_k^L (\hat{c}_k)^{n_k} \left(\sum_q e^{iqx_j} \hat{c}_q^\dagger \right) \left(\sum_p e^{-ipx_i} \hat{c}_p \right) \prod_k^L \left(\hat{c}_k^\dagger\right)^{n_k} \middle| 0 \right\rangle \\ &= \frac{1}{L} (-1)^{N-1} \sum_{q,p} e^{iqx_j} e^{-ipx_i} \left\langle 0 \middle| \prod_k^L (\hat{c}_k)^{n_k} \hat{c}_q^\dagger \hat{c}_p \prod_k^L \left(\hat{c}_k^\dagger\right)^{n_k} \middle| 0 \right\rangle \end{aligned} \tag{35}$$

where in the last line we used the linearity of expectation values to factor out the summations. It remains, then, to determine the matrix elements $(-1)^{1-\sum_k n_k} \left\langle 0 \middle| \prod_k^L (\hat{c}_k)^{n_k} \hat{c}_q^\dagger \hat{c}_p \prod_k^L \left(\hat{c}_k^\dagger\right)^{n_k} \middle| 0 \right\rangle$. To do this, we consider the action of the operators $\hat{c}_q^\dagger, \hat{c}_p$ on an arbitrary energy eigenstate $|\{n_k\}\rangle$. We note as an aside that the explicit representation of $|\{n_k\}\rangle$ and its dual in terms of the operators $\hat{c}_k, \hat{c}_k^\dagger$ and the vacuum was not totally necessary. Because of the fermionic algebra, we should find that

$$\hat{c}_q^\dagger |\{n_k\}\rangle = (1 - n_q) (-1)^{P_q} |\{n_k, n_q = 1\}\rangle \tag{36}$$

where $P_q = \pm 1$ is the *parity* of the site q (which, in practice, counts how many n_k are "to the left" of n_q). More rigorously, $P_q \equiv \mathrm{sgn}(\sigma_q)$ where σ_q is a permutation of the set of all occupied $\{k\}$

including q. Thus, $P_q = 1$ if one must commute $\hat{c}_q^\dagger$ past an even number of $\hat{c}_k^\dagger$ and $P_q = -1$ if the number of $\hat{c}_q^\dagger$ is odd. The notation $|\{n_k, n_q = 1\}\rangle = \hat{c}_q^\dagger |n_1, n_2 \ldots, n_q, \ldots\rangle = |n_1, n_2 \ldots, n_q = 1, \ldots\rangle$. The situation where $n_q = 1$ in the original state is accounted for by the prefactor $1 - n_q$. Likewise,

$$\hat{c}_p |\{n_k\}\rangle = n_p (-1)^{P_p} |\{n_k, n_p = 0\}\rangle \tag{37}$$

in the same notation. Now, provided that we are taking expectation values, we need $\hat{c}_q^\dagger \hat{c}_p |\{n_k\}\rangle \propto |\{n_k\}\rangle$ in order for the matrix element to be non-zero. This occurs only when $q = p$ and therefore

$$\left\langle \{n_k\} \left| \hat{c}_q^\dagger \hat{c}_p \right| \{n_k\} \right\rangle = n_q \delta_{qp} \tag{38}$$

where of course $n_q \in \{0, 1\}$. Inserting this expression back into $C(i, j)$, we find that

$$C(i, j) = \frac{1}{L} \sum_{q,p} e^{iqx_j} e^{-ipx_i} n_q \delta_{qp} = \frac{1}{L} \sum_q e^{iq(x_j - x_i)} n_q. \tag{39}$$

Note that, in particular, when $i = j$ we have

$$C(j, j) = \left\langle \hat{c}_j^\dagger \hat{c}_j \right\rangle = \frac{N}{L}, \tag{40}$$

i.e. that the average number of fermions at the site j is given by the total number of fermions divided by the total number of sites. This value is real, as it necessarily should be provided $\hat{c}_j^\dagger \hat{c}_j$ is an observable. Moreover, when $N = L$ we have $C(j, j) = 1$, meaning that all sites are occupied. The same value is obtained for the single-particle ground state $q = 0$.

3.2 Random On-site Potential

Here, the procedure is very similar to the one followed above. Namely, because of the non-interacting nature of the present system, we expect–even in the case of broken translational symmetry–that the N body eigenstates are simply Slater determinants of the single particle eigenstates. When we

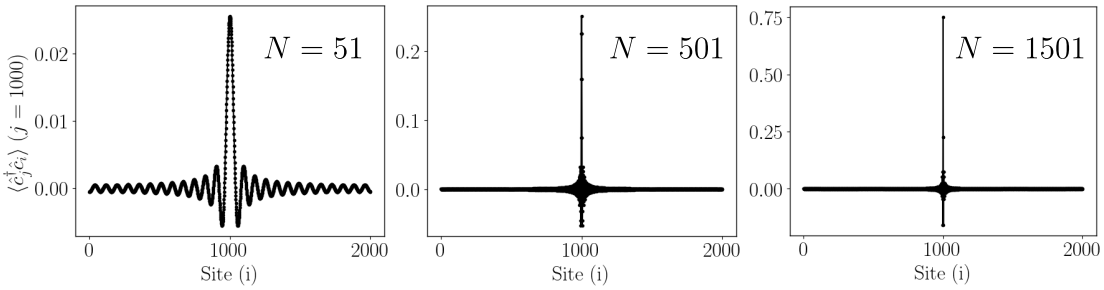

Figure 3: Equal-time one-particle ground-state correlation functions $\langle \hat{c}_j^\dagger \hat{c}_i \rangle$ for one-dimensional free fermions. The Hamiltonian is given by equation 7 with $v = 0.1$ and $t = 1$. See that as the number of particles is increased from 51 to 1501, the correlation function becomes increasingly localized about the site $j = 1000$ (which we keep fixed throughout).

diagonalize the single particle Hamiltonian (eq. 1), we make the mapping $\Psi^\dagger \mathcal{H} \Psi \mapsto \Phi^\dagger \mathcal{D} \Phi$, where $\Psi = \begin{pmatrix} \hat{c}_1 & \hat{c}_2 & \cdots & \hat{c}_L \end{pmatrix}^{\mathrm{T}}$,

$$\mathcal{H} = \begin{pmatrix} v_1 & -t & 0 & \cdots & -t \\ -t & v_2 & -t & & \\ 0 & -t & v_3 & & \vdots \\ \vdots & & & \ddots & \\ -t & & \cdots & & v_L \end{pmatrix}, \tag{41}$$

$\Phi = U^\dagger \Psi \equiv \begin{pmatrix} \hat{c}_{E_1} & \hat{c}_{E_2} & \cdots & \hat{c}_{E_L} \end{pmatrix}$ with U a unitary whose elements are given by the overlap of the on-site basis states and the diagonal basis states, and $\mathcal{D} = \mathrm{diag}\,(E_1, E_2, \ldots, E_L)$ where E_i $1 \leq i \leq L$ are the single-particle energy eigenvalues. For a given eigenvalue E_m, we can identify the mapping

$$\hat{c}_{E_m}^\dagger = \sum_j \psi_j^{E_m} \hat{c}_j^\dagger \tag{42}$$

where $\psi_j^{E_m}$ is the (E_m, j) component of U (the set $\left\{ \psi_j^{E_m} \right\}_j$ forming the eigenvectors of the matrix representation of the Hamiltonian). Because the eigenstates of a Hermitian operator form a basis of

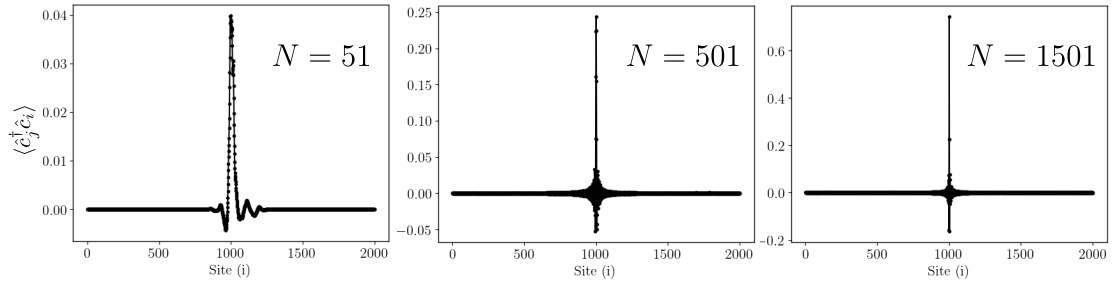

Figure 4: Equal-time one-particle ground-state correlation functions $\langle \hat{c}_j^\dagger \hat{c}_i \rangle$ for one-dimensional free fermions on a "strongly disordered" lattice. The Hamiltonian is given by equation 7 with $v = v + g\epsilon_i$ for $g = 0.1$. Interestingly, we see that even though there is disorder, the single-particle correlation because highly localized about the position of the particle, which in this case is $j = 1000$.

the Hilbert space (i.e. because U is unitary), we can invert the above equation in order to identify:

$$\hat{c}_j^\dagger = \sum_m \left(\psi_j^{E_m}\right)^* \hat{c}_{E_m}^\dagger \tag{43}$$

where $(\cdots)^*$ denotes complex conjugation.

The determination of the equal-time one particle correlations in arbitrary N-particle energy eigenkets thus boils down to solving

$$\begin{aligned}\left\langle \hat{c}_j^\dagger \hat{c}_i \right\rangle &= \left\langle 0 \middle| \prod_m \left(\hat{c}_{E_m}\right)^{n_{E_m}} \left(\sum_l \left(\psi_j^{E_l}\right)^* \hat{c}_{E_l}^\dagger\right) \left(\sum_n \psi_i^{E_n} \hat{c}_{E_n}\right) \prod_m \left(\hat{c}_{E_m}^\dagger\right)^{n_{E_m}} \middle| 0 \right\rangle \\ &= \sum_{l,n} \left(\psi_j^{E_l}\right)^* \psi_i^{E_n} \left\langle 0 \middle| \prod_m \left(\hat{c}_{E_m}\right)^{n_{E_m}} \hat{c}_{E_l}^\dagger \hat{c}_{E_n} \prod_m \left(\hat{c}_{E_m}^\dagger\right)^{n_{E_m}} \middle| 0 \right\rangle . \end{aligned} \tag{44}$$

Comparing the above expression with equation 35, we see that in the limit $v_i \to v$ for all i, we can identity $\hat{c}_{E_n} \leftrightarrow \hat{c}_{k_n}$ and $\psi_i^{E_n} \leftrightarrow L^{-1/2} e^{ik_n x_i}$. We may reasonably expect, then, that the matrix element in equation 44 yields similar results. Indeed, adopting the obvious notation $|\{n_E\}\rangle = \prod_m \left(\hat{c}_{E_m}^\dagger\right)^{n_{E_m}} |0\rangle$ we should find that

$$\hat{c}_{E_l}^\dagger \hat{c}_{E_m} |\{n_E\}\rangle = \delta_{lm} n_{E_m} |\{n_E\}\rangle \tag{45}$$

such that

$$\left\langle \hat{c}_j^\dagger \hat{c}_i \right\rangle = \sum_m \left(\psi_j^{E_m}\right)^* \psi_i^{E_m} n_{E_m} \tag{46}$$

where $\sum_m n_{E_m} = N$ is the total particle number. Figure 4 shows equation 46 for $L = 2000$ sites and various N. The Hamiltonian is given by equation 7 with $v = v + g\epsilon_i$ for $g = 0.1$, and the expectation value is taken with respect to the N particle ground state. Here, we choose $j = 1000$. Amazingly, we see that, even in the case of rather strong "disorder," the single-particle correlation function becomes strongly peaked about the location of the particle. This behavior is consistent with the exact case, including our observation that $\left\langle \hat{c}_j^\dagger \hat{c}_j \right\rangle \to 1$ in the limit $L \to N$. It is truly amazing that this property holds even in strongly disordered systems.

It is useful (and interesting) to observe that the nature of spinless non-interacting fermions is such that the single particle correlation *matrix* may be constructed simply as follows. Suppose the equilibrium state is characterized by a set of N single particle energies $\{\mathcal{E}_n\}$ with $1 \leq n \leq N$. Let $\mathbf{P}$ be the matrix of single-particle expansion coefficients, that is

$$\mathbf{P} = \begin{bmatrix} \psi_1^{\mathcal{E}_1} & \psi_1^{\mathcal{E}_2} & \cdots & \psi_1^{\mathcal{E}_N} \\ \psi_2^{\mathcal{E}_1} & \psi_2^{\mathcal{E}_2} & \cdots & \psi_2^{\mathcal{E}_N} \\ \vdots & \vdots & \ddots & \vdots \\ \psi_L^{\mathcal{E}_1} & \psi_L^{\mathcal{E}_2} & \cdots & \psi_L^{\mathcal{E}_N} \end{bmatrix}_{L \times N} \tag{47}$$

then we claim that

$$C = \mathbf{P}\mathbf{P}^\dagger \tag{48}$$

where $C_{ij} = \left\langle \hat{c}_i^\dagger \hat{c}_j \right\rangle$. Indeed, we have

$$\mathbf{P}\mathbf{P}^\dagger = \begin{bmatrix} \psi_1^{\mathcal{E}_1} & \psi_1^{\mathcal{E}_2} & \cdots & \psi_1^{\mathcal{E}_N} \\ \psi_2^{\mathcal{E}_1} & \psi_2^{\mathcal{E}_2} & \cdots & \psi_2^{\mathcal{E}_N} \\ \vdots & \vdots & \ddots & \vdots \\ \psi_L^{\mathcal{E}_1} & \psi_L^{\mathcal{E}_2} & \cdots & \psi_L^{\mathcal{E}_N} \end{bmatrix}_{L\times N} \begin{bmatrix} \left(\psi_1^{\mathcal{E}_1}\right)^* & \left(\psi_2^{\mathcal{E}_1}\right)^* & \cdots & \left(\psi_L^{\mathcal{E}_1}\right)^* \\ \left(\psi_1^{\mathcal{E}_2}\right)^* & \left(\psi_2^{\mathcal{E}_2}\right)^* & \cdots & \left(\psi_L^{\mathcal{E}_2}\right)^* \\ \vdots & \vdots & \ddots & \vdots \\ \left(\psi_1^{\mathcal{E}_N}\right)^* & \left(\psi_2^{\mathcal{E}_N}\right)^* & \cdots & \left(\psi_L^{\mathcal{E}_N}\right)^* \end{bmatrix}_{N\times L} \tag{49}$$

$$= \begin{bmatrix} \sum_{\mathcal{E}} \psi_1^{\mathcal{E}} \left(\psi_1^{\mathcal{E}}\right)^* & \sum_{\mathcal{E}} \psi_1^{\mathcal{E}} \left(\psi_2^{\mathcal{E}}\right)^* & \cdots & \sum_{\mathcal{E}} \psi_1^{\mathcal{E}} \left(\psi_L^{\mathcal{E}}\right)^* \\ \sum_{\mathcal{E}} \psi_2^{\mathcal{E}} \left(\psi_1^{\mathcal{E}}\right)^* & \sum_{\mathcal{E}} \psi_2^{\mathcal{E}} \left(\psi_2^{\mathcal{E}}\right)^* & \cdots & \sum_{\mathcal{E}} \psi_2^{\mathcal{E}} \left(\psi_L^{\mathcal{E}}\right)^* \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{\mathcal{E}} \psi_L^{\mathcal{E}} \left(\psi_1^{\mathcal{E}}\right)^* & \sum_{\mathcal{E}} \psi_L^{\mathcal{E}} \left(\psi_2^{\mathcal{E}}\right)^* & \cdots & \sum_{\mathcal{E}} \psi_L^{\mathcal{E}} \left(\psi_L^{\mathcal{E}}\right)^* \end{bmatrix}_{L\times L} \tag{50}$$

as advanced. See that, remarkably, this reduces the computation of the one-particle correlation functions to the multiplication of two $N \times L$ matrices.

4 Out of Equilibrium Dynamics

In this section we study the effects of quenches on the dynamics of the many-particle eigenstates of the Hamiltonian 7. The basic idea is that, via some process whose details are not important, the Hamiltonian $\hat{\mathcal{H}}$ is suddenly mapped to the Hamiltonian $\hat{\mathcal{H}}'$ on a timescale of order $T \ll 2\pi/\Delta E$. Here, $\Delta E = E_m - E_n$ can be regarded as the "smallest" (or otherwise characteristic) difference in levels of the spectrum of $\hat{\mathcal{H}}$. A sufficient value of ΔE is the difference between the ground and first excited state energy of a single particle: $\Delta E = E_{k=k_1} - E_{k=0}$ which, for large system sizes, is approximately $\Delta E \approx t\,(2\pi/L)^2$. Ideally, then, we require $T \ll \frac{2\pi\hbar}{t}\left(\frac{L}{2\pi}\right)^2$.

4.1 Dynamics of the Ground State

Let us first see how the ground state of the N (odd) particle system described by Hamiltonian 7 evolves with time. This can be achieved in one of two ways, corresponding to the Schrodinger and Heisenberg pictures, respectively. Obviously, each are equivalent (with respect to the expectation value of observables). In the Schrodinger picture (SP), we evolve the eigenstate with the operator $\hat{U}(t) = \exp\left(-i\hat{\mathcal{H}}t\right)$, while in the Heisenberg picture (HP), the operators evolve according to the Heisenberg equation of motion. Starting with the SP, we define $|\Psi(t)\rangle = \hat{U}(t)\,|GS\rangle$ where $|GS\rangle = \prod_{k<k_F} \hat{c}_k^\dagger\,|0\rangle$ is the N (odd) particle ground state. Expanding the time evolution operator in the energy eigenbasis, it is easy to see that

$$|\Psi(t)\rangle = e^{-iE_{GS}t}\,|GS\rangle \tag{51}$$

where, taking $\hbar = 1$, $E_{GS} = \sum_{k<k_F} \omega_k$. Written another way, the time evolution of the ground state is of the form

$$|\Psi(t)\rangle = \prod_{k<k_F} e^{-i\omega_k t}\hat{c}_k^\dagger\,|0\rangle\,. \tag{52}$$

In the HP, on the other hand, we simply need to consider the time dependence of a single mode. Namely, we need to solve the Heisenberg equation of motion for $\hat{c}_k^\dagger$:

$$\frac{d}{dt}\hat{c}_k^\dagger = i\left[\hat{\mathcal{H}}, \hat{c}_k^\dagger\right]. \tag{53}$$

Expanding the Hamiltonian in the energy eigenbasis (and noting that the Hamiltonian is equivalent in both pictures), we have that

$$\frac{d}{dt}\hat{c}_k^\dagger = i\sum_{k'}\omega_{k'}\left[\hat{c}_{k'}^\dagger\hat{c}_{k'}, \hat{c}_k^\dagger\right] \tag{54}$$

where

$$\begin{aligned}\left[\hat{c}_{k'}^\dagger\hat{c}_{k'}, \hat{c}_k^\dagger\right] &= \hat{c}_{k'}^\dagger\hat{c}_{k'}\hat{c}_k^\dagger - \hat{c}_k^\dagger\hat{c}_{k'}^\dagger\hat{c}_{k'} \\ &= \hat{c}_{k'}^\dagger\hat{c}_{k'}\hat{c}_k^\dagger + \hat{c}_{k'}^\dagger\hat{c}_k^\dagger\hat{c}_{k'} \\ &= \hat{c}_{k'}^\dagger\hat{c}_{k'}\hat{c}_k^\dagger + \hat{c}_{k'}^\dagger\left(\delta_{kk'} - \hat{c}_{k'}\hat{c}_k^\dagger\right) \\ &= \hat{c}_{k'}^\dagger\delta_{kk'}.\end{aligned} \tag{55}$$

Thus, plugging the above expression back into the Heisenberg equations of motion, we arrive at the differential equation $\frac{d}{dt}\hat{c}_k^\dagger = i\omega_k\hat{c}_k^\dagger$ which yields the solution $\hat{c}_k^\dagger(t) = e^{i\omega_k t}\hat{c}_k^\dagger(0) \equiv e^{i\omega_k t}\hat{c}_k^\dagger$, where in the last line we define the notation $\hat{c}_k^\dagger(0) \equiv \hat{c}_k^\dagger$. In what follows, we will adopt the SP as we are interested in the dynamical properties of the states themselves.

4.2 Many-particle Pure State Quench Dynamics

Interestingly, the only system parameters upon which the eigenstates of the Hamiltonian 7 depend is the number of sites L and the lattice parameter a. Thus, any quench which changes t or v (while keeping v constant) will have no effect on the eigenstates. One can imagine that in such a case all of the energy injected (or released) into (from) the system goes into the hopping/on-site energy–it does not effect the momentum of the particles at all. To drive the system out of equilibrium, then,

we can do three things: (i) change the lattice parameters, i.e. by taking $L \mapsto L'$ or $a \mapsto a'$ (they are equivalent), (ii) add some interaction, or (iii) break translational symmetry. The second option can be achieved by adding, e.g., a term of the form $\sum_i U_i \hat{n}_i \hat{n}_{i+1}$ where U_i is some interaction strength and $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$, or a term $\Delta \sum_i \left(\hat{c}_i^\dagger \hat{c}_{i+1}^\dagger + h.c. \right)$. Note that the latter option introduces bilinear terms and does not conserve the total number of particles–a Bogoliubov transformation is required to diagonalize the resulting Hamiltonian. In taking the first option, one must proceed carefully. One must insure that when increasing the number of sites the $t = 0$ wavefunction is well-defined. If, for example, one simply takes $L \mapsto L + 2$ while keeping periodic boundary conditions, one (I did this) should find exactly this. The best way to proceed in this regard is to use open boundary conditions. Case (iii) can be achieved for any boundary conditions simply by mapping $g = 0 \mapsto g \neq 0$. It is this case we will have in mind in the following considerations.

4.2.1 Naive Approach

The basic premise is as such: before the quench (which is assumed to occur at $t_0 = 0$), the system is taken to be in the N (odd) particle ground state $|GS\rangle = \prod_{k<k_F} \hat{c}_k^\dagger |0\rangle$. *It is important to note that the index k need not necessarily be the quasi-momentum, it is simply an index for the first k_F occupied single-particle eigenenergies.* At $t = 0$, some process occurs which suddenly changes the Hamiltonian, driving the resulting system far from equilibrium. The new Hamiltonian is assumed to admit a known basis, which we denote as $\{|E\rangle\}$, such that $\hat{\mathcal{H}}' |E\rangle = E |E\rangle$. Since we are not considering any additional interactions, the non-interacting nature of the pre-quench Hamiltonian remains. In other words, E can be regarded as the sum of N unique single-particle energies.

Now, according to the sudden quench approximation, immediately after the quench the system remains in the pre-quench ground state. The time evolution, however, is now dictated by the post-quench Hamiltonian, i.e.

$$|\Psi(t)\rangle = \exp\left(-i\hat{\mathcal{H}}'t\right)|GS\rangle = \sum_E e^{-iEt} \langle E|GS\rangle |E\rangle \tag{56}$$

where in the last line we inserted an identity of the form $\sum_E |E\rangle \langle E|$. Really, then, the only work

we need to do is to determine the overlap $\langle E|GS\rangle$.

Here is a good place to pause for a moment and consider at a deeper level what the states $|GS\rangle$ really represent. Given L sites, the full Fock space characterizing non-interacting free-fermions is a direct sum of anti-symmetrized $0, 1, \ldots, L$ single-particle tensor product Hilbert spaces. That is,

$$F_L = \oplus_{m=0}^{L} \tilde{S}\left(\mathbb{H}_1^{\otimes^m}\right) = \mathbb{H}_0 \oplus \mathbb{H}_1 \oplus \tilde{S}\left(\mathbb{H}_1 \otimes \mathbb{H}_1\right) \oplus \ldots \oplus \tilde{S}\underbrace{\left(\mathbb{H}_1 \otimes \ldots \otimes \mathbb{H}_1\right)}_{L \text{ times}}. \tag{57}$$

When we fix $0 \leq N \leq L$, we restrict our considerations to a block-diagonal subspace of the space F_L. Given the Hamiltonian we are now considering is non-interacting, there is no mixing between different particle sectors (and hence why F_L is block diagonal). The most general state belonging to F_L can be written

$$\begin{aligned} \|\Psi\rangle = \mu_0 |0\rangle \oplus \sum_{i=1}^{L} \mu_i |\psi_i\rangle \oplus \sum_{i,j=1}^{L} \mu_{i,j} |\psi_i\rangle \wedge |\psi_j\rangle \oplus \ldots \\ \oplus \sum_{i_1,i_2,\ldots,i_L}^{L} \mu_{i_1,i_2,\ldots,i_L} |\psi_{i_1}\rangle \wedge |\psi_{i_2}\rangle \wedge \ldots \wedge |\psi_{i_{L:}}\rangle \end{aligned} \tag{58}$$

where "$\wedge$" is the wedge product and $|\psi_{i_1}\rangle \wedge |\psi_{i_2}\rangle \wedge \ldots \wedge |\psi_{i_{L:}}\rangle = \epsilon_{i_1 i_2 \ldots i_L} |\psi_{i_1}\rangle \otimes |\psi_{i_2}\rangle \otimes \ldots \otimes |\psi_{i_L}\rangle$ with $\epsilon_{i_1 i_2 \ldots i_L}$ the L-dimensional Levi-Civita tensor and summation implied by repeated indices. When restricting our focus to a single N particle sector, the coefficients corresponding to all other sectors are zero. In the absence of interactions, the $\mu_{i_1 \ldots}$ are all the same for the N particle sector, and, through normalization, we find that

$$\|\Psi\rangle_N = \frac{1}{\sqrt{N!}} \epsilon_{i_1 i_2 \ldots i_N} |\psi_{i_1}\rangle \otimes |\psi_{i_2}\rangle \otimes \ldots \otimes |\psi_{i_N}\rangle. \tag{59}$$

In particular, this means that we can write

$$|GS\rangle = \frac{1}{\sqrt{N!}} \epsilon_{i_1 i_2 \ldots i_N} \left|\psi_{k_{i_1}}\right\rangle \otimes \left|\psi_{k_{i_2}}\right\rangle \otimes \ldots \otimes \left|\psi_{k_{i_n}}\right\rangle \tag{60}$$

and

$$|E\rangle = \frac{1}{\sqrt{N!}}\epsilon_{j_1 j_2 \ldots j_N} \left|\phi_{\mathcal{E}_{j_1}}\right\rangle \otimes \left|\phi_{\mathcal{E}_{j_2}}\right\rangle \otimes \ldots \otimes \left|\phi_{\mathcal{E}_{j_n}}\right\rangle$$

where $\mathcal{E}_{i_j}$ is the i_j^{th} single particle energy of the quenched state. Note that because we are assuming the quench breaks all single-particle degeneracy, the set $\{\mathcal{E}_j\}$ admits a well-defined ordering. From these considerations, it follows that

$$\begin{aligned}\left\langle E\middle|GS\right\rangle &= \frac{1}{N!}\epsilon^{j_1 j_2 \ldots j_N}\epsilon_{i_1 i_2 \ldots i_N}\left\langle\phi_{\mathcal{E}_{j_1}}\middle|\psi_{k_{i_1}}\right\rangle\left\langle\phi_{\mathcal{E}_{j_2}}\middle|\psi_{k_{i_2}}\right\rangle\cdots\left\langle\phi_{\mathcal{E}_{j_N}}\middle|\psi_{k_{i_N}}\right\rangle \\ &= \begin{vmatrix} \left\langle\phi_{\mathcal{E}_1}\middle|\psi_{k_1}\right\rangle & \left\langle\phi_{\mathcal{E}_1}\middle|\psi_{k_2}\right\rangle & \cdots & \left\langle\phi_{\mathcal{E}_1}\middle|\psi_{k_N}\right\rangle \\ \left\langle\phi_{\mathcal{E}_2}\middle|\psi_{k_1}\right\rangle & \left\langle\phi_{\mathcal{E}_2}\middle|\psi_{k_2}\right\rangle & \cdots & \left\langle\phi_{\mathcal{E}_2}\middle|\psi_{k_N}\right\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \left\langle\phi_{\mathcal{E}_N}\middle|\psi_{k_1}\right\rangle & \left\langle\phi_{\mathcal{E}_N}\middle|\psi_{k_2}\right\rangle & \cdots & \left\langle\phi_{\mathcal{E}_N}\middle|\psi_{k_N}\right\rangle \end{vmatrix}\end{aligned} \tag{61}$$

where the second line comes from the definition of the determinant $|\cdots|$ [13].

It remains, then, to calculate the single-particle overlaps. This is straightforward, as all we need to do is introduce an identity in the form $\sum_i |x_i\rangle\langle x_i|$ and use the fact that $\left\langle x_i\middle|\phi_{\mathcal{E}_j}\right\rangle = \varphi_{\mathcal{E}_j}(x_i)$ and $\left\langle x_i\middle|\psi_{k_m}\right\rangle = \psi_{k_m}(x_i) = L^{-1/2}e^{ik_m x_i}$. Thus, the matrix elements of $\langle E|GS\rangle$ go like

$$\left\langle\phi_{\mathcal{E}_j}\middle|\psi_{k_m}\right\rangle = \sum_{i=0}^{L-1}\varphi^*_{\mathcal{E}_j}(x_i)\,\psi_{k_m}(x_i) = \frac{1}{\sqrt{L}}\sum_{i=0}^{L-1}\varphi^*_{\mathcal{E}_j}(x_i)\,e^{ik_m x_i} \tag{62}$$

which can be readily calculated on a computer. Note that in the special case $|E\rangle = |GS\rangle$, $\left\langle\phi_{\mathcal{E}_j}\middle|\psi_{k_m}\right\rangle = \delta_{jm}$ and $\left\langle GS\middle|GS\right\rangle = 1$ as expected. Moreover, if any row or column is identically zero, then the total overlap is zero. This means that $|E\rangle$ and $|GS\rangle$ must have the same number of particles, also as expected.

One can easily convince themselves that although theoretically possible, the numerical implementation of equation 56 is unfeasible. This is due to the fact that for L sites and N particles, there are $\begin{pmatrix} L \\ N \end{pmatrix} = L!/\left(N!\,(L-N)!\right)$ possible values of $\{E\}$. For $L = 100$ and $N = 51$, this amounts

to order 10^{29} possible combinations. Another method must be used here.

4.2.2 Gaussian State Approach

Let us cast this problem in another light using the special properties of fermionic Gaussian states [Cite some stuff]. Consider the stationary ground state, i.e. the Fermi sea $\prod_{k<k_F} \hat{c}_k^\dagger |0\rangle$. We can rewrite this state in the lattice site basis by insertion of N identities $\sum_j |j\rangle \langle j|$ which gives

$$|\Psi\rangle = \prod_k^N \sum_j \left\langle j \middle| \hat{c}_k^\dagger \middle| 0 \right\rangle |j\rangle \tag{63}$$

where, by equation 9, we have $\left\langle j \middle| \hat{c}_k^\dagger \middle| 0 \right\rangle = L^{-1/2} e^{ikx_j}$. This means we can write

$$|\Psi\rangle = \prod_k^N \sum_j \frac{1}{\sqrt{L}} e^{ikx_j} \hat{c}_j^\dagger |0\rangle = \prod_k^N \sum_j P_{kj} \hat{c}_j^\dagger |0\rangle \tag{64}$$

where in the last line we defined an $L \times N$ matrix $\mathbf{P}$ whose elements $P_{kj} = \frac{1}{\sqrt{L}} e^{ikx_j}$. Suppose now that we evolve the state with equation 7 (no quench yet), we simply have

$$|\Psi(t)\rangle = \hat{U}(t) |\Psi(t=0)\rangle = \hat{U}(t) \prod_k^N \hat{c}_k^\dagger |0\rangle, \tag{65}$$

the result of which is given by equation 52. We can then recast this expression in exactly the same way as above, only now the matrix will have a time dependence owing to $\hat{U}(t)$. Indeed, all of the steps will be the same, and it is easy to conclude that

$$|\Psi(t)\rangle = \prod_k^N \sum_{j=1}^L P_{kj}(t) \hat{c}_j^\dagger |0\rangle \tag{66}$$

with $P_{kj}(t) = \frac{1}{\sqrt{L}} e^{ikx_j} e^{-i\omega_k t}$. It should not come as a surprise that the time dependence of the ground state of non-interacting spinless fermions can be described in terms of plane waves moving freely on a lattice–we have, in fact, already reached this conclusion.

So, what about a quenched state? Or, more generally, how can we represent a state in the manner

of equation 66 which is time-evolved according to a Hamiltonian to which it is not an eigenstate? Let us assume that the quench does not alter the non-interacting nature of the system, and that the new (i.e. post-quench) Hamiltonian $\hat{\mathcal{H}}'$ admits a *single particle* basis $\{|\mathcal{E}\rangle\}$. Similarly, we assume that the number of particles N pre- and post-quench does not change. Since the Hamiltonian remains non-interacting, it can be written as a sum over N single-particle Hamiltonians $\hat{\mathcal{H}}'_I$. Therefore, the time-evolution operator takes the convenient form

$$\hat{U}(t) = \prod^{N} e^{-i\hat{\mathcal{H}}'_I t} = \prod^{N} \sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \tag{67}$$

where the last equality is achieved by expanding the single particle Hamiltonian in the basis $\{|\mathcal{E}\rangle\}$. Then, we have that

$$|\Psi(t)\rangle = \hat{U}(t) \prod_{k}^{N} \hat{c}_k^\dagger |0\rangle \tag{68}$$

$$= \prod^{N} \sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \prod_{k}^{N} \hat{c}_k^\dagger |0\rangle \tag{69}$$

$$= \left(\sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \right) \cdots \left(\sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \right) \hat{c}_{k_1}^\dagger \cdots \hat{c}_{k_N}^\dagger |0\rangle \tag{70}$$

$$= \left(\sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \right) \cdots \left(\sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \right) \hat{c}_{k_1}^\dagger |0\rangle_{k_1} \cdots \hat{c}_{k_N}^\dagger |0\rangle_{k_N} \tag{71}$$

$$= \left(\sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \hat{c}_{k_1}^\dagger |0\rangle_{k_1} \right) \cdots \left(\sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \hat{c}_{k_N}^\dagger |0\rangle_{k_N} \right) \tag{72}$$

where, in order of appearance, we used the fact that $|0\rangle \equiv \otimes_k^N |0\rangle_k$ and $\left[\hat{c}_k^\dagger, |\mathcal{E}\rangle \langle\mathcal{E}|\right] = 0$. The latter equality can be seen by taking the inner product with an arbitrary Fock state and using the fact that for any particle number conserving Hamiltonian, wavefunctions in different N sectors are orthogonal (see e.g. equation 61). Therefore, we can write

$$|\Psi(t)\rangle = \prod_{k}^{N} \sum_{\mathcal{E}} e^{-i\mathcal{E}t} |\mathcal{E}\rangle \langle\mathcal{E}| \hat{c}_k^\dagger |0\rangle \tag{73}$$

where we dropped the subscript k on the vacuum state for notational simplicity. Note also that we index the product by k. To write this expression in the desired form, we insert two identities of the from $\sum_j |j\rangle \langle j|$ to give

$$|\Psi(t)\rangle = \prod_k^N \sum_{\mathcal{E}} \sum_j \sum_l e^{-i\mathcal{E}t} |j\rangle \langle j|\mathcal{E}\rangle \langle \mathcal{E}|l\rangle \langle l| \hat{c}_k^\dagger |0\rangle \tag{74}$$

$$= \prod_k^N \sum_{\mathcal{E}} \sum_j \left(\sum_l \phi_{\mathcal{E}}^*(x_l) \psi_k(x_l) \right) e^{-i\mathcal{E}t} \phi_{\mathcal{E}}(x_j) |j\rangle \tag{75}$$

$$= \prod_k^N \sum_j \left(\sum_{\mathcal{E}} \mathcal{C}_{k\mathcal{E}} e^{-i\mathcal{E}t} \phi_{\mathcal{E}}(x_j) \right) \hat{c}_j^\dagger |0\rangle \tag{76}$$

where in the last line we defined the expansion coefficients $\mathcal{C}_{k\mathcal{E}} = \sum_l \phi_{\mathcal{E}}^*(x_l) \psi_k(x_l)$ which are nothing more than the overlap between the pre- and post-quench wavefunctions.

Now, we claim that we can write equation 76 as

$$|\Psi(t)\rangle = \prod_k^N \sum_j \tilde{P}_{kj}(t) \hat{c}_j^\dagger |0\rangle \tag{77}$$

where $\tilde{\mathbf{P}} = \mathbf{U} e^{-i\mathbf{E}t} \mathbf{U}^\dagger \mathbf{P}$ with $\mathbf{E}$ the $L \times L$ diagonal matrix representation of $\hat{\mathcal{H}}'$ and $\mathbf{U}$ the $L \times L$ unitary diagonalization matrix of the matrix representation of $\hat{\mathcal{H}}'$. At a working level, $\mathbf{U}$ is the matrix of eigenvectors of the matrix representation of $\hat{\mathcal{H}}'$, i.e. $U_{\mathcal{E}j} = \phi_{\mathcal{E}}(x_j)$. Note that $\mathbf{P}$ is the same matrix defined earlier, i.e. the matrix of coefficients of the pre-quench state. Let us verify

now that this is the case. First, we note that

$$\begin{aligned}\mathbf{U}^{\dagger}\mathbf{P} &= \begin{bmatrix} \phi^{*}_{\mathcal{E}_1}(x_1) & \phi^{*}_{\mathcal{E}_1}(x_2) & \cdots & \phi^{*}_{\mathcal{E}_1}(x_L) \\ \phi^{*}_{\mathcal{E}_2}(x_1) & \phi^{*}_{\mathcal{E}_2}(x_2) & \cdots & \phi^{*}_{\mathcal{E}_2}(x_L) \\ \vdots & \vdots & \ddots & \vdots \\ \phi^{*}_{\mathcal{E}_L}(x_1) & \phi^{*}_{\mathcal{E}_L}(x_2) & \cdots & \phi^{*}_{\mathcal{E}_L}(x_L) \end{bmatrix} \begin{bmatrix} \psi_{k_1}(x_1) & \psi_{k_2}(x_1) & \cdots & \psi_{k_N}(x_1) \\ \psi_{k_1}(x_2) & \psi_{k_2}(x_2) & \cdots & \psi_{k_N}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{k_1}(x_L) & \psi_{k_2}(x_L) & \cdots & \psi_{k_N}(x_L) \end{bmatrix}_{L\times N} \\ &= \begin{bmatrix} \mathcal{C}_{k_1\mathcal{E}_1} & \mathcal{C}_{k_2\mathcal{E}_1} & \cdots & \mathcal{C}_{k_N\mathcal{E}_1} \\ \mathcal{C}_{k_1\mathcal{E}_2} & \mathcal{C}_{k_2\mathcal{E}_2} & \cdots & \mathcal{C}_{k_N\mathcal{E}_2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{C}_{k_1\mathcal{E}_N} & \mathcal{C}_{k_2\mathcal{E}_N} & \cdots & \mathcal{C}_{k_N\mathcal{E}_N} \end{bmatrix}_{L\times N} \end{aligned} \tag{78}$$

where we use the the definition of $\mathcal{C}_{k\mathcal{E}}$ provided above. It follows that

$$\begin{aligned} e^{-i\mathbf{E}t}\mathbf{U}^{\dagger}\mathbf{P} &= \begin{bmatrix} e^{-i\mathcal{E}_1 t} & 0 & \cdots & 0 \\ 0 & e^{-i\mathcal{E}_2 t} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{-i\mathcal{E}_N t} \end{bmatrix} \begin{bmatrix} \mathcal{C}_{k_1\mathcal{E}_1} & \mathcal{C}_{k_2\mathcal{E}_1} & \cdots & \mathcal{C}_{k_N\mathcal{E}_1} \\ \mathcal{C}_{k_1\mathcal{E}_2} & \mathcal{C}_{k_2\mathcal{E}_2} & \cdots & \mathcal{C}_{k_N\mathcal{E}_2} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{C}_{k_1\mathcal{E}_N} & \mathcal{C}_{k_2\mathcal{E}_N} & \cdots & \mathcal{C}_{k_N\mathcal{E}_N} \end{bmatrix}_{L\times N} \\ &= \begin{bmatrix} \mathcal{C}_{k_1\mathcal{E}_1}e^{-i\mathcal{E}_1 t} & \mathcal{C}_{k_2\mathcal{E}_1}e^{-i\mathcal{E}_1 t} & \cdots & \mathcal{C}_{k_N\mathcal{E}_1}e^{-i\mathcal{E}_1 t} \\ \mathcal{C}_{k_1\mathcal{E}_2}e^{-i\mathcal{E}_2 t} & \mathcal{C}_{k_2\mathcal{E}_2}e^{-i\mathcal{E}_2 t} & \cdots & \mathcal{C}_{k_N\mathcal{E}_2}e^{-i\mathcal{E}_2 t} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{C}_{k_1\mathcal{E}_N}e^{-i\mathcal{E}_N t} & \mathcal{C}_{k_2\mathcal{E}_N}e^{-i\mathcal{E}_N t} & \cdots & \mathcal{C}_{k_N\mathcal{E}_N}e^{-i\mathcal{E}_N t} \end{bmatrix}_{L\times N} \end{aligned} \tag{79}$$

so that, using

$$\mathbf{U} = \begin{bmatrix} \phi_{\mathcal{E}_1}(x_1) & \phi_{\mathcal{E}_2}(x_1) & \cdots & \phi_{\mathcal{E}_N}(x_1) \\ \phi_{\mathcal{E}_1}(x_2) & \phi_{\mathcal{E}_2}(x_2) & \cdots & \phi_{\mathcal{E}_N}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\mathcal{E}_1}(x_N) & \phi_{\mathcal{E}_2}(x_N) & \cdots & \phi_{\mathcal{E}_N}(x_N) \end{bmatrix}_{L\times L} \tag{80}$$

it is clear that

$$\tilde{\mathbf{P}} = \begin{bmatrix} \sum_{\mathcal{E}} \mathcal{C}_{k_1\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_1) & \sum_{\mathcal{E}} \mathcal{C}_{k_2\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_1) & \cdots & \sum_{\mathcal{E}} \mathcal{C}_{k_N\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_1) \\ \sum_{\mathcal{E}} \mathcal{C}_{k_1\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_2) & \sum_{\mathcal{E}} \mathcal{C}_{k_2\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_2) & \cdots & \sum_{\mathcal{E}} \mathcal{C}_{k_N\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{\mathcal{E}} \mathcal{C}_{k_1\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_N) & \sum_{\mathcal{E}} \mathcal{C}_{k_2\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_N) & \cdots & \sum_{\mathcal{E}} \mathcal{C}_{k_N\mathcal{E}} e^{-i\mathcal{E}t}\phi_{\mathcal{E}}(x_N) \end{bmatrix}_{L\times N} \tag{81}$$

as advanced. A simpler, but less explicit, way of viewing this is noticing that we can write the time evolution of the state in matrix form as

$$\tilde{\mathbf{P}}(t) = \exp(-i\mathbf{H}'t)\,\mathbf{P} \tag{82}$$

where $\mathbf{H}$ is the matrix representation of the single-particle Hamiltonian 7. Since the post-quench state is assumed not to introduce interaction terms or violate particle-number conservation, we know that we can find a unitary $\mathbf{U}$ which diagonalizes $\mathbf{H}'$. Inserting two identities of the form $\mathbf{U}\mathbf{U}^\dagger$, we see that

$$\tilde{\mathbf{P}}(t) = \mathbf{U}\mathbf{U}^\dagger \exp(-i\mathbf{H}'t)\,\mathbf{U}\mathbf{U}^\dagger\mathbf{P} = \mathbf{U}\exp(-i\mathbf{E}t)\,\mathbf{U}^\dagger\mathbf{P} \tag{83}$$

where $\mathbf{E} = \mathbf{U}^\dagger\mathbf{H}'\mathbf{U}$.

Notice that if the quench is "trivial," and the resulting eigenstates are the same as the initial states, we recover equation 66. Immediately, one observes that we no longer have to sum over $L!/(N!\,(L-N)!)$ energy eigenvalues. Indeed, we only have to multiply $L\times L$ and $L\times N$ matrices, the elements of which are simply sums over L single-particle eigenenergies.What we have shown above is, in fact, nothing but a special case of a more general principle:

Theorem 1 The action of an exponential operator who's argument is bilinear in fermionic creation and annihilation operators[1] on a Slater determinant yields a new Slater determinant, that is

$$\exp\left(\sum_{i,j}\hat{c}_i^\dagger X_{ij}\hat{c}_j\right)|\Psi_I\rangle = \prod_k^N \sum_{j=1}^L P'_{kj}\hat{c}_j^\dagger|0\rangle \tag{84}$$

where X_{ij} is the ij component of some $L \times L$ matrix $\mathbf{X}$ and $\mathbf{P'} = e^{\mathbf{X}}\mathbf{P}$.

A proof of this relation is given in section 7, and is very similar to what was shown above. Theorem 1, in words, tells us that the action of some exponential operator whose argument is quadratic in fermion creation and annihilation operators simply rotates the original lattice-site basis. Indeed, supposing $\mathbf{X}$ is not diagonal in the lattice site basis, and assuming the spectrum of $\mathbf{X}$ is known, one may insert into the equation for $\mathbf{P'}$ two identities of the form $\mathbf{U}^\dagger\mathbf{U}$ where $\mathbf{U}$ is the $L \times L$ unitary matrix of single particle overlaps in the lattice-site basis and eigenbasis of $\mathbf{X}$. This results in $\mathbf{P'} = \mathbf{U}e^{\tilde{\mathbf{X}}}\mathbf{U}^\dagger\mathbf{P}$ where $\tilde{\mathbf{X}}$ is a diagonal matrix of eigenvalues of $\mathbf{X}$ (compare with equation 77). Using the special properties introduced here and above, we develop two methods for calculating the equal-time one-body density matrix for a system of N non-interacting spinless fermions on a lattice of L sites driven far from equilibrium by means of a quench.

Method 1 The first method we develop holds only for spinless fermions–it will not extend to our considerations of hard core bosons, the complication of the latter arising from the Jordan-Wigner string operators. The main idea is similar to that developed above, only at present we wish to remain in the initial energy eigenbasis representation. The matrix $\mathbf{P}$ defined above serves as nothing more than the transformation matrix between the lattice-site and energy eigenbasis for the initial (or pure) states *with N total particles* (see for instance section 3.2). This differentiates $\mathbf{P}$ from the usual unitary transformation matrix $\mathbf{U}$, the latter of which contains all information about the possible combinations of particles (i.e. contains sums over all possible modes). So, for an equilibrium state with a conserved number of particles, there is a transformation between

[1] It is assumed here that the exponential operator is well defined. That is, $\hat{X}$ is a bounded linear operator such that $e^{\hat{X}} = \sum_n \hat{X}^n/n!$, which is valid in the case of the lattice Hamiltonian 7 and the number operator $\hat{N}$ (given the lattice constraint, i.e. $N \leq L$).

$\Phi_k^\dagger = \begin{pmatrix} \hat{c}_{k_1}^\dagger & \cdots & \hat{c}_{k_N}^\dagger \end{pmatrix}$ and $\Psi^\dagger = \begin{pmatrix} \hat{c}_1^\dagger & \cdots & \hat{c}_L^\dagger \end{pmatrix}$, namely

$$\Phi_k^\dagger = \Psi^\dagger \mathbf{P} \tag{85}$$

and, likewise,

$$\Phi_k = \mathbf{P}^\dagger \Psi. \tag{86}$$

See that the above equations are nothing more than a matrix representation of the transformation evoked in equation 64.

We now ask the question of how a unitary operator, and in particular the unitary time evolution operator, changes this mapping. Let $\hat{\mathcal{H}}'$ be some Hamiltonian under which the system evolves for all times $t > 0$. Assume that the original state is of the form $\prod_k^N \hat{c}_k^\dagger |0\rangle$ where $\{k\}$ indexes a set of N single particle eigenenergies. The time evolution operator can be written as $\hat{U}(t) = \exp\left(-it \sum_{ij} \hat{c}_i^\dagger H'_{ij} \hat{c}_j\right)$ such that the state for all times $t \geq 0$ is given by $|\Psi(t)\rangle = \hat{U}(t) \prod_k^N \hat{c}_k^\dagger |0\rangle$. In lieu of equations 77 and 64, as well as the above mappings, we construct a set of *instantaneous* creation and annihilation operators $\hat{c}_k^\dagger(t)$ and $\hat{c}_k(t)$, respectively, such that

$$\Psi^\dagger \mathcal{U} \exp(-i\mathbf{E}t) \mathcal{U}^\dagger \mathbf{U} \equiv \Psi^\dagger \tilde{\mathbf{U}}(t) = \varphi_k^\dagger(t) \tag{87}$$

and

$$\mathbf{U}^\dagger \mathcal{U} \exp(i\mathbf{E}t) \mathcal{U}^\dagger \Psi \equiv \tilde{\mathbf{U}}^\dagger(t) \Psi = \varphi_k(t) \tag{88}$$

where $\varphi_k^\dagger(t) = \begin{pmatrix} \hat{c}_{k_1}^\dagger(t) & \cdots & \hat{c}_{k_N}^\dagger(t) \end{pmatrix}$ and $\mathcal{U}$ and $\mathbf{E}$ are as defined in equation 83. These operators are said to be instantaneous in the sense that we are still working in the Schrodinger picture, i.e. these operators do not evolve in time according to, e.g., the Heisenberg equation of

motion. Instead, *at each instant in time* $t \geq 0$, the state of the system can be written

$$|\Psi(t)\rangle = \prod_k^N \hat{c}_k^\dagger(t)|0\rangle = \prod_k^N \sum_j \tilde{P}_{kj}(t)\hat{c}_j^\dagger|0\rangle \tag{89}$$

where $\tilde{P}_{kj}(t) = \sum_\epsilon \mathcal{C}_{k\epsilon} e^{-i\epsilon t}\phi_\epsilon(x_j)$ just as we showed above. Note that, in particular, $\hat{c}_k(0) = \hat{c}_k$.

With this mapping, the equal-time one-body density matrix can be written as

$$\rho_{ij}(t) = \langle 0|\prod_k^N \hat{c}_k \hat{U}^\dagger(t)\hat{c}_i^\dagger \hat{c}_j \hat{U}\prod_k^N \hat{c}_k^\dagger|0\rangle = \langle 0|\prod_k^N \hat{c}_k(t)\hat{c}_i^\dagger \hat{c}_j \prod_k^N \hat{c}_k^\dagger(t)|0\rangle \tag{90}$$

$$= \sum_{k',k''} \tilde{U}_{k'i}^\dagger(t)\tilde{U}_{k''j}(t)\langle 0|\prod_k^N \hat{c}_k(t)\hat{c}_{k'}^\dagger(t)\hat{c}_{k''}(t)\prod_k^N \hat{c}_k^\dagger(t)|0\rangle \tag{91}$$

where in the last line we made use of the mapping

$$\Psi^\dagger = \varphi_{\mathcal{E}}^\dagger(t)\tilde{\mathbf{U}}^\dagger(t) = \varphi_k^\dagger(t)\mathbf{U}^\dagger\mathcal{U}\exp(i\mathbf{E}t)\mathcal{U}^\dagger \tag{92}$$

which is similar to that defined in equation 85 but with all possible modes allowed. The N particle information is now contained in the expectation value

$$\langle 0|\prod_k^N \hat{c}_k(t)\hat{c}_{k'}^\dagger(t)\hat{c}_{k''}(t)\prod_k^N \hat{c}_k^\dagger(t)|0\rangle = \delta_{k'k''}n_{k'} \tag{93}$$

which yields

$$\rho_{ij}(t) = \sum_k \tilde{U}_{ki}^\dagger(t)\tilde{U}_{kj}(t)n_k \tag{94}$$

where, to be sure, $\sum_{\sigma'} n_{\sigma'} = N$. It is easy to convince oneself that, as a consequence (compare the above expression to equation 48),

$$\mathbf{C}(t) = \exp(-i\mathbf{H}'t)\mathbf{P}\mathbf{P}^\dagger\exp(i\mathbf{H}'t) \tag{95}$$

where $[\mathbf{C}(t)]_{ij} = \rho_{ij}(t)$. To see that this is indeed true, recognize first that $\tilde{\mathbf{P}}$ is $L \times N$ which makes $\tilde{\mathbf{P}}\tilde{\mathbf{P}}^{\dagger}$ $L \times L$, as it necessarily must be. Second, the definitions of $\tilde{\mathbf{U}} = \mathcal{U}\exp(-i\mathbf{E}t)\mathcal{U}^{\dagger}\mathbf{U}$ and $\tilde{\mathbf{P}} = \mathcal{U}\exp(-i\mathbf{E}t)\mathcal{U}^{\dagger}\mathbf{P}$ are remarkably similar–one can imagine constructing $\mathbf{P}$ out of N rows of $\mathbf{U}$, as is indeed the case. Then, so long as $\mathbf{P}$ corresponds to the N occupied modes–as by construction–we see that equations 94 and 95 are in fact equivalent.

Method 2 The next method uses explicitly the properties of real (lattice) space Slater determinants. We start by writing the equal-time one-body density matrix in the convenient form

$$\rho_{ij}(t) = \left\langle \Psi(t) \left| \hat{c}_i^{\dagger}\hat{c}_j \right| \Psi(t) \right\rangle \tag{96}$$

$$= \delta_{ij} - \langle 0| \left(\prod_k^N \sum_l \tilde{P}_{kl}^{\dagger}(t)\,\hat{c}_l \right) \hat{c}_j\hat{c}_i^{\dagger} \left(\prod_q^N \sum_m \tilde{P}_{qm}(t)\,\hat{c}_m^{\dagger} \right) |0\rangle \tag{97}$$

where, of course, the P_{qm} are the elements of the matrix of components $\mathbf{P}$. See that we can represent

$$\hat{c}_j^{\dagger} \left(\prod_q^N \sum_m \tilde{P}_{qm}(t)\,\hat{c}_m^{\dagger} \right) |0\rangle = \prod_q^{N+1} \sum_{m=1}^{L} \tilde{P}_{qm}^{j}(t)\,\hat{c}_m^{\dagger}|0\rangle \tag{98}$$

where $\tilde{P}_{qm}^{j}(t)$ is equivalent to $\tilde{P}_{qm}(t)$ up to an additional column whose only entry is a 1 at the site j, that is $\tilde{P}_{N+1,i}^{j}(t) = \delta_{ij}$. Likewise, by dual correspondence, we have

$$\langle 0| \left(\prod_k^N \sum_l \tilde{P}_{kl}(t)\,\hat{c}_l^{\dagger} \right)^{\dagger} \hat{c}_i = \langle 0| \prod_k^{N+1} \sum_l \tilde{P}_{kl}^{i,\dagger}(t)\,\hat{c}_l \tag{99}$$

with $\tilde{P}_{kl}^{i}(t)$ equivalent to $\tilde{P}_{kl}(t)$ up to an additional column for which $\tilde{P}_{N+1,m}^{i}(t) = \delta_{mi}$. The equal-time one-body density matrix can thus be written

$$\rho_{ij}(t) = \delta_{ij} - \langle 0| \prod_k^{N+1} \sum_{l=1}^{L} \tilde{P}_{kl}^{\dagger,i}(t)\,\hat{c}_l \prod_q^{N+1} \sum_{m=1}^{L} \tilde{P}_{qm}^{j}(t)\,\hat{c}_m^{\dagger}|0\rangle\,. \tag{100}$$

To evaluate this expression further, we recognize that or a general set of complex numbers $\{\mathcal{A}_{ij}\}$:

$$\prod_{i=1}^{N}\sum_{j=1}^{L}\mathcal{A}_{ij}=\sum_{j_1=1}^{L}\sum_{j_2=1}^{L}\cdots\sum_{j_N=1}^{L}\mathcal{A}_{1j_1}\mathcal{A}_{2j_2}\cdots\mathcal{A}_{N,j_N} \tag{101}$$

which implies that

$$\prod_{q}^{N+1}\sum_{m=1}^{L}\tilde{P}_{qm}\left(t\right)\hat{c}_{m}^{\dagger}\left|0\right\rangle=\sum_{\{m\}}\tilde{P}_{q_1m_1}^{j}\left(t\right)\tilde{P}_{q_2m_2}^{j}\left(t\right)\cdots\tilde{P}_{q_{N+1}m_{N+1}}^{j}\left(t\right)\hat{c}_{m_1}^{\dagger}\hat{c}_{m_2}^{\dagger}\cdots\hat{c}_{m_{N+1}}^{\dagger}\left|0\right\rangle \tag{102}$$

where we adopt the notation $\sum_{\{m\}}\equiv\sum_{m_1=1}^{L}\sum_{m_2=1}^{L}\cdots\sum_{m_{N+1}=1}^{L}$. Here, the modes $\{q_i\}$ are ordered according to increasing absolute value. By the dual correspondence, we also have

$$\left\langle 0\right|\prod_{k}^{N+1}\sum_{l}\tilde{P}_{kl}^{\dagger}\left(t\right)\hat{c}_{l}=\sum_{\{l\}}\left\langle 0\right|\hat{c}_{l_{N+1}}\cdots\hat{c}_{l_2}\hat{c}_{l_1}\tilde{P}_{k_{N+1}l_{N+1}}^{i,\dagger}\left(t\right)\cdots\tilde{P}_{k_2l_2}^{i,\dagger}\left(t\right)\tilde{P}_{k_1l_1}^{i,\dagger}\left(t\right) \tag{103}$$

whereby $\tilde{P}_{k_{N+1}l_{N+1}}^{i,\dagger}\left(t\right)$ we mean $\left(\tilde{P}^{\dagger}\right)_{k_{N+1}l_{N+1}}^{i}\left(t\right)$. Written this way, we can rewrite the RHS of equation 100 as

$$\begin{aligned}\rho_{ij}\left(t\right)=\delta_{ij}-\sum_{\{m\}}\sum_{\{l\}}&\tilde{P}_{k_{N+1}l_{N+1}}^{\dagger,i}\cdots\tilde{P}_{k_2l_2}^{\dagger,i}\tilde{P}_{k_1l_1}^{\dagger,i}\tilde{P}_{k_1m_1}^{j}\tilde{P}_{k_2m_2}^{j}\cdots\tilde{P}_{k_{N+1}m_{N+1}}^{j}\\&\times\left\langle 0\right|\hat{c}_{l_{N+1}}\cdots\hat{c}_{l_2}\hat{c}_{l_1}\hat{c}_{m_1}^{\dagger}\hat{c}_{m_2}^{\dagger}\cdots\hat{c}_{m_{N+1}}^{\dagger}\left|0\right\rangle\end{aligned} \tag{104}$$

where we dropped the argument t for notational simplicity. It remains here to calculate the final matrix elements, which we do using the special properties of Slater determinants:

Theorem 2 Given $N+1$ fermionic operators $\{\hat{c}_j\}$, we have

$$\left\langle 0\right|\hat{c}_{l_{N+1}}\cdots\hat{c}_{l_2}\hat{c}_{l_1}\hat{c}_{m_1}^{\dagger}\hat{c}_{m_2}^{\dagger}\cdots\hat{c}_{m_{N+1}}^{\dagger}\left|0\right\rangle=\epsilon^{\gamma_1\cdots\gamma_{N+1}}\delta_{l_1m_{\gamma_1}}\cdots\delta_{l_{N+1}m_{\gamma_{N+1}}} \tag{105}$$

where $\epsilon^{\gamma_1\cdots\gamma_{N+1}}$ is the Levi-Civita symbol and summation is implied.

With this, we have (making explicit the summation over dummy indices)

$$\begin{aligned}
\rho_{ij}(t) &= \delta_{ij} - \sum_{\{m\}}\sum_{\{l\}} \tilde{P}^{i,\dagger}_{k_{N+1}l_{N+1}} \cdots \tilde{P}^{i,\dagger}_{k_1 l_1} \tilde{P}^{j}_{k_1 m_1} \cdots \tilde{P}^{j}_{k_{N+1} m_{N+1}} \sum_{\{\gamma\}} \epsilon^{\gamma_1 \cdots \gamma_{N+1}} \delta_{l_1 m_{\gamma_1}} \cdots \delta_{l_{N+1} m_{\gamma_{N+1}}} \\
&= \delta_{ij} - \sum_{\{m\}}\sum_{\{\gamma\}} \epsilon^{\gamma_1 \cdots \gamma_{N+1}} \tilde{P}^{i,\dagger}_{k_1 m_{\gamma_1}} \cdots \tilde{P}^{i,\dagger}_{k_{N+1} m_{\gamma_{N+1}}} \tilde{P}^{j}_{k_1 m_1} \cdots \tilde{P}^{j}_{k_{N+1} m_{N+1}} \quad \text{(sum over } l\text{)} \\
&= \delta_{ij} - \sum_{\{\gamma\}} \epsilon^{\gamma_1 \cdots \gamma_{N+1}} \sum_{m_1} \tilde{P}^{i,\dagger}_{k_1 m_{\gamma_1}} \tilde{P}^{j}_{k_1 m_1} \cdots \sum_{m_{N+1}} \tilde{P}^{i,\dagger}_{k_{N+1} m_{\gamma_{N+1}}} \tilde{P}^{j}_{k_{N+1} m_{N+1}} \\
&= \delta_{ij} - \det\left[\left(\mathbf{P}^i(t)\right)^\dagger \mathbf{P}^j(t) \right] \qquad (106)
\end{aligned}$$

where the last line is made apparent by ample reorganizing of the factors $\tilde{P}^{i,\dagger}_{k_p m_{\gamma_q}}, \tilde{P}^{j}_{k_p m_{\gamma_q}}$ for each set $\{\gamma\}$. As mentioned above, for spinless non-interacting fermions, this method is not the most efficient. Indeed, the complexity of calculating just one element of the correlation matrix is proportional to $(N+1)^2$ where N is the number of particles. The first method, in comparison, allows one to calculate the entire correlation matrix simply by multiplying $L \times L$ matrices. However, the first method will prove to be unfeasible for hard core bosons, and the method just developed turns out to be the most efficient.

4.3 Numerics

Using the results of section 4.2, we can simulate the out-of-equilibrium dynamics for a number of quantum quenches. In this section, we report on a few such schemes and briefly discuss the results.

4.3.1 Random Potential Quench

The first quench we consider takes $v_i \equiv v$ for all i and $t < 0$ to $v_i = v + g\epsilon_i$ for $\epsilon_i \in [0,1]$ random and $t \geq 0$. The local number density is shown as a function of time for $L = 1000$ sites, $t = 1$, $v = 0$, and $g = 0.5$ for open and closed boundary conditions in Figure 5. There are $N = 11$ total particles. It is interesting to note that the behavior of the system after the quench is more or less uniform with respect to open and closed boundaries–the only major difference occuring near the edges of the lattice.

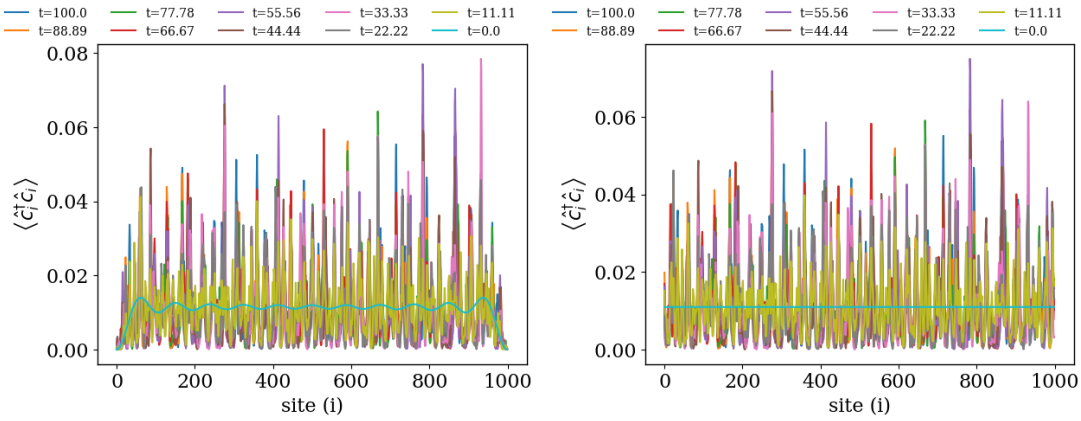

Figure 5: Local number density dynamics for a random quench. The left panel shows open boundary conditions, and the right shows periodic boundary conditions. The local number density is shown at ten different times, which is in units of $\hbar/J$ where J is the hopping parameter. The number of sites is $L = 1000$, the number of particles $N = 11$, $J = 1$, $v = 0$, and the random on-site potential strength is $g = 0.5$.

4.3.2 Half-step Potential Quench

Next, we consider what happens when a system is initially constrained to a box of width $L/2$ for $t < 0$ and then allowed to expand freely for all $t \geq 0$. The height of the initial confining box is t, $L = 1000$, $t = 1$, and $v = 0$. The local number density is shown as a function of time for both open and closed boundaries in Figure . There are $N = 51$ total particles.

4.3.3 Quadratic Trap Potential Quench

Finally, we consider the free expansion of a system initially confined to a trap of the form $v = gx_i^2$ where $x_i = ia$ with $x_0 = 0$. Again, $L = 1000$, $t = 1$ and $v = 0$. We take $g = 10t/L^2$ so that $v = 10t$ at its highest point. The local number density is shown as a function of time for open and closed boundaries. The total number of particles is $N = 101$.

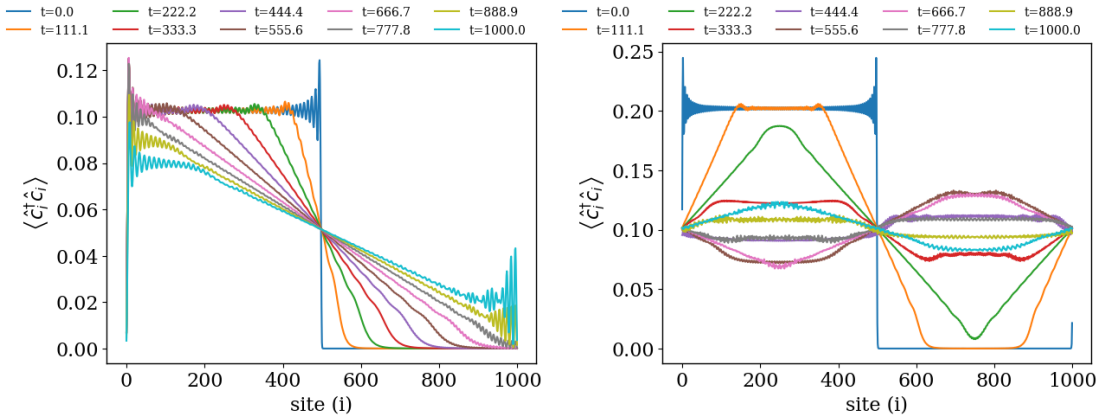

Figure 6: Local number density dynamics for a finite half-step quench. The left panel shows open boundary conditions, and the right shows periodic boundary conditions. The local number density is shown at ten different times, which is in units of $\hbar/J$ where J is the hopping parameter. The number of sites is $L = 1000$, the number of particles $N = 51$, $J = 1$, $v = 0$, and the half-step potential strength is $g = 1$.

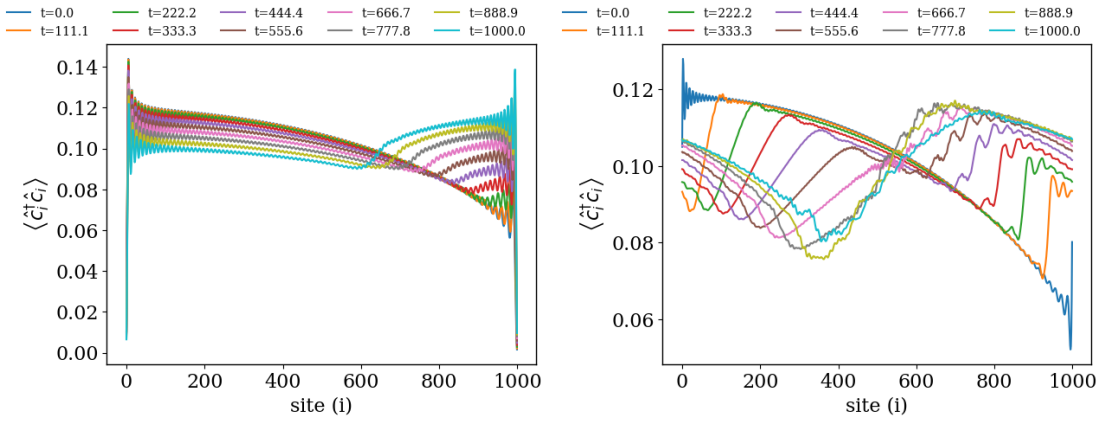

Figure 7: Local number density dynamics of freely expanding fermions after turning off a quadratic trap. The left panel shows open boundary conditions, and the right shows periodic boundary conditions. The local number density is shown at ten different times, which is in units of $\hbar/J$ where J is the hopping parameter. The number of sites is $L = 1000$, the number of particles $N = 101$, $J = 1$, $v = 0$, and the half-step potential strength is $g = 10t/L^2$.

5 Mixed State Correlations

In this section, we extend the previous analyses to account for correlations between mixed states. Particular attention will be paid to thermal states described by the grand canonical ensemble.

5.1 Density Operators and Thermal Ensembles

To begin, we review briefly the density operator formalism and its use in the description of statistical mechanical ensembles in quantum mechanics. For simplicity, we will consider here a single particle before later generalizing to many-particles. Let us suppose we have a system described by states in some single-particle Hilbert space $\mathbb{H}$. The density operator is then *defined* as

$$\hat{\rho} = \sum_j p_j \left|\psi_j\right\rangle \left\langle\psi_j\right| \tag{107}$$

where $p_j \in [0,1]$ is identified as a probability with the property that $\sum_j p_j = 1$. This latter fact immediately suggests $\mathrm{Tr}\left\{\hat{\rho}\right\} = \sum_n \left\langle\phi_n\right|\hat{\rho}\left|\phi_n\right\rangle = 1$ where $\{\left|\phi_n\right\rangle\}$ is any set of states which spans the Hilbert space. From similar considerations, we may conclude that $\hat{\rho}$ is positive semi-definite, that is $\left\langle\phi\right|\hat{\rho}\left|\phi\right\rangle = \sum_j p_j \left|\left\langle\phi\right|\left.\psi_j\right\rangle\right|^2 \geq 0$ where, again, $\left|\phi\right\rangle$ is any state in the Hilbert space. We *define* a pure state as any state $\left|\psi_i\right\rangle$ for which $p_j = \delta_{ji}$, that is

$$\hat{\rho} = \left|\psi_i\right\rangle \left\langle\psi_i\right| \tag{108}$$

and we see that the density operator is nothing but a projector onto the subspace spanned by $\left|\psi_i\right\rangle$. A state is called mixed if it is not pure. It is clear that $\mathrm{Tr}\left\{\hat{\rho}^2\right\} = 1$ only if $\hat{\rho}$ is a pure state. Indeed, if $\hat{\rho}$ is mixed, then there are at least two $p_j \neq 0$, say p_1 and p_2, for which $p_1 + p_2 = 1$. But then $\mathrm{Tr}\left\{\hat{\rho}^2\right\} = p_1^2 + p_2^2 < 1$, and the claim is proved.

The density operator is unique in the sense that it is an operator defined in terms of the states of a system. This means that for $\hat{\rho}$ to be dynamical, we must consider it in the Schrodinger picture, whereby the states evolve in time according to some Hamiltonian $\hat{\mathcal{H}}$ by means of the Schrodinger

equation. In the Schrodinger picture, then, the density operator evolves as

$$\partial_t \hat{\rho} = \sum_j p_j \partial_t \left(|\psi_j\rangle \langle\psi_j| \right) = \sum_j p_j \left[\left(\partial_t |\psi_j\rangle \right) \langle\psi_j| + |\psi_j\rangle \left(\partial_t \langle\psi_j| \right) \right] \tag{109}$$

$$= \frac{1}{i\hbar} \sum_j p_j \left[\hat{\mathcal{H}} |\psi_j\rangle \langle\psi_j| - |\psi_j\rangle \langle\psi_j| \hat{\mathcal{H}} \right] = \frac{1}{i\hbar} \left[\hat{\mathcal{H}}, \hat{\rho} \right] \tag{110}$$

where in the last line we used the fact that $\partial_t |\psi_j\rangle = (i\hbar)^{-1} \hat{\mathcal{H}} |\psi_j\rangle \leftrightarrow (-i\hbar)^{-1} \langle\psi_j| \hat{\mathcal{H}} = \partial_t \langle\psi_j|$ and $\hat{\mathcal{H}}^\dagger = \hat{\mathcal{H}}$. The above equality is known as the Von Neumann equation.

The power of the density matrix formalism becomes apparent when we consider the expectation values of observables. Indeed, let $\hat{\mathcal{O}}$ be some observable. Then we have

$$\left\langle \hat{\mathcal{O}} \right\rangle = \mathrm{Tr} \left\{ \hat{\rho} \hat{\mathcal{O}} \right\}. \tag{111}$$

The usefulness of this result is that the trace has some nice properties [10], among which is the independence of basis choice. This fact is easy enough to prove: suppose $\{|a_n\rangle\}$ and $\{|b_n\rangle\}$ are two complete bases of the Hilbert space, then

$$\left\langle \hat{\mathcal{O}} \right\rangle = \sum_l \left\langle a_l \middle| \hat{\rho} \hat{\mathcal{O}} \middle| a_l \right\rangle = \sum_{l,m,n} \langle a_l | b_m \rangle \left\langle b_m \middle| \hat{\rho} \hat{\mathcal{O}} \middle| b_n \right\rangle \langle b_n | a_l \rangle \tag{112}$$

$$= \sum_{l,m,n} \langle b_n | a_l \rangle \langle a_l | b_m \rangle \left\langle b_m \middle| \hat{\rho} \hat{\mathcal{O}} \middle| b_n \right\rangle = \sum_{m,n} \langle b_n | b_m \rangle \left\langle b_m \middle| \hat{\rho} \hat{\mathcal{O}} \middle| b_n \right\rangle \tag{113}$$

$$= \sum_n \left\langle b_n \middle| \hat{\rho} \hat{\mathcal{O}} \middle| b_n \right\rangle \tag{114}$$

as we claimed. Another important property of the trace is the so-called *cyclic property* which states that the trace is invariant under "circular" permutations, e.g.

$$\mathrm{Tr}\{ABCD\} = \mathrm{Tr}\{BCDA\} = \mathrm{Tr}\{CDAB\} = \ldots \tag{115}$$

where A, B, C, D are arbitrary square matrices.

5.1.1 Statistical Mechanical Ensembles

An important class of density operators are those pertaining to statistical mechanical ensembles. Examples include the microcanonical ensemble:

$$\hat{\rho}_\mu = \left[\int d\mu \delta \left(E - \mathcal{H} \left(\mu \right) \right) \right]^{-1} \delta \left(E - \mathcal{H} \left(\mu \right) \right) \tag{116}$$

wherein each microstate μ is equally probable; the canonical ensemble:

$$\hat{\rho}_C = \frac{1}{Z} e^{-\beta \hat{\mathcal{H}}} \tag{117}$$

where $\hat{\mathcal{H}}$ is the Hamiltonian, $\beta = \left(k_B T \right)^{-1}$, and $Z = \mathrm{Tr} \left\{ e^{-\beta \hat{\mathcal{H}}} \right\}$, which describes a closed system in contact with a thermal reservoir; and the grand canonical ensemble:

$$\hat{\rho}_{GC} = \frac{1}{\mathcal{Z}} e^{-\beta \left(\hat{\mathcal{H}} - \mu \hat{N} \right)} \tag{118}$$

where μ is the chemical potential, $\hat{N} = \sum_j \hat{n}_j$ the particle number operator, and $\mathcal{Z} = \mathrm{Tr} \left\{ e^{-\beta \left(\hat{\mathcal{H}} - \mu \hat{N} \right)} \right\}$. The grand canonical ensemble is important for two reasons. First, it introduces the notion of a chemical potential which, in fermionic systems, is closely related to the Fermi energy. Second, it accounts for the possibility of particle non-conservation, which will be crucial in our studies of the one-body density matrix.

As an instructive example, we calculate the thermal expectation value of the local number density $\hat{n}_k$ in the grand canonical ensemble where the Hamiltonian $\hat{\mathcal{H}}$ is given by equation 17. We have that

$$\langle \hat{n}_k \rangle = \left\langle \hat{c}_k^\dagger \hat{c}_k \right\rangle \tag{119}$$

where

$$\hat{\rho}_{GC} = \frac{e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}}{\mathrm{Tr}\left\{e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}\right\}} = \frac{1}{\mathcal{Z}}\prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger\hat{c}_k} \tag{120}$$

where we defined the partition function $\mathcal{Z} = \mathrm{Tr}\left\{e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}\right\}$ with the trace taken with respect to the total fermionic Fock space (equations 57 and 58). Given L sites, there are $\sum_{N=0}^{L}\begin{pmatrix} L \\ N \end{pmatrix} = 2^L$ total states in the Fock space, suggesting that the above partition function is, in general, very hard to compute. At present, however, the non-interacting nature of the system can be used to our advantage–namely the fact that in the quasi-momentum basis the eigenstates are product states. Indeed, each product of $e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger\hat{c}_k}$ only "reacts" to the occupation of the k^{th} mode–it is insensitive to the occupation of all others. This therefore factorizes the trace into the product of the sum of the factors $e^{-\beta(\epsilon_k-\mu)n_k}$ for all possible *single-particle* occupations $n_k \in \{0,1\}$. Explicitly, this means that

$$\mathcal{Z} = \prod_k \sum_{n_k} e^{-\beta(\epsilon_k-\mu)n_k} = \prod_k \left[1 + e^{-\beta(\epsilon_k-\mu)}\right] \tag{121}$$

as is well known [cite].

A more interesting (and insightful) derivation is presented in [4], which makes use of the properties of Gaussian states. As we saw in section 4.2.2, the equilibrium state $|\Psi_I\rangle = \prod_{k \text{ filled}} \hat{c}_k^\dagger |0\rangle$ may be recast as $|\Psi_I\rangle = \prod_k^N \sum_j P_{kj}\hat{c}_j^\dagger |0\rangle$ where the P_{kj} are elements of the matrix $\mathbf{P}$ of components of $|\Psi_I\rangle$. We make use here Theorem one above as well as the following theorem that will be proved in section 7.

Theorem 3 The trace over the fermionic Fock space of such Gaussian operators takes the following form:

$$\mathrm{Tr}\left\{\exp\left(\sum_{i,j}\hat{c}_i^\dagger X_{ij}\hat{c}_j\right)\exp\left(\sum_{m,n}\hat{c}_m^\dagger Y_{mn}\hat{c}_n\right)\cdots\right\} = \det\left[\mathbf{I} + e^{\mathbf{X}}e^{\mathbf{Y}}\cdots\right] \tag{122}$$

where $\mathbf{I}$ is the $L \times L$ identity operator and $\mathbf{X}, \mathbf{Y}, \ldots$ are $L \times L$ matrices.

With these, along with the observation that the Hamiltonian 7 can be written

$$\hat{\mathcal{H}} = \sum_{i,j} \hat{c}_i^\dagger H_{ij} \hat{c}_j \tag{123}$$

where H_{ij} is ij^{th} element of $\mathbf{H}$–an $L \times L$ matrix of the form of equation 41, we may immediately conclude that the partition function takes the form

$$\mathcal{Z} = \mathrm{Tr}\left\{ \exp\left(-\beta \sum_{i,j} \hat{c}_i^\dagger H_{ij} \hat{c}_j \right) \exp\left(\beta\mu \sum_{i,j} \hat{c}_i^\dagger I_{ij} \hat{c}_j \right) \right\} \tag{124}$$

$$= \det\left[\mathbf{I} + e^{-\beta(\mathbf{H} - \mu\mathbf{I})} \right] \tag{125}$$

where $\mathbf{I}$ is the $L \times L$ identity matrix. By inserting two identities of the form $\mathbf{U}\mathbf{U}^\dagger$ where $\mathbf{H}\mathbf{U} = \mathbf{U}\mathbf{E}$ with $\mathbf{E}$ the diagonal matrix of eigenvalues of $\mathbf{H}$, we arrive at

$$\mathcal{Z} = \det\left[\mathbf{U}\mathbf{U}^\dagger \left(\mathbf{1} + e^{-\beta(\mathbf{H} - \mu\mathbf{I})} \right) \mathbf{U}\mathbf{U}^\dagger \right] = \det\left[\mathbf{U} \left(\mathbf{1} + e^{-\beta(\mathbf{E} - \mu\mathbf{I})} \right) \mathbf{U}^\dagger \right] \tag{126}$$

$$= \prod_k^L \left[1 + e^{-\beta(\epsilon_k - \mu)} \right] \tag{127}$$

where in the last line we used the fact that $\det\left[\mathbf{U}\mathbf{D}\mathbf{U}^\dagger\right] = \det\left[\mathbf{D}\mathbf{U}\mathbf{U}^\dagger\right] = \det[\mathbf{D}]$ where $\mathbf{D}$ is a diagonal matrix. This can be seen from the fact that for any $L \times L$ matrices $\mathbf{A}$ and $\mathbf{B}$, $\det(\mathbf{A}\mathbf{B}) = \det(\mathbf{A}) \det(\mathbf{B})$. Comparing our final result equation 127 to the "hand-waving" result shows that they are identical.

Taking the limit $T \to 0$ takes $\beta \to \infty$ in which case the factor $e^{-\beta(\epsilon_k - \mu)} \to 0$, leaving $\mathcal{Z} = 1$. On the other hand, if we take $T \to \infty$, $\beta \to 0$ and $e^{-\beta(\epsilon_k - \mu)} \to 1$, leaving $\mathcal{Z} = 2^L$. Interestingly, we see that we regain the microcanonical ensemble in the infinite temperature limit.

It is now straightforward to calculate the number density $\hat{n}_k$ in the grand canonical ensemble.

Namely, we need only calculate

$$\langle \hat{n}_k \rangle = \frac{\mathrm{Tr}\left\{ \hat{c}_k^\dagger \hat{c}_k \prod_{k'} e^{-\beta(\epsilon_{k'}-\mu)\hat{c}_{k'}^\dagger \hat{c}_{k'}} \right\}}{\prod_k^L \left[1 + e^{-\beta(\epsilon_k - \mu)}\right]} \tag{128}$$

$$= \sum_{n_k} \frac{n_k e^{-\beta(\epsilon_k-\mu)n_k}}{1 + e^{-\beta(\epsilon_k-\mu)}} \tag{129}$$

where the last line comes from the observations that, (i) the trace is basis independent and may therefore be taken over the product basis of eigenstates of $\hat{\mathcal{H}}$ and (ii) the action of $\hat{n}_k$ on those states is independent of all $k' \neq k$. Hence, the problem is reduced to a single particle one. The resulting sum is trivial, and we find that

$$\langle \hat{n}_k \rangle = \frac{1}{e^{\beta(\epsilon_k-\mu)} + 1} \tag{130}$$

which is just the Fermi-Dirac distribution. Generically, the chemical potential μ is a function of temperature, $\mu = \mu(T)$, and can be determined by requiring that $\sum_k \langle \hat{n}_k \rangle = N$ for all temperatures. There are approximate methods for determining analytic forms of $\mu(T)$–usually by expanding around $\mu(T=0) = \epsilon_F$ where ϵ_F is the Fermi energy (e.g. the Sommerfeld expansion)–but for our purposes it suffices to know that μ can be calculated numerically.

5.2 Finite Temperature Correlations in Equilibrium

In this section, we are interested in calculating the equal-time one-body density matrix at finite temperatures in equilibrium. There are, like when solving quench dynamics, two ways to calculate the one-body density matrix. The first is far simpler, but is special to spinless non-interacting fermions. The second is more involved, but will be useful when considering hard core bosons.

Method 1 This method is inspired by [5]. We will again assume that the equilibrium states can be characterized by a momentum k. The total Fock space is spanned by states of the form $|\Psi_I\rangle = \prod_{k\ \mathrm{filled}}^N \hat{c}_k^\dagger |0\rangle$ where $0 \leq N \leq L$. At finite temperatures, the equal-time one-body density

matrix is given by

$$\left\langle \hat{c}_i^\dagger \hat{c}_j \right\rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left\{ \hat{c}_i^\dagger \hat{c}_j e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} \right\} \tag{131}$$

$$= \frac{\mathrm{Tr}\left\{ \hat{c}_i^\dagger \hat{c}_j \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\}}{\prod_k^L \left[1+e^{-\beta(\epsilon_k-\mu)}\right]} \tag{132}$$

$$= \delta_{ij} \frac{\mathrm{Tr}\left\{ \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\}}{\prod_k^L \left[1+e^{-\beta(\epsilon_k-\mu)}\right]} - \frac{\mathrm{Tr}\left\{ \hat{c}_j \hat{c}_i^\dagger \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\}}{\prod_k^L \left[1+e^{-\beta(\epsilon_k-\mu)}\right]} \tag{133}$$

where in the last line we used the canonical anticommutation relations. The first term on the last line of the RHS is trivial. The second term requires more work. In this case, we proceed as we usually would, namely, by expanding the $\hat{c}_j, \hat{c}_i^\dagger$ in the eigenbasis of the Hamiltonian. Doing so leaves

$$\mathrm{Tr}\left\{ \hat{c}_j \hat{c}_i^\dagger \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\} = \mathrm{Tr}\left\{ \sum_{k',k''} \psi_{k'}(x_j)\, \psi_{k''}^*(x_i)\, \hat{c_{k'}} \hat{c}_{k''}^\dagger \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\} \tag{134}$$

$$= \sum_{k',k''} \psi_{k'}(x_j)\, \psi_{k''}^*(x_i)\, \mathrm{Tr}\left\{ \hat{c_{k'}} \hat{c}_{k''}^\dagger \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\} \tag{135}$$

and so it remains only to calculate the last trace. By inspection, it is clear that the trace is non-zero only when $k' = k''$. This follows from two observations. First, because the trace is basis independent, we may choose to sum over the eigenstates of the Hamiltonian. Second, up to a phase the operators $\hat{c_{k'}}, \hat{c}_{k''}^\dagger$ care only about the occupation of the k', k'' mode, respectively. In conjunction, these observations imply that $\mathrm{Tr}\left\{ \hat{c_{k'}} \hat{c}_{k''}^\dagger \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\} \propto \delta_{kk'}$, as advanced. Thus, we have that

$$\mathrm{Tr}\left\{ \hat{c}_j \hat{c}_i^\dagger \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\} = \sum_{k'} \psi_{k'}(x_j)\, \psi_{k'}^*(x_i)\, \mathrm{Tr}\left\{ \hat{c_{k'}} \hat{c}_{k'}^\dagger \prod_k e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\} \tag{136}$$

$$= \sum_{k'} \psi_{k'}(x_j)\, \psi_{k'}^*(x_i)\, \mathrm{Tr}\left\{ \prod_{k\neq k'} e^{-\beta(\epsilon_k-\mu)\hat{c}_k^\dagger \hat{c}_k} \right\} \tag{137}$$

$$= \sum_{k'} \psi_{k'}(x_j)\, \psi_{k'}^*(x_i) \prod_{k\neq k'}^{L} \left[1+e^{-\beta(\epsilon_k-\mu)}\right] \tag{138}$$

where, in order of appearance, we used the fact that for any Fock state $|\{n_k\}\rangle$, $\left\langle \{n_k\} \left| \hat{c_{k'}} \hat{c}^\dagger_{k'} \right| \{n_k\} \right\rangle = 1 - n_{k'}$–and therefore the term $\left\langle \{n_k\} \left| \hat{c_{k'}} \hat{c}^\dagger_{k'} e^{-\beta(\epsilon_k - \mu)\hat{c}^\dagger_{k'}\hat{c}_{k'}} \right| \{n_k\} \right\rangle$ contributes only 0 ($n_k = 1$) or 1 ($n_k = 0$)–and, following the logic of section 5.1.1, $\mathrm{Tr}\left\{ \prod_{k \neq k'} e^{-\beta(\epsilon_k - \mu)\hat{c}^\dagger_k \hat{c}_k} \right\} = \prod_{k \neq k'}^{L} \left[1 + e^{-\beta(\epsilon_k - \mu)} \right]$.

Hence, combing the above result with equation 133, we arrive at

$$\left\langle \hat{c}^\dagger_i \hat{c}_j \right\rangle = \delta_{ij} - \sum_{k'} \psi_{k'}(x_i)\, \psi^*_{k'}(x_j) \left[1 + e^{-\beta(\epsilon_{k'} - \mu)} \right]^{-1} \tag{139}$$

which, we claim, takes the convenient form

$$\mathbf{C} = \mathbf{I} - \mathbf{U} \left[\mathbf{I} + e^{-\beta(\mathbf{E} - \mu \mathbf{I})} \right]^{-1} \mathbf{U}^\dagger \tag{140}$$

where $[\mathbf{C}]_{ij} = \left\langle \hat{c}^\dagger_i \hat{c}_j \right\rangle$, $\mathbf{I}$ is the $L \times L$ identity matrix, and $\mathbf{U}$ is the unitary diagonalization matrix for $\mathbf{H}$–the matrix representation of equation 7–such that $\mathbf{HU} = \mathbf{UE}$ where $\mathbf{E}$ is a diagonal matrix of eigenvalues of $\mathbf{H}$. It is straightforward to show that equation 139 and equation 140 are equivalent.

Method 2 This method is inspired by [4] and serves as an alternative way of calculating the off-diagonal elements of 140. This method is computationally more complex, and will not be helpful for our current endeavors, instead laying the groundwork necessary to study hard core bosons on a lattice. Inspired by our treatment of quench dynamics in section 4.2.2, we write an arbitrary Fock state as $|\Psi_I\rangle = \prod_{k \text{ filled}} \hat{c}^\dagger_k |0\rangle = \prod_k^N \sum_j P_{kj} \hat{c}^\dagger_j |0\rangle$ where the P_{kj} are elements of the matrix $\mathbf{P}$ of components of $|\Psi_I\rangle$. At finite temperatures, the equal-time one-body density matrix is given by

$$\left\langle \hat{c}^\dagger_i \hat{c}_j \right\rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left\{ \hat{c}^\dagger_i \hat{c}_j e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})} \right\} \tag{141}$$

$$= \frac{1}{\mathcal{Z}} \mathrm{Tr}\left\{ \hat{c}^\dagger_i \hat{c}_j \exp\left(-\beta \sum_{i,j} \hat{c}^\dagger_i H_{ij} \hat{c}_j \right) \exp\left(\beta\mu \sum_{i,j} \hat{c}^\dagger_i I_{ij} \hat{c}_j \right) \right\} \tag{142}$$

where the partition function $\mathcal{Z}$ is calculated in section 5.1.1. The claims made in that same section allow us to greatly simplify the calculation of this value for $i \neq j$. We observe that

$$1 + \hat{c}^\dagger_j \hat{c}_i = e^{\hat{c}^\dagger_j \hat{c}_i} \tag{143}$$

owing to the definition of operator exponentials and the fermionic algebra (in particular, the hard core constraint $\left(\hat{c}_i^\dagger\right)^2 = \left(\hat{c}_j\right)^2 = 0$). Thus, we can write

$$\left\langle \hat{c}_i^\dagger \hat{c}_j \right\rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left(\exp\left(\sum_{i,j} \hat{c}_i^\dagger \delta_{ij} \hat{c}_j \right) \exp\left(-\beta \sum_{i,j} \hat{c}_i^\dagger H_{ij} \hat{c}_j \right) \exp\left(\beta\mu \sum_{i,j} \hat{c}_i^\dagger I_{ij} \hat{c}_j \right) \right) - \frac{1}{\mathcal{Z}} \mathrm{Tr}\left\{ \exp\left(-\beta \sum_{i,j} \hat{c}_i^\dagger H_{ij} \hat{c}_j \right) \exp\left(\beta\mu \sum_{i,j} \hat{c}_i^\dagger I_{ij} \hat{c}_j \right) \right\} \tag{144}$$

$$= \frac{1}{\mathcal{Z}} \left(\det\left[\mathbf{I} + e^{\mathbf{\Delta}} e^{-\beta(\mathbf{H}-\mu\mathbf{I})} \right] - \det\left[\mathbf{I} + e^{-\beta(\mathbf{H}-\mu\mathbf{I})} \right] \right) \tag{145}$$

$$= \frac{1}{\mathcal{Z}} \det\left[\left(\mathbf{I} + (\mathbf{I} + \mathbf{\Delta})\, e^{-\beta(\mathbf{H}-\mu\mathbf{I})} \right) \right] - 1 \tag{146}$$

where $\mathbf{\Delta}$ is the matrix representation of δ_{ij}. In order of appearance, we used equation 122, equation 127, and the fact that, in matrix form, equation 143 reads $e^{\mathbf{\Delta}} = \mathbf{I} + \mathbf{\Delta}$. Again, we emphasize that this formalism is not useful for free fermions. The above expression is computationally expensive, and calculates only one element of $\mathbf{C}$ at a time.

5.2.1 Numerics

Here we show various numerical results. All of the following are done using the formalism of Method 1 in the previous section.

Constant On-site Potential with OBC Here, we consider a system of non-interacting spinless fermions on a lattice of $L = 1000$ sites with a constant on-site potential $v = 0.1t$. The local number density and two-point correlation function for fixed $j = 500$ are shown as a function of inverse temperature in Figure 8. Here, the number of particles is fixed to $N = 101$, and the chemical potential μ for each temperature is set by $\sum_i \rho_{ii} = N$.

Interestingly, as the temperature T increases (β decreases), the local number density becomes increasingly uniform (i.e. flat) and the two-point correlator becomes increasingly localized about $j = 500$. This suggests that as the temperature increases, the phase coherence of the states decreases. This, in effect, leads to increased interference between states with different quasi-

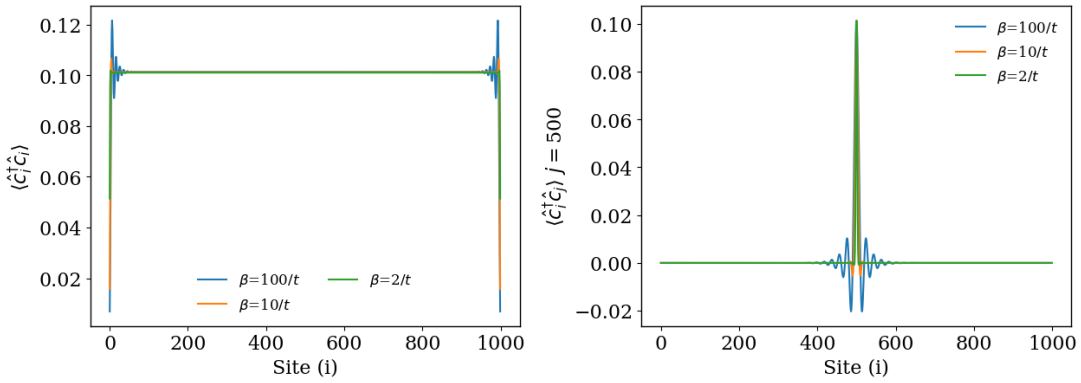

Figure 8: Local number density (left) and two-point correlation function for a particle at $j = 500$ (right) as a function of site i and temperature.

momentum, causing the local number density to flatten and the two-point correlator to localize. Note that this should not come as a surprise given the state evolves from a pure state to a mixed state as T increases from 0.

We also would like to consider a new experimentally relevant physical (which will prove useful in our later studies of hydrodynamization [cite]) called the momentum distribution function (MDF) n_k. The MDF is *defined* as the Fourier transform of the one-body density matrix ρ_{ij} [cite], that is

$$n_k = \frac{1}{L} \sum_{i,j} e^{ik(x_i - x_j)} \rho_{ij} \tag{147}$$

where, of course, L is the number of lattice sites[2]. We plot this quantity in Figure 9 for a system with open boundary conditions and constant v and compare it to the analytic case described by equation 130. The results for $N = 51, L = 100$, $N = 101, L = 1000$, and $N = 501, L = 1000$ are shown.

There are a number of interesting observations to be made with regards to this figure. First, for $L = 100$ sites we see that at low temperatures (high β), the MDF deviates rather significantly from the Fermi-Dirac distribution (FDD). This should not come as a surprise given that the FDD

[2]This is, of course, nothing but the normalization constant. It will turn out in our later studies of hard core bosons that this constant depends on the particulars of the lattice potential, e.g. the strength and shape of a trap.

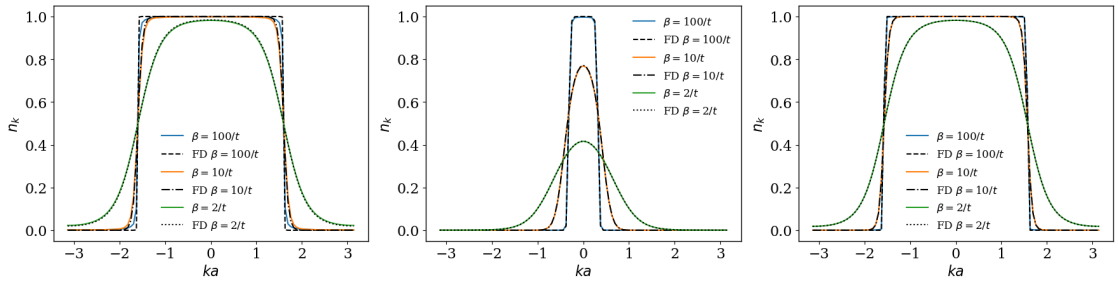

Figure 9: Momentum distribution function (MDF) as a function of quasi-momentum ka and inverse temperature $\beta = (k_B T)^{-1}$. From left to right, we show the MDF at temperatures $\beta = 100, 10$, and 2 for 51 particles on 100 sites, 101 particles on 1000 sites, and 501 particles on 1000 sites.

is exact and relies on the existence of well-defined quasi-momenta. Indeed, one may show that by inserting the one-body density matrix corresponding to a translationally invariant system with periodic boundary conditions yields the FDD. What is perhaps more surprising is that the FDD predicts well the behavior of ,one, the high temperature (low β) MDF for $L = 100$ and, two, the MDF for large system sizes. Concerning the former, a possible explanation is the fact that, near the middle of the lattice, the highly excited states for open and periodic boundaries are qualitatively similar. This suggests that, at high temperatures when highly excited modes are thermally more probable, the open system is qualitatively indistinguishable from the periodic system, at least away from the edges. Indeed, as we already pointed out, the local number density becomes flat as the temperature increases. This "flatness" is exactly the same behavior admitted by the periodic system *at all temperatures*, and hence the agreement. A reasonable refute to this argument, to which I do not have a good answer, is that fermions–especially those in periodic systems–are highly non-local objects, and therefore *must* be aware of the boundary conditions. Concerning the second point, it is likely that near the "edges" of the MDF, a similar trend is seen as in the $L = 100$ case, only here we do not have the resolution to make it clear.

Random Potential with OBC Here we consider the same quantities as above but for a system with potential $v_i = v + g\epsilon_i$ where v is a constant, $\epsilon_i \in [0, 1]$ is a random parameter, and g is the potential strength. The local number density, two-point correlator, and momentum distribution

function are all shown as a function of temperature in figure 10.

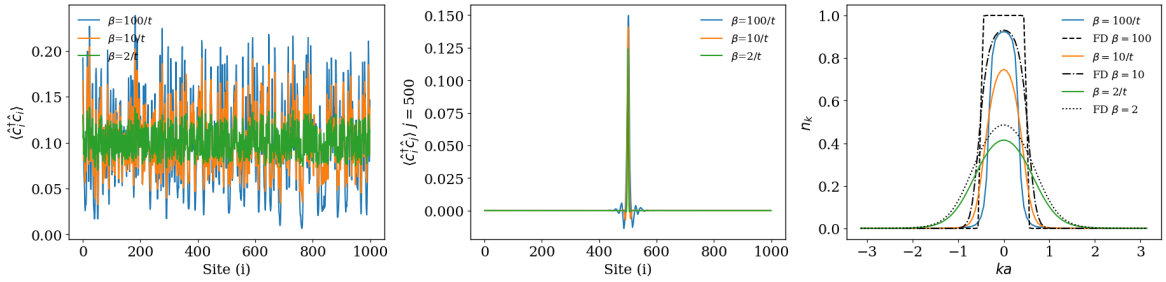

Figure 10: Local number density (left), two-point correlator (middle), and momentum distribution function (right) for $N = 101$ spinless fermions on a lattice of $L = 1000$ sites with a random on-site potential. The strength of the potential is $g = 0.5t$. The dotted and dashed lines on the rightmost figure show the FDD expectation.

Inspection of this figure shows a number of qualitative differences from the previous case $(g = 0)$. Most striking is the difference of the MDF to the FDD. This should not come as a surprise, although the momentum profile is peculiar. One might expect that the MDF be more delocalized given that the single particle eigenstates are extremely localized in space. The fact that the profile is actually *more* localized than in the translationally invariant case is curious. On the other hand, we do see that as the temperature is increased, the local number density tends towards a uniform density about the same value as in the exact and previous cases.

Half-step Potential with OBC Here we consider a potential of the form $v_i = v + g\theta\left(x_i - x_{L/2}\right)$ where $g = 1t$ is the "strength" of the step. The local number density, two-point correlator, and momentum distribution function as a function of temperature for $L = 1000$ sites, $N = 101$ particles, and open boundary conditions are all shown in figure 11.
Discuss.

Trap Potential with OBC The last and possibly most relevant scenario we will consider is a potential trap, i.e. $v_i = g\left(x_i - x_{L/2}\right)^2$ with g the trap strength. Potentials of this kind are particularly pertinent to trapped atom experiments, and will be considered heavily in our treatment of hard core bosons. The local number density, two-point correlator, and momentum distribution

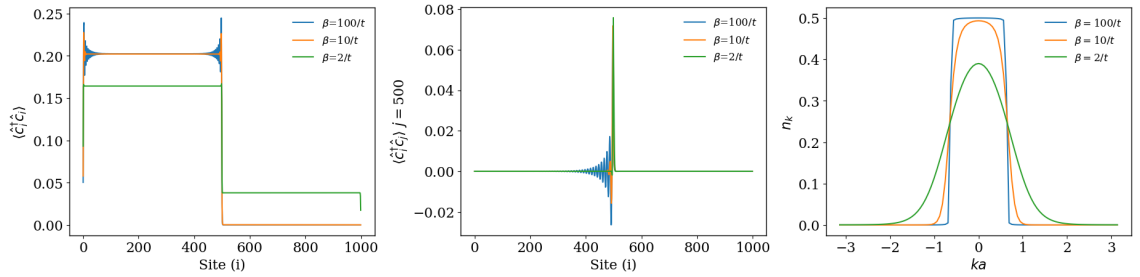

Figure 11: Local number density (left), two-point correlator (middle), and momentum distribution function (right) for $N = 101$ spinless fermions on a lattice of $L = 1000$ sites with a half-step potential.

function are all shown as a function of temperature in figure for a trapped system with $L = 1000$ sites, $N = 101$ particles, and open boundary conditions (also physically relevant) in figure 12.

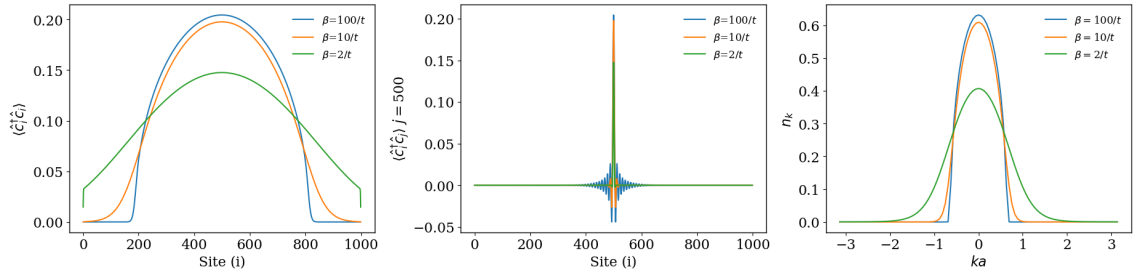

Figure 12: Local number density (left), two-point correlator (middle), and momentum distribution function (right) for $N = 101$ spinless fermions on a lattice of $L = 1000$ sites with a trap potential.

Discuss.

5.3 Finite Temperature Correlations out of Equilibrium

The natural next step is to consider non-equilibrium dynamics of non-interacting spinless fermions at finite temperature. Our approach will combine those developed in sections 4.2.2 and 5.2. The pre-quench Hamiltonian is taken to be $\hat{\mathcal{H}}$, which is assumed to admit an eigenbasis of the form $|\{\mathcal{E}\}\rangle = \prod_{\mathcal{E}} \hat{c}^\dagger_{\mathcal{E}} |0\rangle$, where $\{\mathcal{E}\}$ is the set of L single-particle eigenvalues, and eigenenergy $E = \sum_{\mathcal{E}} n_{\mathcal{E}} \mathcal{E}$. At $t = 0$, the Hamiltonian is quenched in some way such that the resulting Hamiltonian is given by $\hat{\mathcal{H}}'$ which admits some eigenbasis $|\{\epsilon\}\rangle$. So far, the set up is identical to that presented in section 4.2.

We here make matters more interesting by also taking the initial state to be in equilibrium with a thermal reservoir of inverse temperature β. In this way, the initial state is no longer pure, but is instead characterized by the density operator 118 where, to be sure, the Hamiltonian is given by $\hat{\mathcal{H}}$.

The equal-time one-body density operator can be calculated at a time t via

$$\rho_{ij}(t) = \frac{1}{\mathcal{Z}}\mathrm{tr}\left\{\hat{c}_i^\dagger \hat{c}_j e^{-i\hat{\mathcal{H}}'t} e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} e^{i\hat{\mathcal{H}}'t}\right\} \tag{148}$$

$$= \delta_{ij} - \frac{1}{\mathcal{Z}}\mathrm{tr}\left\{\hat{c}_j \hat{c}_i^\dagger e^{-i\hat{\mathcal{H}}'t} e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)} e^{i\hat{\mathcal{H}}'t}\right\} \tag{149}$$

where, again, the trace is taken with respect to the entire fermionic Fock space. Note that due to the equivalence between expectation values in the Schrodinger and Heisenberg pictures, the expectation value of a quantity $\left\langle \Psi(t)\middle|\hat{\mathcal{O}}\middle|\Psi(t)\right\rangle$ can be calculated as $\mathrm{tr}\left\{\hat{\mathcal{O}}\hat{\rho}(t)\right\}$, where $\hat{\rho}(t)$ evolves according to the Schrodinger equation, or as $\mathrm{tr}\left\{\hat{\mathcal{O}}(t)\hat{\rho}\right\}$, where $\hat{\mathcal{O}}(t) = e^{i\hat{\mathcal{H}}t}\hat{\mathcal{O}}e^{-i\hat{\mathcal{H}}t}$.

This method combines the first methods of sections 4.2.2 and 5.2. The idea is straightforward: first we find the diagonal representation of the operator $e^{-i\hat{\mathcal{H}}'t}e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}e^{i\hat{\mathcal{H}}'t}$ and then use this basis to rewrite the lattice operators. Once this is done, the procedure is exactly as in section 5.2. With this in mind, we express the time evolved density operator as

$$e^{-i\hat{\mathcal{H}}'t}e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}e^{i\hat{\mathcal{H}}'t} = \exp\left(-it\sum_{ij}\hat{c}_i^\dagger H'_{ij}\hat{c}_j\right)\exp\left(-\beta\sum_{lm}\hat{c}_l^\dagger H_{lm}\hat{c}_m\right)\exp\left(\beta\mu\sum_{no}\hat{c}_n^\dagger I_{no}\hat{c}_o\right)$$
$$\times\exp\left(it\sum_{pq}\hat{c}_p^\dagger H'_{pq}\hat{c}_q\right) \tag{150}$$

$$\doteq \Psi^\dagger e^{-i\mathbf{H}'t}e^{-\beta(\mathbf{H}-\mu\mathbf{I})}e^{i\mathbf{H}'t}\Psi \tag{151}$$

where in the last line we take $\Psi^\dagger = \begin{pmatrix}\hat{c}_1^\dagger & \cdots & \hat{c}_L\end{pmatrix}$, $\Psi = \left(\Psi^\dagger\right)^\dagger$, and $\mathbf{H}'$ and $\mathbf{H}$ the matrix representation of the post- and pre-quench Hamiltonian in the lattice site basis, respectively. Written in this way, it is clear how we should diagonalize this operator. Namely, we insert two types of identities, $\mathbf{U}\mathbf{U}^\dagger$ and $\mathcal{U}\mathcal{U}^\dagger$, corresponding to unitary transformations which map the lattice basis to

the energy eigenbasis of the post- and pre-quench Hamiltonian, respectively. The result is

$$e^{-i\mathbf{H}'t}e^{-\beta(\mathbf{H}-\mu\mathbf{I})}e^{i\mathbf{H}'t} = \Psi^\dagger\mathbf{U}e^{-i\mathbf{E}'t}\mathbf{U}^\dagger\mathcal{U}e^{-\beta(\mathbf{E}-\mu\mathbf{I})}\mathcal{U}^\dagger\mathbf{U}e^{i\mathbf{E}'t}\mathbf{U}^\dagger\Psi \tag{152}$$

$$\equiv \varphi_E^\dagger(t)\, e^{-\beta(\mathbf{E}-\mu\mathbf{I})}\varphi_E(t) \tag{153}$$

where in the last line we *defined* the instantaneous creation and annihilation operators, $\varphi_E^\dagger(t) = \begin{pmatrix} \hat{c}_{\mathcal{E}_1}^\dagger(t) & \cdots & \hat{c}_{\mathcal{E}_L}^\dagger(t) \end{pmatrix}$ and $\varphi_E(t) = \left(\varphi_E^\dagger(t)\right)^\dagger$, respectively, such that the time evolved density operator can be written explicitly as

$$e^{-i\hat{\mathcal{H}}'t}e^{-\beta\left(\hat{\mathcal{H}}-\mu\hat{N}\right)}e^{i\hat{\mathcal{H}}'t} = \prod_\sigma e^{-\beta(\mathcal{E}_\sigma-\mu)\hat{c}_{\mathcal{E}_\sigma}^\dagger(t)\hat{c}_{\mathcal{E}_\sigma}(t)}. \tag{154}$$

This allows us to write the equal-time one-body density matrix as

$$\rho_{ij}(t) = \delta_{ij} - \frac{1}{\mathcal{Z}}\mathrm{tr}\left\{\hat{c}_j\hat{c}_i^\dagger\prod_\sigma e^{-\beta(\mathcal{E}_\sigma-\mu)\hat{c}_{\mathcal{E}_\sigma}^\dagger(t)\hat{c}_{\mathcal{E}_\sigma}(t)}\right\} \tag{155}$$

$$= \delta_{ij} - \frac{1}{\mathcal{Z}}\sum_{\sigma',\sigma''}\tilde{U}_{\sigma',i}(t)\,\tilde{U}_{\sigma'',j}^\dagger(t)\,\mathrm{tr}\left\{\hat{c}_{\mathcal{E}_{\sigma'}}(t)\,\hat{c}_{\mathcal{E}_{\sigma''}}^\dagger(t)\prod_\sigma e^{-\beta(\mathcal{E}_\sigma-\mu)\hat{c}_{\mathcal{E}_\sigma}^\dagger(t)\hat{c}_{\mathcal{E}_\sigma}(t)}\right\} \tag{156}$$

where in the last line we defined the unitary transformation matrix $\tilde{\mathbf{U}}^\dagger(t) = \mathcal{U}^\dagger\mathbf{U}\exp(i\mathbf{E}t)\,\mathbf{U}^\dagger$ which maps the lattice operators to the instantaneous operators. See that the above expression is exactly analogous to equation 135 (in fact for $t = 0$ it is identical). Thus, we expect that the ensuing algebra is the same. To be explicit, we take the trace over the states $\prod_\sigma \hat{c}_{\mathcal{E}_\sigma}^\dagger(t)\,|0\rangle$, which implies that σ' must be equal to σ'' for otherwise the expectation value is zero. Moreover, the action of $\hat{c}_{\mathcal{E}_{\sigma'}}(t)\,\hat{c}_{\mathcal{E}_{\sigma'}}^\dagger(t)$ on any instantaneous fermionic state returns 0 if the state is occupied and 1 otherwise. This means that the only non-zero contribution to the product $\prod_\sigma e^{-\beta(\mathcal{E}_\sigma-\mu)\hat{c}_{\mathcal{E}_\sigma}^\dagger(t)\hat{c}_{\mathcal{E}_\sigma}(t)}$ from the σ' orbital is 1, meaning

$$\hat{c}_{\mathcal{E}_{\sigma'}}(t)\,\hat{c}_{\mathcal{E}_{\sigma'}}^\dagger(t)\prod_\sigma e^{-\beta(\mathcal{E}_\sigma-\mu)\hat{c}_{\mathcal{E}_\sigma}^\dagger(t)\hat{c}_{\mathcal{E}_\sigma}(t)} = \prod_{\sigma\neq\sigma'} e^{-\beta(\mathcal{E}_\sigma-\mu)\hat{c}_{\mathcal{E}_\sigma}^\dagger(t)\hat{c}_{\mathcal{E}_\sigma}(t)} \tag{157}$$

and we are left with

$$\rho_{ij}(t) = \delta_{ij} - \frac{1}{\mathcal{Z}} \sum_{\sigma'} \tilde{U}_{\sigma',j}(t) \tilde{U}^{\dagger}_{\sigma',i}(t) \operatorname{tr} \left\{ \prod_{\sigma \neq \sigma'} e^{-\beta(\mathcal{E}_\sigma - \mu) \hat{c}^{\dagger}_{\mathcal{E}_\sigma}(t) \hat{c}_{\mathcal{E}_\sigma}(t)} \right\} \tag{158}$$

$$= \delta_{ij} - \sum_{\sigma'} \tilde{U}_{\sigma',j}(t) \tilde{U}^{\dagger}_{\sigma',i}(t) \frac{\prod_{\sigma \neq \sigma'}^{L} \left[1 + e^{-\beta(\mathcal{E}_\sigma - \mu)}\right]}{\prod_{\sigma}^{L} \left[1 + e^{-\beta(\mathcal{E}_\sigma - \mu)}\right]} \tag{159}$$

$$= \delta_{ij} - \sum_{\sigma'} \tilde{U}_{\sigma',j}(t) \tilde{U}^{\dagger}_{\sigma',i}(t) \left[1 + e^{-\beta(\mathcal{E}_{\sigma'} - \mu)}\right]^{-1} \tag{160}$$

or

$$\mathbf{C}(t) = \mathbf{I} - \tilde{\mathbf{U}}(t) \left[\mathbf{I} + e^{-\beta(\mathbf{E} - \mu \mathbf{I})}\right]^{-1} \tilde{\mathbf{U}}^{\dagger}(t) \tag{161}$$

$$= \mathbf{I} - \mathbf{U} \exp(-i\mathbf{E}'t) \mathbf{U}^{\dagger} \mathcal{U} \left[\mathbf{I} + e^{-\beta(\mathbf{E} - \mu \mathbf{I})}\right]^{-1} \mathcal{U}^{\dagger} \mathbf{U} \exp(i\mathbf{E}'t) \mathbf{U}^{\dagger} \tag{162}$$

$$= \mathbf{I} - \exp(-i\mathbf{H}'t) \left[\mathbf{I} + e^{-\beta(\mathbf{H} - \mu \mathbf{I})}\right]^{-1} \exp(i\mathbf{H}'t) \tag{163}$$

which is just what we found in section 5.2 but with $\mathbf{U} \mapsto \tilde{\mathbf{U}}(t)$.

Here we begin to see a trend, namely, that the time dependence of the one-body density matrix for spinless non-interacting fermions goes simply as

$$\mathbf{C}(t) = e^{-i\mathbf{H}'t} \mathbf{C}(0) e^{i\mathbf{H}'t} \tag{164}$$

where $\mathbf{C}(0)$ is the initial correlation matrix in equilibrium. This should not come as a surprise if $\rho_{ij}(t)$ is to truly be interpreted as a density matrix. Indeed, given we are working in the Schrodinger representation, the time dependence of an arbitrary density matrix $\hat{\rho}$ is contained fully within the states which represent it, namely, $\hat{\rho}(t) = \sum_j p_j |\psi_j(t)\rangle \langle \psi_j(t)|$. But we know that $|\psi_j(t)\rangle = \hat{U}(t) |\psi_j(0)\rangle$, and therefore $\hat{\rho}(t) = \sum_j p_j \hat{U}(t) |\psi_j(0)\rangle \langle \psi_j(0)| \hat{U}^{\dagger}(t) = e^{-i\hat{\mathcal{H}}t} \hat{\rho}(0) e^{i\hat{\mathcal{H}}t}$.

5.3.1 Numerics

We show here a number of numerical results regarding the post-quench dynamics of non-interacting spinless fermion systems initially coupled to a thermal reservoir of temperature T.

Free Expansion (Open Boundary Conditions) In figure 13 we show the dynamics of the local particle density after turning off a trapping potential of some sort (quadratic or finite step) at various inverse temperatures.

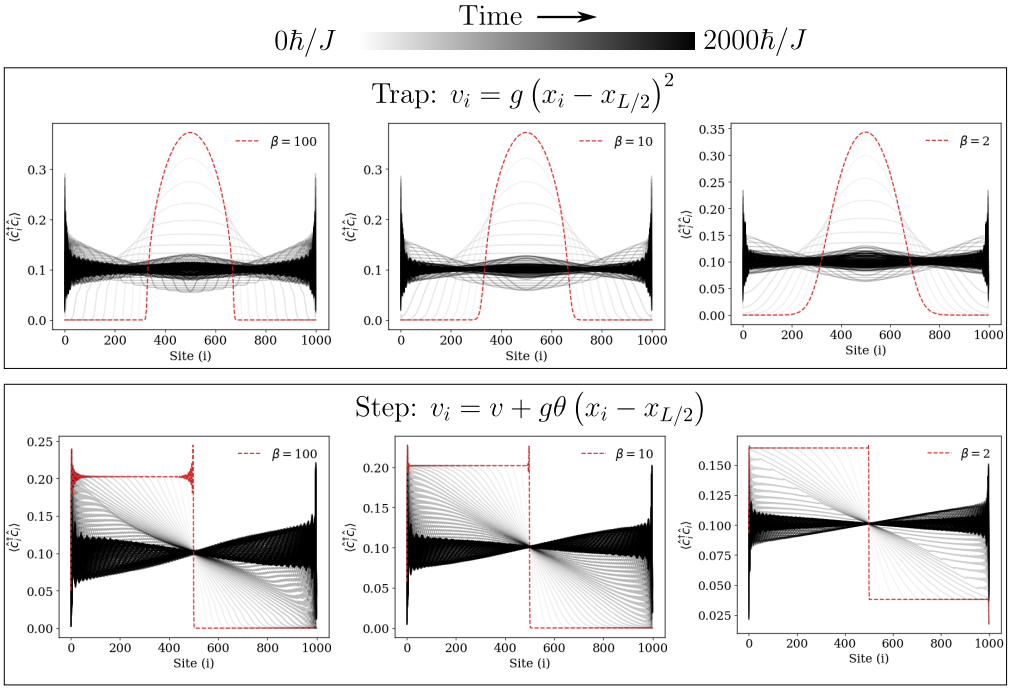

Figure 13: Free expansion of local density following the termination of a trapping potential (**top:** quadratic; **bottom:** half-step) at finite temperature. The plot lines grow darker with time. The trap functions are shown above their respective results. The inverse temperatures are shown to be 100,10, and 2 $\hbar/J$ where J is the hopping strength (not to be confused with the time parameter t). The dashed red lines show the initial local density.

In all cases, the local density is seen to become more or less uniform with time. This is to be expected, even in the case of open boundary conditions. It is interesting also to observe that the fermions "pile-up" near the edges of the lattice for even long times.

Dynamics of Momentum Distribution Function Special attention will be paid here to the role of open versus periodic boundary conditions. In figure 14, we show the dynamics of the momentum distribution function for the free expansion of spinless fermions following a quadratic potential trap.

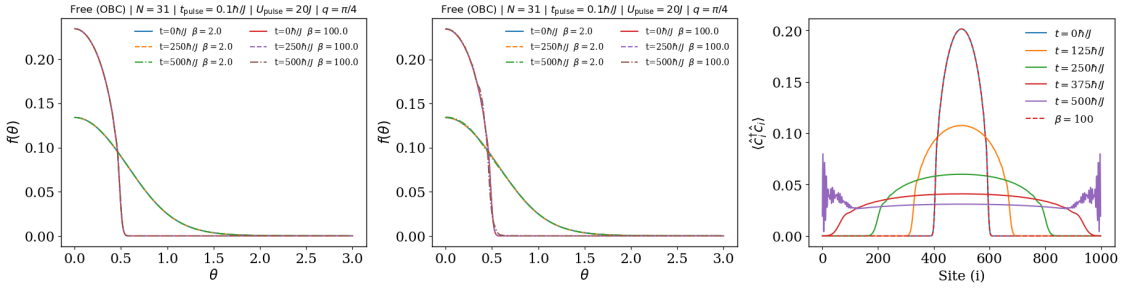

Figure 14: Momentum distribution function for freely expanding fermions following a quadratic trap with **Left:** periodic boundary conditions and **Middle:** open boundary conditions. **Right:** local density dynamics for same time stamps shown in the first two figures. The temperature here is $\beta = 100$.

See that for free expansion with periodic boundary conditions (i.e., free expansion into continuum; left panel), the MDF does not change with time. Indeed, one may show that this is indeed the case *for all subsequent times*. In contrast, for free expansion into a box with hard walls (open boundary conditions; middle panel), the MDF is observed to be static for all times $t \lessapprox 500\hbar/J$ before (albeit, slightly) deviating at $t = 500\hbar/J$. Comparing the central panel to the rightmost panel, wherein the local density dynamics are shown for the same time steps, we see that the MDF becomes dynamic only *after* the particles have had time to interact with the wall. One should find that the MDF oscillates about its $t = 0$ position for all subsequent times after interacting with the wall.

6 Bragg Pulse Quench

Here, we consider in detail a quench of great experimental importance: the Bragg pulse quench. Recall that Bragg diffraction was originally developed to determine the structure of crystalline solids by measuring the intensity profile of scattered X-rays. The basic idea there was that the crystal acted as a periodic array of localized scattering potentials which caused the X-rays to interfere in a way which depended on the reciprocal lattice. Here, the idea is more or less the same, only now the reverse process occurs. Indeed, we subject a gas of atoms to a standing wave of light at some fixed frequency. The latter acts as our "crystal," and the atoms trade momentum with the electromagnetic field in such a way that their momentum distribution function shows a diffraction pattern. In the 1930's Kapitza and Dirac showed that, in fact, one can think about this as a true diffraction phenomenon, i.e. that the standing waves can be though to diffract matter waves (deBroglie waves) [CITE]. To date, Bragg diffraction of atoms has proven to be of utmost importance to atomic, molecular, and optical physics [CITE], and in particular plays a key role in probing hydrodynamization in hard core bosons.

6.1 Theory

At a microscopic level, the trapped atoms interact with the electromagnetic field of the standing wave through their induced dipole moments [7]. The interaction of a single atom with the electromagnetic field can be modeled as $\hat{\mathcal{H}}_{\text{int}} = \mathbf{d} \cdot \mathbf{E}$ where $\mathbf{d} \propto \hat{x}$ is the dipole operator, $\hat{x}$ the coordinate operator, and $\mathbf{E}$ is the electromagnetic field evaluated at the position of the atom. Such an interaction generally results in a Jaynes-Cummings type Hamiltonian after quantizing the electromagnetic field. Presently, we are not interested in modeling such an interaction. Instead, we follow Ref. [6], wherein the authors use an effective minimal coupling Hamiltonian, which models the dipole interaction as a one-body potential of the form $U(x) = U_{\text{pulse}} \cos qx$ coupled to a bosonic field $\hat{\Psi}^{\dagger}(x)\hat{\Psi}(x)$. We acknowledge that in employing a minimal coupling Hamiltonian, we should in theory also include the vector potential $\mathbf{A}$ by mapping the conjugate momentum to $\mathbf{p} \mapsto \mathbf{p} - \frac{q}{c}\mathbf{A}$ in the initial Hamiltonian. However, here and in Ref. [6] it is assumed that the amplitude of the

pulse U_{pulse} is large and the temporal extent τ of the pulse is small while $U_{\text{pulse}}\tau$ is kept relatively constant. In this way, for the duration of the quench, the Hamiltonian–and therefore the dynamics–is dominated by $U(x)$. In other words, $\hat{\mathcal{H}}_0\tau \ll 1$ including any terms which couple to the vector potential.

On a lattice, the pulse Hamiltonian takes the form

$$\hat{\mathcal{H}}_{\text{pulse}} = \sum_j U_{\text{pulse}} \cos^2(kx_j)\, \hat{c}_j^\dagger \hat{c}_j \tag{165}$$

where the full Hamiltonian (during the quench) is $\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{SF}} + \hat{\mathcal{H}}_{\text{pulse}}$ where $\hat{\mathcal{H}}_{\text{SF}}$ is of the form 17. Note that the above Hamiltonian differs from the one presented in Ref. [6] by an additive constant (use $\cos qx = 2\cos^2(qx/2) - 1$ and define $2k = q$) and is written in the current form to be consistent with Refs. [8, 9]. The problem we would like to study is: given some initial state $|\Psi_I\rangle = \prod_{|\theta|<\theta_F} \hat{c}_\theta^\dagger |0\rangle$[3] at $t_0 = 0$, what are the dynamics for $t > 0$ when we quench the Hamiltonian by $\hat{\mathcal{H}}_{\text{pulse}}$ for some time τ and then return the system to its original Hamiltonian? In other words, how do the unitary dynamics look if we time-evolve the initial state according to some time-dependent Hamiltonian of the form:

$$\hat{H}(t) = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{pulse}}\Theta(t-\tau) \quad (t > 0) \tag{166}$$

where

$$\Theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases} \tag{167}$$

is the Heaviside step function and in general $\left[\hat{\mathcal{H}}_{\text{pulse}}, \hat{\mathcal{H}}_0\right] \neq 0$. The answer lies, of course, in the time-evolution operator. In all previous cases, the Hamiltonian for all times $t > t_0$ were time-

[3] Again to be consistent with Refs. [8, 9], we denote the single-particle quasi-momenta (rapidities) by θ and by θ_F the largest occupied mode.

independent, and so

$$\hat{U}(t) = \exp\left(-i\int_0^t dt'\hat{\mathcal{H}}\right) = e^{-i\hat{\mathcal{H}}t} \tag{168}$$

trivially. At present, however, the Hamiltonian *is* time-dependent and, what's more, $\left[\hat{H}(t_1), \hat{H}(t_2)\right] \neq 0$ for $t_1 \neq t_2$ generally (let, e.g., $0 < t_1 < \tau$) . Thus, we need to use the Dyson series:

$$\hat{U}(t) = \hat{\mathcal{T}} \exp\left(-i\int_0^t dt' \hat{H}(t)\right) \tag{169}$$

where $\hat{\mathcal{T}}$ is the time-ordering operator, i.e.

$$\begin{aligned}\hat{\mathcal{T}}\left(\hat{A}_1(t_1)\hat{A}_2(t_2)\cdots\hat{A}_n(t_n)\right) = \sum_{p\in P_n} &\Theta(t_{p_1} - t_{p_2})\Theta(t_{p_2} - t_{p_3})\cdots\Theta\left(t_{p_{n-1}} - t_{p_n}\right) \\ &\times \hat{A}_{p_1}(t_{p_1})\hat{A}_{p_2}(t_{p_2})\cdots\hat{A}_{p_n}(t_{p_n})\end{aligned} \tag{170}$$

with P_n the set of all permutations of $\{1, 2, \ldots, n\}$. The time dependence of the Hamiltonian in the present case is trivial, and therefore we may conclude that

$$\hat{U}(t) = \begin{cases} \exp\left(-i\hat{H}_p t\right) & t < \tau \\ \exp\left(-i\hat{\mathcal{H}}_0(t-\tau)\right)\exp\left(-i\hat{H}_p\tau\right) & t > \tau \end{cases} \tag{171}$$

where for notational simplicity we write $\hat{H}_p = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{pulse}}$.

As a final remark, it is fun to note that we can apply the same reasoning above to a sequence of Bragg pulses, which differ perhaps in amplitude or in wavelength. Indeed, suppose we apply m pulses with corresponding pulse Hamiltonians

$$\hat{\mathcal{H}}^{(m)}_{\text{pulse}} = \sum_j U^{(m)}_{\text{pulse}} \cos^2\left(k^{(m)}x_j\right)\hat{c}^\dagger_j\hat{c}_j \tag{172}$$

one after another (this is not necessary but is simpler) for times $\tau_1, \tau_2, \ldots, \tau_m$. It is easy to see that

for $t > T = \sum_{i=1}^{m} \tau_i$ the time evolution operator is of the form

$$\hat{U}(t) = \exp\left(-i\hat{\mathcal{H}}_0 (t-T)\right) \exp\left(-i\hat{H}_p^{(m)}\tau_m\right) \cdots \exp\left(-i\hat{H}_p^{(2)}\tau_2\right) \exp\left(-i\hat{H}_p^{(1)}\tau_1\right) \tag{173}$$

where we again use the notation $\hat{H}_p^{(k)} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{pulse}}^{(m)}$.

6.1.1 Raman-Nath Regime

This derivation follows that of Ref. [6]. Taking the limit $\tau \to 0$ while keeping $U_{\text{pulse}}\tau$ constant is known as the Raman-Nath regime, and corresponds to timescales wherein the constituent particles do not have time to react to the pulse. In this regime, the unitary time evolution operator (called the Bragg pulse operator in Ref. [6]) can be written as

$$\hat{U}_B = \exp\left(-iA \sum_j \cos^2(kx_j)\, \hat{c}_j^\dagger \hat{c}_j\right) \tag{174}$$

where we defined $A = U_{\text{pulse}}\tau$. The initial state, as above, is assumed to be in equilibrium and (for now) zero temperature: $|\Psi_I\rangle = \prod_{|\theta|<\theta_F} \hat{c}_\theta^\dagger |0\rangle$. The action of the quench is as before, namely, we propagate the state $|\Psi_I\rangle$ according to the quenched Hamiltonian. The only difference here is that the quench is instantaneous, after which the state evolves according to the initial Hamiltonian.

Applying the Bragg pulse operator to the initial state results in

$$\hat{U}_B |\Psi_I\rangle = \prod_j^L e^{-iA\cos^2(kx_j)\hat{c}_j^\dagger \hat{c}_j} \prod_{|\theta|<\theta_F} \hat{c}_\theta^\dagger |0\rangle \tag{175}$$

$$= \prod_j^L e^{-iA\cos^2(kx_j)\hat{c}_j^\dagger \hat{c}_j} \prod_{|\theta|<\theta_F} \sum_l P_{\theta l} \hat{c}_l^\dagger |0\rangle \tag{176}$$

$$= \prod_{|\theta|<\theta_F} \sum_l e^{-iA\cos^2(kx_l)} P_{\theta l} \hat{c}_l^\dagger |0\rangle \tag{177}$$

where in the middle line we used the expansion described in Section 4.2 and one can obtain the last line by noticing that $\left[\hat{c}_j^\dagger \hat{c}_j, \hat{c}_l^\dagger\right] = 0$ for all $j \neq l$. We further simplify this expression by expanding

the $e^{-iA\cos^2(kx_l)}$ contribution in terms of plane waves:

$$e^{-i2A\cos^2(kx_l)} = e^{-iA}e^{-iA\cos(2kx_l)} \tag{178}$$

$$= e^{-iA}\sum_{n=-\infty}^{\infty}(-i)^n J_n(-iA)\, e^{-i2knx_l} \tag{179}$$

where in the last line we used the Jacobi-Anger expansion (see Section 7 for proof). Using $(-i)^n = i^{-n}$ and $I_n(-iA) = i^{-n}J_n(-iA)$ (see e.g. [10]), we arrive at

$$\hat{U}_B|\Psi_I\rangle = \prod_{|\theta|<\theta_F}\sum_{n=-\infty}^{\infty} I_n(-iA)\sum_l e^{-i2knx_l}P_{\theta l}\hat{c}_l^\dagger|0\rangle \tag{180}$$

where we disregarded the overall phase e^{-iA}.

Restricting our attention to the case where the initial system is homogeneous, we see that the phase e^{-i2knx_l} on the single particle states indicates the gain/loss of $2kn$ rapidity (momentum). Explicitly writing $P_{\theta l} = e^{i\theta x_l}/\sqrt{L}$, we see that

$$\frac{1}{\sqrt{L}}\sum_l e^{-i(\theta+2kn)x_l}\hat{c}_l^\dagger|0\rangle = \sum_l P_{\theta+2kn,l}\hat{c}_l^\dagger|0\rangle = \hat{c}_{\theta+2kn}^\dagger|0\rangle \tag{181}$$

so that the state of the system immediately following a Bragg pulse in the Raman-Nath regime can be written

$$|\Psi(t=0)\rangle = \prod_{|\theta|<\theta_F}\sum_{n=-\infty}^{\infty} I_n(-iA)\,\hat{c}_{\theta+2kn}^\dagger|0\rangle\,. \tag{182}$$

The ensuing time dynamics are driven by the initial Hamiltonian, under which the state evolves

like

$$|\Psi(t)\rangle = e^{-i\hat{\mathcal{H}}_0 t} \prod_{|\theta|<\theta_F} \sum_{n=-\infty}^{\infty} I_n(-iA)\, \hat{c}^\dagger_{\theta+2kn} |0\rangle \tag{183}$$

$$= \prod_{\theta'}^{L} e^{-i\mathcal{E}_{\theta'} t \hat{c}^\dagger_{\theta'} \hat{c}_{\theta'}} \prod_{|\theta|<\theta_F} \sum_{n=-\infty}^{\infty} I_n(-iA)\, \hat{c}^\dagger_{\theta+2kn} |0\rangle \tag{184}$$

$$= \prod_{|\theta|<\theta_F} \sum_{n=-\infty}^{\infty} I_n(-iA)\, e^{-i\mathcal{E}_{\theta+2kn} t} \hat{c}^\dagger_{\theta+2kn} |0\rangle \tag{185}$$

where $\mathcal{E}_{\theta+2kn}$ is the single particle eigenenergy evaluated at $\theta + 2kn$ (compare to eq. A9 of Ref. [8]).

6.2 Zero Temperature Correlations

We calculate here the equal-time one-body correlation functions for non-interacting spinless fermions following a Bragg pulse quench (or sequence of such quenches) as a function of time for initially pure states. Then, we calculate the total one-body density matrix and experimentally relevant momentum distribution functions. Inspired by Ref. [8], we perform such calculations using both theoretical methods described above in hopes that we find qualitatively similar results.

6.2.1 "Exact" Approach

Here, we follow the approach of section 6.1 which involves applying a Bragg pulse quench for a finite amount of time. We will here be primarily interested in the dynamics for times $t > \tau$ where τ is the duration of the Bragg pulse. Thus, we consider the one-body correlation function

$$\left\langle \Psi(t) \left| \hat{c}^\dagger_i \hat{c}_j \right| \Psi(t) \right\rangle = \langle 0| \prod_{|\theta|<\theta_F} \hat{c}_\theta e^{i\hat{H}_p \tau} e^{i\hat{\mathcal{H}}_0 (t-\tau)} \hat{c}^\dagger_i \hat{c}_j e^{-i\hat{\mathcal{H}}_0 (t-\tau)} e^{-i\hat{H}_p \tau} \prod_{|\theta|<\theta_F} \hat{c}^\dagger_\theta |0\rangle \tag{186}$$

and recognize, by exactly the same reasoning as invoked in section 4.2.2, that

$$|\Psi(t)\rangle = e^{-i\hat{\mathcal{H}}_0 (t-\tau)} e^{-i\hat{H}_p \tau} \prod_{|\theta|<\theta_F} \hat{c}^\dagger_\theta |0\rangle \equiv \prod_{|\theta|<\theta_F} \hat{c}^\dagger_\theta(t) |0\rangle \tag{187}$$

where the instantaneous creation and annihilation operators $\hat{c}_\theta^\dagger(t)$ and $\hat{c}_\theta(t)$ are related to the lattice operators via

$$\Psi^\dagger = \varphi_\theta^\dagger(t)\,\mathcal{U}^\dagger e^{i\mathbf{H}_p\tau}e^{i\mathbf{H}_0(t-\tau)} \equiv \varphi_\theta^\dagger(t)\,\tilde{\mathbf{U}}^\dagger(t) \tag{188}$$

where $\mathbf{H}_0$ is the matri x representation of $\hat{\mathcal{H}}_0$ and $\mathbf{H}_p$ the matrix representation of $\hat{H}_p$, and

$$\Psi = e^{-i\mathbf{H}_0(t-\tau)}e^{-i\mathbf{H}_p\tau}\mathcal{U}\varphi_\theta(t) \equiv \tilde{\mathbf{U}}(t)\,\varphi_\theta(t) \tag{189}$$

respectively. We use here the same notation developed in section 4.2.2, namely $\Psi^\dagger = \begin{pmatrix} \hat{c}_1^\dagger & \cdots & \hat{c}_L^\dagger \end{pmatrix}$ and $\varphi_\theta^\dagger(t) = \begin{pmatrix} \hat{c}_{\theta_1}^\dagger(t) & \cdots & \hat{c}_{\theta_L}^\dagger(t) \end{pmatrix}$. The ensuing steps are exactly the same, and we simply state here the result:

$$\mathbf{C}(t) = e^{-i\mathbf{H}_0(t-\tau)}e^{-i\mathbf{H}_p\tau}\mathbf{P}\mathbf{P}^\dagger e^{i\mathbf{H}_p\tau}e^{i\mathbf{H}_0(t-\tau)} \tag{190}$$

$$= \mathbf{U}_0^\dagger e^{-i\mathbf{E}_0(t-\tau)}\mathbf{U}_0\mathbf{U}_p^\dagger e^{-i\mathbf{E}_p\tau}\mathbf{U}_p\mathbf{P}\mathbf{P}^\dagger\mathbf{U}_p e^{i\mathbf{E}_p\tau}\mathbf{U}_p^\dagger\mathbf{U}_0 e^{i\mathbf{E}_0(t-\tau)}\mathbf{U}_0^\dagger \tag{191}$$

where, of course, $\mathbf{P}$ is the $L \times N$ matrix formed from columns of $\mathcal{U}^\dagger$ which corresponds to single-particle phase at each site for each of the N momentum modes. The last line is of course obtained by inserting identities of the form $\mathbf{U}_0^\dagger\mathbf{U}_0$ and $\mathbf{U}_p^\dagger\mathbf{U}_p$ where $\mathbf{U}_0$ and $\mathbf{U}_p$ are unitary transformation matrices from the lattice space to the diagonal space of $\mathbf{H}_0$ and $\mathbf{H}_p$, respectively. Note that the matrix representations of the time evolution operator are time ordered, that is we "sandwich" the initial equilibrium correlation matrix $\mathbf{P}\mathbf{P}^\dagger$ with time evolution operators in order of increasing time. The momentum distribution function is calculated as a function of time by simply replacing ρ_{ij} by $\rho_{ij}(t)$ in equation 147.

6.2.2 Raman-Nath Approach

At zero temperature and for homogeneous systems, we can derive an analytic result for the MDF using equation 185. The advantage of doing this over simply using, e.g., equation 177 is that

the former provides us with theoretical control over the orders of the Bragg peaks. The rapidity distribution simply goes like

$$f(\theta) = \left\langle \Psi(t) \left| \hat{c}_\theta^\dagger \hat{c}_\theta \right| \Psi(t) \right\rangle \tag{192}$$

where

$$|\Psi(t)\rangle = \prod_{|\theta|<\theta_F} \sum_{n=-\infty}^{\infty} \mathcal{I}_n(\theta, t)\, \hat{c}_{\theta+2kn}^\dagger |0\rangle \tag{193}$$

with the definition $\mathcal{I}_n(\theta, t) = I_n(-iA)\, e^{-i\mathcal{E}_{\theta'+2kn}t}$ (it is assumed throughout that A is kept fixed). Now, in the quasi-momentum space the state $|\Psi(t)\rangle$ is a linear superposition of product states. As a result, it suffices to look at the action of the local mode operator $\hat{c}_\theta^\dagger \hat{c}_\theta$ on each single-particle state. By the canonical anticommutation algebra, it follows that

$$\hat{c}_\theta^\dagger \hat{c}_\theta \sum_{n=-\infty}^{\infty} \mathcal{I}_n(\theta', t)\, \hat{c}_{\theta'+2kn}^\dagger |0\rangle = \sum_{n=-\infty}^{\infty} \delta_{\theta,\theta'+2kn} \mathcal{I}_n(\theta', t)\, \hat{c}_{\theta'+2kn}^\dagger |0\rangle \tag{194}$$

which, we note, for a single mode will (at most) kill all but one term in the sum. So, for a given θ, the rapidity distribution goes like

$$\begin{aligned}
f(\theta) &= \langle 0| \prod_{|\theta'|<\theta_F} \sum_{n=-\infty}^{\infty} \mathcal{I}_n^*(\theta', t)\, \hat{c}_{\theta'+2kn} \hat{c}_\theta^\dagger \hat{c}_\theta \prod_{|\theta'|<\theta_F} \sum_{n=-\infty}^{\infty} \mathcal{I}_n(\theta', t)\, \hat{c}_{\theta'+2kn}^\dagger |0\rangle \\
&= \langle 0| \prod_{\substack{|\theta'|<\theta_F \\ \theta'\neq\theta}} \sum_{n=-\infty}^{\infty} \mathcal{I}_n^*(\theta', t)\, \hat{c}_{\theta'+2kn} \prod_{\substack{|\theta'|<\theta_F \\ \theta'\neq\theta}} \sum_{n=-\infty}^{\infty} \mathcal{I}_n(\theta', t)\, \hat{c}_{\theta'+2kn}^\dagger |0\rangle \\
&\quad \times \langle 0| \sum_{n=-\infty}^{\infty} \mathcal{I}_n^*(\theta', t)\, \hat{c}_{\theta'+2kn} \hat{c}_\theta^\dagger \hat{c}_\theta \sum_{n=-\infty}^{\infty} \mathcal{I}_n(\theta', t)\, \hat{c}_{\theta'+2kn}^\dagger |0\rangle \\
&= \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \delta_{\theta,\theta+2kn} \mathcal{I}_m^*(\theta, t)\, \mathcal{I}_n(\theta, t) \langle 0| \hat{c}_{\theta+2km} \hat{c}_{\theta+2kn}^\dagger |0\rangle \\
&= \sum_{n=-\infty}^{\infty} \delta_{\theta,\theta'+2kn} \left| \mathcal{I}_n(\theta', t) \right|^2
\end{aligned} \tag{195}$$

where, in the second line, we made use of the fact that the local mode operator–being a one-body operator–will act only on a particular θ mode pertaining to the sector where it acts non-trivially (we assume here the such sector exists, for otherwise $f(\theta)$ is trivially zero). The remaining factor (the first line of the RHS of second equality), is simply the overlap of an $N-1$ body Slater determinant with itself and is thus unity. The third line is the result of what we showed above, and in the fourth line we use the orthogonality of the single-particle eigenstates.

Some remarks are in store. First, even though the above argument in some sense relied on the existence of a quasi-momentum θ state upon which the action of the local mode operator was non-trivial, we find that the above result should hold even in absence. That is, the above expression yields 0 when $\theta \neq \theta' + 2kn$. Second, our derivation was for a fixed value of θ, in which case at most one $\theta' + 2kn$ is non-trivial. What we would actually like to consider is the full range of $\theta \in [-\pi/a, \pi/a)$ in which the quasi-momentum is defined. It is rather straightforward to see that the above reasoning can be applied at every value of θ, and that the only non-trivial results occur when $|\theta'| \leq \theta_F$, where $\theta_F = \frac{\pi(N-1)}{L}$ is the Fermi momentum (assuming N odd). In this way, we can write $f(\theta)$ as an almost everywhere smooth function of its argument:

$$f(\theta) = \sum_{n=-\infty}^{\infty} |I_n(-iA)|^2 \Theta(\theta_F - |\theta + 2kn|) \tag{196}$$

where we made use here of the fact that $|\mathcal{I}_n(\theta', t)|^2 = \left|I_n(-iA)\, e^{-i\mathcal{E}_{\theta'+2kn}t}\right|^2 = |I_n(-iA)|^2$. Here we see another interesting result: the rapidity distribution does not evolve with time for homogeneous systems! What is remarkable is, as we shall soon see, in spite of this, the momentum distribution for hard core bosons (which are mappable to spinless fermions) *does*.

6.2.3 Raman-Nath Alternative Approach:

It is interesting to point out that there is but another way to calculate the rapidity distribution function using the Raman-Nath limit. It should turn out that this approach is not particularly useful–for one because in the previous section we calculated an analytic expression for the RDF, while the ensuing approach is analytic, and two because the approach mirrors the "exact" one,

suggesting one just opts for that instead. Regardless, we quickly go through the details here. Starting with equation equation 185, we see that

$$\prod_{|\theta|<\theta_F} \sum_l e^{-iA\cos^2(kx_l)} P_{\theta l} \hat{c}_l^\dagger |0\rangle = \prod_{|\theta|<\theta_F} \sum_l \tilde{P}_{\theta l} \hat{c}_l^\dagger |0\rangle \tag{197}$$

where $\tilde{\mathbf{P}} = \mathbf{DP}$ is an $L \times N$ matrix where $\mathbf{P}$ is the matrix of coefficients of the initial (pre-quench) state and

$$\mathbf{D} = \begin{bmatrix} e^{-iA\cos^2(kx_1)} & & & 0 \\ & e^{-iA\cos^2(kx_2)} & & \\ & & \cdots & \\ 0 & & & e^{-iA\cos^2(kx_L)} \end{bmatrix} \tag{198}$$

is an $L \times L$ diagonal matrix. It follows that the equal-time one-body density matrix is

$$\rho_{ij}(t) = \langle 0| \prod_{|\theta|<\theta_F} \sum_l \tilde{P}_{\theta l}^\dagger \hat{c}_l \hat{c}_i^\dagger \hat{c}_j \prod_{|\theta|<\theta_F} \sum_l \tilde{P}_{\theta l} \hat{c}_l^\dagger |0\rangle \tag{199}$$

which takes exactly the same form as, e.g., equation 97. From this, we may immediately conclude (by following exactly the same steps as in those calculations) that

$$\mathbf{C} = \mathbf{DPP}^\dagger \mathbf{D}^\dagger \tag{200}$$

is the one-body correlation matrix.

6.3 Finite Temperature Correlations

Next, we envision a scenario wherein a system of non-interacting spinless fermions is initially coupled to a bath at temperature T and then quenched via a Bragg pulse. Unsurprisingly, as in the previous section, most of our work is already done. The only insight needed here is to note that the time

dependence of the density matrix should go like

$$\hat{\rho}(t) = \hat{U}(t)\,\hat{\rho}(0)\,\hat{U}^{\dagger}(t)$$

where $\rho(0) = \mathcal{Z}^{-1}\exp\left(-\beta\left(\hat{\mathcal{H}}_0 - \mu\hat{N}\right)\right)$ with $\mathcal{Z} = \mathrm{tr}\left\{\exp\left(-\beta\left(\hat{\mathcal{H}}_0 - \mu\hat{N}\right)\right)\right\}$ and, for times $t > \tau$, $\hat{U}(t)$ is given by 171. Hence, we only need to calculate

$$\rho_{ij}(t) = \frac{1}{\mathcal{Z}}\mathrm{tr}\left\{\hat{c}_i^{\dagger}\hat{c}_j e^{-i\hat{\mathcal{H}}_0(t-\tau)}e^{-i\hat{H}_p\tau}e^{-\beta\left(\hat{\mathcal{H}}_0-\mu\hat{N}\right)}e^{i\hat{H}_p\tau}e^{i\hat{\mathcal{H}}_0(t-\tau)}\right\} \tag{201}$$

$$= \delta_{ij} - \frac{1}{\mathcal{Z}}\mathrm{tr}\left\{\hat{c}_j\hat{c}_i^{\dagger}e^{-i\hat{\mathcal{H}}_0(t-\tau)}e^{-i\hat{H}_p\tau}e^{-\beta\left(\hat{\mathcal{H}}_0-\mu\hat{N}\right)}e^{i\hat{H}_p\tau}e^{i\hat{\mathcal{H}}_0(t-\tau)}\right\} \tag{202}$$

which amounts to diagonalizing the matrix

$$\Psi^{\dagger}e^{-i\mathbf{H}_0(t-\tau)}e^{-i\mathbf{H}_p\tau}e^{-\beta(\mathbf{H}_0-\mu\mathbf{I})}e^{i\mathbf{H}_p\tau}e^{i\mathbf{H}_0(t-\tau)}\Psi = \varphi_{\theta}^{\dagger}(t)\,e^{-\beta(\mathbf{E}_0-\mu\mathbf{I})}\varphi_{\theta}(t) \tag{203}$$

where we defined $\varphi_{\theta}^{\dagger}(t) = \Psi^{\dagger}e^{-i\mathbf{H}_0(t-\tau)}e^{-i\mathbf{H}_p\tau}\hat{\mathcal{U}}$ as in section 6.2.1. The trace over the fermionic Fock space can then be taken over the $\hat{c}_{\theta}(t)$, $\hat{c}_{\theta}^{\dagger}(t)$ states, resulting in

$$\rho_{ij}(t) = \delta_{ij} - \frac{1}{\mathcal{Z}}\sum_{\theta',\theta''}\tilde{U}_{\theta',i}(t)\,\tilde{U}^{\dagger}_{\theta'',j}(t)\,\mathrm{tr}\left\{\hat{c}_{\theta'}\hat{c}^{\dagger}_{\theta''}\prod_{\theta}e^{-\beta(\mathcal{E}_{\theta}-\mu)\hat{c}^{\dagger}_{\theta}(t)\hat{c}_{\theta}(t)}\right\} \tag{204}$$

$$= \delta_{ij} - \frac{1}{\mathcal{Z}}\sum_{\theta'}\tilde{U}_{\theta',i}(t)\,\tilde{U}^{\dagger}_{\theta',j}(t)\,\mathrm{tr}\left\{\hat{c}_{\theta'}\hat{c}^{\dagger}_{\theta'}\prod_{\theta}e^{-\beta(\mathcal{E}_{\theta}-\mu)\hat{c}^{\dagger}_{\theta}(t)\hat{c}_{\theta}(t)}\right\} \tag{205}$$

$$= \delta_{ij} - \sum_{\theta'}\tilde{U}_{\theta',i}(t)\,\tilde{U}^{\dagger}_{\theta',j}(t)\left[1+e^{-\beta(\mathcal{E}_{\theta'}-\mu)}\right]^{-1} \tag{206}$$

where we defined $\tilde{\mathbf{U}} = e^{-i\mathbf{H}_0(t-\tau)}e^{-i\mathbf{H}_p\tau}\hat{\mathcal{U}}$. Comparing the final line to what we found in section 5.3, we may immediately conclude that

$$\mathbf{C}(t) = \mathbf{I} - \tilde{\mathbf{U}}(t)\left[\mathbf{I} + e^{-\beta(\mathbf{E}-\mu\mathbf{I})}\right]^{-1}\tilde{\mathbf{U}}^\dagger(t) \tag{207}$$

$$= \mathbf{I} - \mathbf{U}_0 e^{-i\mathbf{E}_0(t-\tau)}\mathbf{U}_0^\dagger\mathbf{U}_p e^{-i\mathbf{E}_p\tau}\mathbf{U}_p^\dagger\hat{\mathcal{U}}\left[\mathbf{I} + e^{-\beta(\mathbf{E}-\mu\mathbf{I})}\right]^{-1}\hat{\mathcal{U}}^\dagger\mathbf{U}_p e^{i\mathbf{E}_p\tau}\mathbf{U}_p^\dagger\mathbf{U}_0 e^{i\mathbf{E}_0(t-\tau)}\mathbf{U}_0^\dagger \tag{208}$$

$$= \mathbf{I} - e^{-i\mathbf{H}_0(t-\tau)}e^{-i\mathbf{H}_p\tau}\left[\mathbf{I} + e^{-\beta(\mathbf{H}-\mu\mathbf{I})}\right]^{-1}e^{i\mathbf{H}_p\tau}e^{i\mathbf{H}_0(t-\tau)}, \tag{209}$$

which should not come as a surprise. See that we may easily generalize this result to arbitrary sequences of pulses:

$$\mathbf{C}(t) = \mathbf{I} - e^{-i\mathbf{H}_0(t-T)}e^{-i\mathbf{H}_{p_m}\tau_m}\cdots e^{-i\mathbf{H}_{p_1}\tau_1}\left[\mathbf{I} + e^{-\beta(\mathbf{H}-\mu\mathbf{I})}\right]^{-1}e^{i\mathbf{H}_{p_1}\tau_1}\cdots e^{i\mathbf{H}_{p_m}\tau_m}e^{i\mathbf{H}_0(t-T)} \tag{210}$$

where we defined $T = \sum_i^m \tau_i$.

6.4 Numerics

We focus here on the dynamics of the momentum distribution function of homogeneous and inhomogeneous (trapped) non-interacting fermions immediately following a Bragg pulse. Particular attention is paid to the difference between open and periodic boundary conditions, as well as the long and short time scale evolution. In all cases (except the analytical Raman-Nath results), we take $U_{\text{pulse}} = 20J$, $\tau = 0.1\hbar/J$, and $qa = \frac{\pi}{4}ka$. For the Raman-Nath regime, we write, inspired by Ref. [9], a generic three-peak state of the form

$$|\Psi(t)\rangle = \prod_{|\theta|<\theta_F}\left(-iA_{-1}\hat{c}_{\theta-2k}^\dagger + A_0\hat{c}_\theta^\dagger + iA_1\hat{c}_{\theta+2k}\right)|0\rangle \tag{211}$$

where $A_0 = 2/\sqrt{6}$ and $A_1 = A_{-1} = 1/\sqrt{6}$. The resulting momentum distribution function can, of course, be written explicitly as

$$f(\theta) = \frac{1}{6}\Theta(\theta_F - |\theta - 2k|) + \frac{2}{3}\Theta(\theta_F - |\theta|) + \frac{1}{6}\Theta(\theta_F - |\theta + 2k|) \tag{212}$$

and is depicted in figure .

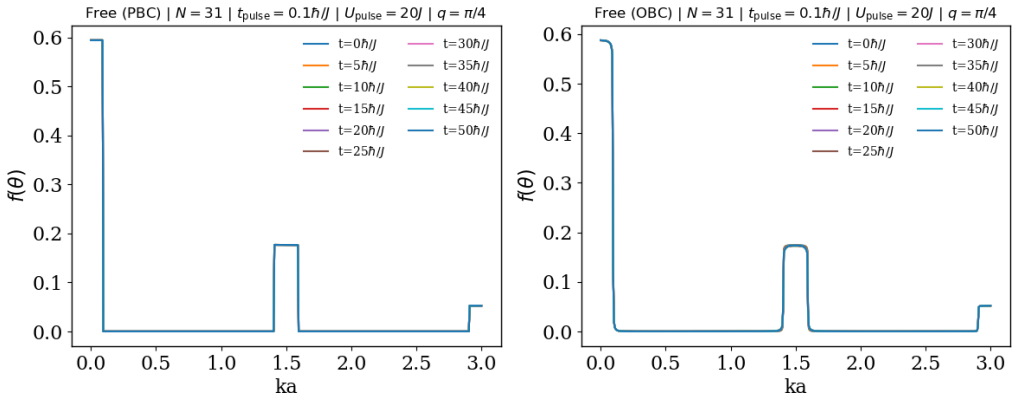

Figure 15: Momentum distribution function for $N = 31$ non-interacting spinless fermions in a homogeneous potential ($v_i \equiv v$) at $T = 0$ for (**left**) periodic and (**right**) open boundary conditions. See that there are slight qualitative differences between the two and, importantly, the OBC case shows slight variations with respect to the $t = 0$ distribution at long times.

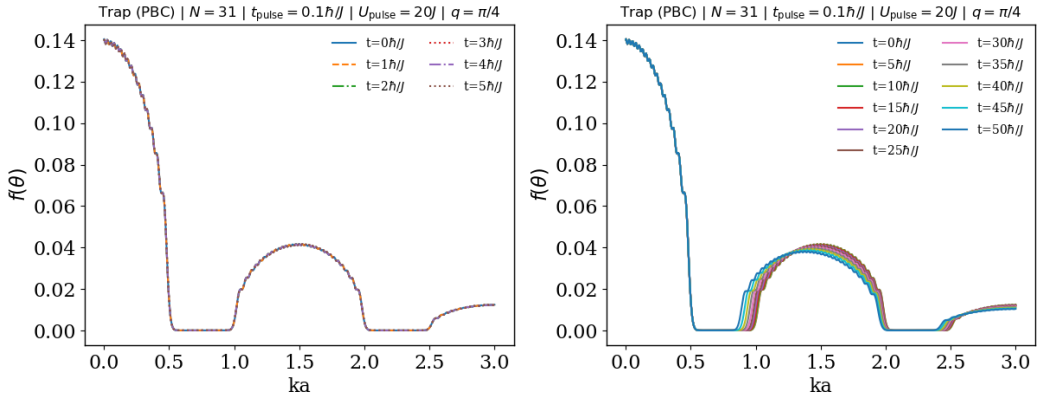

Figure 16: Momentum distribution function for $N = 31$ spinless fermions in a quadratic trapping potential at $T = 0$ with periodic boundary conditions. (**Left**) short time dynamics. (**Right**) long time dynamics. After approximately 50 times the duration of the scattering pulse, the fermions begin to climb the potential wall of the quadratic trap, causing them to slow down and, as a result, the momentum distribution function tends towards $ka = 0$. See files for an animation of the local number density. Note that for open boundary conditions, the same sort of oscillatory behavior is observed.

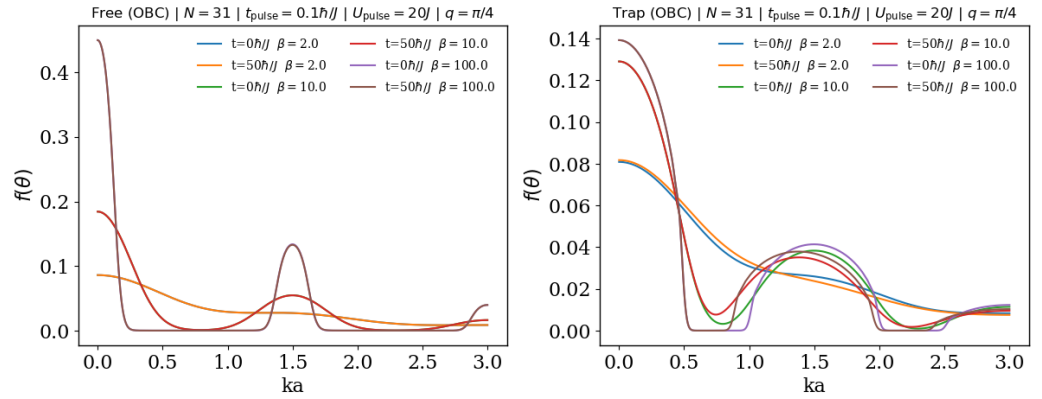

Figure 17: Momentum distribution function for $N = 31$ free (**left**) and trapped (**right**) non-interacting spinless fermions at finite temperatures $\beta = 2, 10$, and $100J$ immediately following and $t = 50\hbar/J$ after a Bragg pulse quench. In both cases, open boundary conditions are used. Similarly to what is observed in figure 15, the MDF does not significantly change at long times for fermions in a homogeneous potential. In contrast, the MDF for trapped fermions is observed to change significantly at long times, consistent with figure 16.

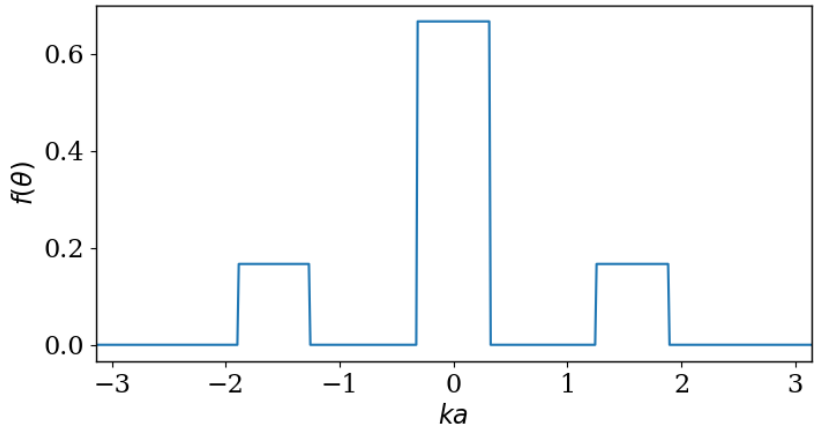

Figure 18: Momentum distribution function as predicted by equation 212. This corresponds to a three-peak state in a homogeneous potential. Note that one can show analytically in this case that the MDF will not evolve in time for all times after the quench.

7 Various Proofs

Here we prove various claims and theorems presented throughout our notes.

7.1 Proof of Theorem 1

Theorem 1 The action of an exponential operator who's argument is bilinear in fermionic creation and annihilation operators on a Slater determinant yields a new Slater determinant, that is

$$\exp\left(\sum_{i,j}\hat{c}_i^\dagger X_{ij}\hat{c}_j\right)|\Psi_I\rangle = \prod_k^N \sum_{j=1}^L P'_{kj}\hat{c}_j^\dagger|0\rangle \tag{213}$$

where X_{ij} is the ij component of some $L\times L$ matrix $\mathbf{X}$ and $\mathbf{P'} = e^{\mathbf{X}}\mathbf{P}$.

Proof The idea of this proof is very similar to the derivation performed in section 4.2.2. We will assume that $\mathbf{X}$ fulfills the necessary requirements to be diagonalizable by a unitary transformation, as this is the only case which concerns us here. In this case, there exists a unitary matrix $\mathbf{U}$ such that $\mathbf{U}\mathbf{U}^\dagger\mathbf{X}\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}\mathbf{D}_\mathbf{x}\mathbf{U}^\dagger$ where $\mathbf{D}_\mathbf{x}$ is a diagonal matrix of eigenvalues of $\mathbf{X}$. Notice that $\mathbf{U}$ can be interpreted as rotating the states from the eigenbasis of $\mathbf{X}$ back to the original lattice site basis. Let $\{|x\rangle\}$ be a complete set of states for which the operator $\hat{X}$ is diagonal, that is, $\hat{X}|x\rangle = x|x\rangle$ and $\langle x|x'\rangle = \delta_{xx'}$. Letting $|\Psi_I\rangle = \prod_\theta^N c_\theta^\dagger|0\rangle$, we insert N identities of the form $\sum_x |x\rangle\langle x|$ such that

$$|\Psi_I\rangle = \prod_\theta^N \sum_x |x\rangle\langle x| c_\theta^\dagger|0\rangle \tag{214}$$

$$= \prod_\theta^N \sum_x \sum_j |x\rangle\langle x|j\rangle\langle j| c_\theta^\dagger|0\rangle \tag{215}$$

$$= \prod_\theta^N \sum_x \sum_j U_{xj}^\dagger P_{\theta j}|x\rangle \tag{216}$$

where in the second line we inserted N lattice-site identities and in the last line we identified $P_{\theta j} = \langle j| c_\theta^\dagger|0\rangle$ as the θj component of $\mathbf{P}$ and $U_{xj}^\dagger = \langle x|j\rangle$ as the xj component of $\mathbf{U}^\dagger$. In the basis

spanned by $|x\rangle$, we can write

$$\exp\left(\sum_{i,j}\hat{c}_i^\dagger X_{ij}\hat{c}_j\right) = \exp\left(\sum_x D_x\hat{c}_x^\dagger\hat{c}_x\right) = \prod_x \exp\left(D_x\hat{c}_x^\dagger\hat{c}_x\right) \tag{217}$$

where the operators $\hat{c}_x^\dagger, \hat{c}_x$ create/annihilate a mode with eigenvalue D_x. Acting this on the original state in the transformed basis, we are left with

$$\exp\left(\sum_{i,j}\hat{c}_i^\dagger X_{ij}\hat{c}_j\right)|\Psi_I\rangle = \prod_\theta^N\sum_x e^{D_x}\sum_j U_{xj}^\dagger P_{\theta j}\,|x\rangle \tag{218}$$

$$= \prod_\theta^N\sum_l\sum_x U_{xl}e^{D_x}\sum_j U_{xj}^\dagger P_{\theta j}\hat{c}_l^\dagger\,|0\rangle \quad (U_{xl} = \langle l|x\rangle) \tag{219}$$

$$= \prod_\theta^N\sum_l P'_{\theta l}\hat{c}_l^\dagger\,|0\rangle \tag{220}$$

where in the last line we defined $P'_{\theta l} = \sum_x U_{xl}e^{D_x}\sum_j U_{xj}^\dagger P_{\theta j}$ which can easily be identified as the matrix elements of $\mathbf{P'} = \mathbf{U}e^{\mathbf{D_x}}\mathbf{U}^\dagger\mathbf{P} = e^{\mathbf{X}}\mathbf{P}$ (compare to section 4.2.2).

7.2 Proof of Theorem 2

Theorem Given $N+1$ fermionic operators $\{\hat{c}_j\}$, we have

$$\left\langle 0\middle|\hat{c}_{l_{N+1}}\cdots\hat{c}_{l_2}\hat{c}_{l_1}\hat{c}_{m_1}^\dagger\hat{c}_{m_2}^\dagger\cdots\hat{c}_{m_{N+1}}^\dagger\middle|0\right\rangle = \epsilon^{\gamma_1\cdots\gamma_{N+1}}\delta_{l_1 m_{\gamma_1}}\cdots\delta_{l_{N+1}m_{\gamma_{N+1}}} \tag{221}$$

where $\epsilon^{\gamma_1\cdots\gamma_{N+1}}$ is the Levi-Civita symbol and summation is implied.

Proof This is trivially true for a bilinear product of fermion operators: $\left\langle \hat{c}_i \hat{c}_j^\dagger \right\rangle = \delta_{ij}$, and is easy to see for quadratic products:

$$\left\langle \hat{c}_{i_2} \hat{c}_{i_1} \hat{c}_{j_1}^\dagger \hat{c}_{j_2}^\dagger \right\rangle = \left\langle \hat{c}_{i_2} \left(\delta_{i_1 j_1} - \hat{c}_{j_1}^\dagger \hat{c}_{i_1} \right) \hat{c}_{j_2}^\dagger \right\rangle = \delta_{i_1 j_1} \left\langle \hat{c}_{i_2} \hat{c}_{j_2}^\dagger \right\rangle - \left\langle \hat{c}_{i_2} \hat{c}_{j_1}^\dagger \hat{c}_{i_1} \hat{c}_{j_2}^\dagger \right\rangle \tag{222}$$

$$= \delta_{i_1 j_1} \delta_{i_2 j_2} - \left\langle \hat{c}_{i_2} \hat{c}_{j_1}^\dagger \left(\delta_{i_1 j_2} - \hat{c}_{j_2}^\dagger \hat{c}_{i_1} \right) \right\rangle = \delta_{i_1 j_1} \delta_{i_2 j_2} - \delta_{i_1 j_2} \delta_{i_2 j_1} \tag{223}$$

$$= \sum_{\gamma_1, \gamma_2} \epsilon^{\gamma_1 \gamma_2} \delta_{i_1 j_{\gamma_1}} \delta_{i_2 j_{\gamma_2}} \tag{224}$$

where in each step we simply employed the canonical anticommutator algebra. For the general case of $2N$-products, we simply use equation 61 and the orthogonality of the single-particle basis states to equate the right and left sides of the expression in the theorem statement.

7.3 Proof of Theorem 3

Theorem 3 The trace over the fermionic Fock space of Gaussian exponential operators takes the following form:

$$\mathrm{Tr} \left\{ \exp\left(\sum_{i,j} \hat{c}_i^\dagger X_{ij} \hat{c}_j \right) \exp\left(\sum_{m,n} \hat{c}_m^\dagger Y_{mn} \hat{c}_n \right) \cdots \right\} = \det\left[\mathbf{I} + e^{\mathbf{X}} e^{\mathbf{Y}} \cdots \right]$$

where $\mathbf{I}$ is the $L \times L$ identity operator and $\mathbf{X}, \mathbf{Y}, \ldots$ are $L \times L$ matrix representations of the operators $\hat{X}, \hat{Y}, \ldots$ in the lattice-site basis.

Proof Let $\Psi^\dagger = \begin{pmatrix} \hat{c}_1^\dagger & \cdots & \hat{c}_L^\dagger \end{pmatrix}$ such that we can write

$$\exp\left(\sum_{i,j} \hat{c}_i^\dagger X_{ij} \hat{c}_j \right) \exp\left(\sum_{m,n} \hat{c}_m^\dagger Y_{mn} \hat{c}_n \right) \cdots = \exp\left(-\Psi^\dagger \mathbf{X} \Psi \right) \exp\left(-\Psi^\dagger \mathbf{Y} \Psi \right) \cdots \tag{225}$$

$$= \exp\left(-\Psi^\dagger \left[\mathbf{X} + \mathbf{Y} + \cdots \right] \Psi \right) \tag{226}$$

$$= \Psi^\dagger \exp\left(-\mathbf{X} \right) \exp\left(-\mathbf{Y} \right) \cdots \Psi \tag{227}$$

mportancewhere $\mathbf{X}, \mathbf{Y}, \ldots$ are as in the statement of the theorem. We assume, as in the proof of theorem 1, that $\mathbf{X}, \mathbf{Y}, \ldots$ satisfy all of the necessary diagonalization requirements such that there exists unitaries $\mathbf{U_x}, \mathbf{U_y}, \ldots$ such that

$$\Psi^\dagger \exp(-\mathbf{X}) \exp(-\mathbf{Y}) \cdots \Psi = \Psi^\dagger \mathbf{U_x} \exp(-\mathbf{D_x}) \mathbf{U_x}^\dagger \mathbf{U_y} \exp(-\mathbf{D_y}) \mathbf{U_y}^\dagger \cdots \Psi \tag{228}$$

$$= \Gamma^\dagger e^{-\mathcal{D}} \Gamma \tag{229}$$

where in the last line we defined the vector of diagonal operators $\Gamma = \mathcal{U}\Psi$ for which the matrix $\exp(-\mathbf{X}) \exp(-\mathbf{Y})$ takes the diagonal representation $\mathcal{D}$. In the simple case of, e.g., the time evolution operator $e^{-i\hat{H}'t}$ considered in section 4.2.2, $\mathcal{D} = -i\mathbf{E}'t$ and $\mathcal{U}$ is the matrix of overlaps between the lattice-site basis and the energy eigenbasis for $\hat{H}'$. Let us now suppose that $\Gamma^\dagger = \begin{pmatrix} c^\dagger_{\gamma_1} & \cdots & \hat{c}^\dagger_{\gamma_L} \end{pmatrix}$ and $\mathcal{D} = \mathrm{diag}(d_{\gamma_1}, \ldots, d_{\gamma_L})$ such that, $\Gamma^\dagger e^{-\mathcal{D}} \Gamma = \prod_\nu e^{-\hat{c}^\dagger_{\gamma_\nu} d_{\gamma_\nu} \hat{c}_{\gamma_\nu}}$. Because the trace is basis independent, we may take it with respect to the orthogonal Γ product-basis. In this way, as we saw in e.g. section 5.1.1, the trace over the fermion Fock space becomes the product of the trace over L single-particle Hilbert spaces:

$$\mathrm{Tr}\left\{ \exp\left(\sum_{i,j} \hat{c}^\dagger_i X_{ij} \hat{c}_j \right) \exp\left(\sum_{m,n} \hat{c}^\dagger_m Y_{mn} \hat{c}_n \right) \cdots \right\} = \sum_{\{\gamma_\mu\}} \langle \gamma_\mu | \prod_\nu e^{-\hat{c}^\dagger_{\gamma_\nu} d_{\gamma_\nu} \hat{c}_{\gamma_\nu}} | \gamma_\mu \rangle \tag{230}$$

$$= \prod_\nu \sum_{\gamma_\mu} e^{-\hat{c}^\dagger_{\gamma_\mu} d_{\gamma_\mu} \hat{c}_{\gamma_\mu}} \tag{231}$$

$$= \prod_\nu \left(1 + e^{-d_{\gamma_\nu}}\right). \tag{232}$$

Comparing this with the RHS of the theorem statement, we see that

$$\det\left[\mathbf{I} + e^{\mathbf{X}} e^{\mathbf{Y}} \cdots\right] = \det\left[\mathbf{I} + \mathbf{U_x} e^{-\mathbf{X}} \mathbf{U_x}^\dagger \mathbf{U_y} e^{-\mathbf{Y}} \mathbf{U_y}^\dagger \cdots\right] \tag{233}$$

$$= \det\left[\mathbf{I} + e^{-\mathcal{D}}\right] \tag{234}$$

$$= \prod_\nu \left(1 + e^{-d_{\gamma_\nu}}\right) \tag{235}$$

which establishes the equality.

7.4 Proof of Jacobi-Anger Identity

Jacobi-Anger Identity Let $z \in \mathbb{C}$, then

$$e^{iz\cos\theta} = \sum_{n=-\infty}^{\infty} i^n J_n(z)\, e^{in\theta} \tag{236}$$

where n is an integer, $\theta \in [-\pi, \pi)$, and J_n is a Bessel function of the first kind.

Proof This proof is inspired by Ref. [12]. Notice that $e^{iz\cos\theta} = e^{iz\sin(\theta+\pi/2)}$, so it suffices to consider here the expansion of $e^{iz\sin\theta}$. This latter function is clearly periodic and integrabale on the compact domain $[-\pi, \pi]$. Hence, it admits a well-defined Fourier expansion [13]:

$$e^{iz\sin\theta} = \sum_{n=-\infty}^{\infty} c_n e^{in\theta} \tag{237}$$

where $c_n = (2\pi)^{-1}\int_{-\pi}^{\pi} dx e^{iz\sin x} e^{-inx}$. Invoking the Euler identity, we can further expand the c_n as

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx \cos(z\sin x - nx) + \frac{i}{2\pi}\int_{-\pi}^{\pi} dx \sin(z\sin x - nx). \tag{238}$$

Now, clearly the argument $z\sin x - nx$ is odd (that is, $x \mapsto -x$ takes $z\sin x - nx \mapsto -(z\sin x - nx)$), and therefore $\sin(z\sin x - nx)$ is also odd. Since we are integrating about an even domain, the last term on the RHS of the above expression must be identically zero, leaving only

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx \cos(z\sin x - nx) \equiv J_n(z) \tag{239}$$

with the last equality coming from an integral representation of the first order Bessel function (see e.g. [14]). Thus, we are left with

$$e^{iz\cos\theta} = e^{iz\sin(\theta+\pi/2)} = \sum_{n=-\infty}^{\infty} J_n(z)\, e^{in(\theta+\pi/2)} = \sum_{n=-\infty}^{\infty} i^n J_n(z)\, e^{in\theta} \tag{240}$$

as desired.

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