Quantum Traffic Wave Modeling

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1 Tight Binding Model for a 1D Ring

Let us consider non-interacting bosons on a strictly 1D ring of radius R and L sites. The single particle Hamiltonian is

$$H = \sum_{i=1}^{L} \epsilon_0 n_i - t \sum_{i=1}^{L} \left(a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} \right) \tag{1}$$

We define the ring by having periodicity: site $L+1$ being equivalent to site 1. We use the ansatz for bloch waves:

$$|\psi_{n\pm1}\rangle = e^{\pm ika} |\psi_n\rangle \tag{2}$$

We get the same dispersion relation as for the 1D tight binding model for a chain. Where a is the lattice spacing, which equals to $2\pi R/L$.

$$\epsilon(k) = \epsilon_0 - 2t\cos(ka) \tag{3}$$

For a finite ring, k takes discrete values. We can consider the additional phase of going around the whole ring to be 1.

$$e^{ikLa} = 1 \Longrightarrow k = \frac{2\pi}{aL} m \quad m \in \mathbb{Z} \tag{4}$$

For suitably small momenta, $k \ll \pi/a$, we can Taylor expand the energy. Setting $\epsilon_0 = 2t$ to yield the dispersion relation of a free particle with an effective mass determined by the properties of the lattice. Essentially, low momentum particles are unaware of the underlying lattice.

The energy spectrum has Z_2 symmetry about $k = 0$ with the ground state having zero k momentum, and thus zero m angular momentum. We want to break Z_2 symmetry about $k = 0$, and this can be done by passing magnetic flux through the ring.

2 Persistent Currents With Magnetic Flux

We now consider a continuum quantum ring with magnetic flux through the ring in such a way that the magnetic field is zero at the radius of the ring. By choosing circular cylindrical coordinate:

$$A_r = A_z = 0$$

$$A_\phi = \begin{cases} \frac{B_0 r}{2} & \text{if } r \leq r_c \\ \frac{B_0 r_c^2}{2r} = \frac{\Phi}{2\pi r} & \text{if } r > r_c \end{cases}$$

Such that there is flux $\Phi = \pi r_c^2 B_0$ through the ring. If the ring is in the field-free region, then the boson states only depend on the total flux penetrating the ring. Writing the potential term as, $V = e\phi - e\mathbf{A}\cdot\mathbf{v}$, we can write down the Lagrangian $L = T - V$ and then switch into the Hamiltonian formalism by finding the conjugate momentum. The general form of the Hamiltonian with an Electromagnetic potential energy term is

$$H = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m} + e\phi_{EM} \tag{5}$$

For our case, we can immediately write down the TISE.

$$\frac{1}{2m}\left(-\frac{i\hbar}{R}\frac{\partial}{\partial\phi} - \frac{e\Phi}{2\pi R}\right)^2 \Psi(\phi) = \epsilon\Psi(\phi) \tag{6}$$

Due to the circle cylindrical symmetry, we use the ansatz $\psi_m = e^{im\phi}$. The dispersion relation written using angular momentum m is

$$\epsilon(m, \Phi) = \frac{\hbar^2}{2mR^2}\left(m - \frac{\Phi}{\Phi_0}\right)^2 \tag{7}$$

Where $\Phi_0 = h/e$ is the flux quantum. The result can be seen as a shift to the spectrum, such that the ground state has non-zero angular momentum.

One can think the same physical situation in a different manner. We can instead have a free-field Hamiltonian with twisted boundary conditions. *I.e. Ahranov-Bohm.* We first choose a gauge $\mathbf{A} = \nabla\chi$ such that $\mathbf{B} = \nabla\times\mathbf{A}$ is zero at the ring; in a strictly one-dimensional ring we can write $\chi(\phi) = \Phi\phi/(2\pi)$. We now write consider the following unitary transformations to the state and the Hamiltonian

$$\psi \rightarrow \psi' = U\psi \tag{8}$$

$$H \rightarrow H' = UHU^{-1} \tag{9}$$

By doing both transformations 8 and 9, the energy spectrum is preserved. We want the unitary transform to take the EM Hamiltonian H to the free-field Hamiltonian H'.

We define the unitary operator U as

$$U = e^{i\frac{e}{\hbar}\int \mathbf{A}d\mathbf{l}} = e^{-i\frac{e}{\hbar}\chi} \tag{10}$$

We act the unitary transform on the Hamiltonian in equation 6.

$$\Longrightarrow \frac{1}{2m}U\left(-\frac{i\hbar}{R}\partial_\phi - \frac{e\Phi}{2\pi R}\right)^2 U^{-1}\ f(\phi) \tag{11}$$

$$\Longrightarrow \frac{1}{2m}U\left(-\frac{i\hbar}{R}\partial_\phi - \frac{e\Phi}{2\pi R}\right)\left(U^{-1}\frac{-i\hbar}{R}\partial_\phi f(\phi)\right) \tag{12}$$

$$\Longrightarrow \frac{-\hbar^2}{2mR^2}\partial_\phi^2 f(\phi) \tag{13}$$

3 Tight Binding Model for a 1D Ring with Flux

We can write down the free-field Hamiltonian for this discrete model with flux by adding an Ahranov-Bohm phase term to the 1D Ring Hamiltonian in equation 1. The angle subtended by hopping from site i to site $i+1$ is $2\pi/L$

$$H = \sum_{i=1}^{L} \epsilon_0 n_i - t\sum_{i=1}^{L}\left(e^{-i2\pi\phi/L}a_{i+1}^\dagger a_i + e^{i2\pi\phi/L}a_i^\dagger a_{i+1}\right) \tag{14}$$

Where $\phi = \Phi/\Phi_0$. To find the dispersion relation, we can rewrite the Hamiltonian in terms of the basis states $a_1^\dagger|vac\rangle = |1\rangle$, $a_2^\dagger|vac\rangle = |2\rangle$ ...

$$H = \epsilon_0\sum_{n=1}^{L}|n\rangle\langle n| - t\sum_{n=1}^{L}\left(e^{-i2\pi\phi/L}|n+1\rangle\langle n| + e^{i2\pi\phi/L}|n\rangle\langle n+1|\right) \tag{15}$$

Considering a general state

$$|\Psi\rangle = \sum_m \psi_m|m\rangle \tag{16}$$

We can form the overlap $\langle p|H|\Psi\rangle = E\langle p|\Psi\rangle$

$$\epsilon_0\sum_n \psi_n\langle p|n\rangle - t\sum_n\left(\psi_n e^{-i2\pi\phi/L}\langle p|n+1\rangle + \psi_{n+1}e^{i2\pi\phi/L}\langle p|n\rangle\right) = E\sum_n \psi_n\langle p|n\rangle$$

$$\epsilon_0\psi_p - t\left(\psi_{p-1}e^{-i2\pi\phi/L} + \psi_{p+1}e^{i2\pi\phi/L}\right) = E\psi_p$$

Again, we use a Bloch wave ansatz $\psi_p = e^{ikpa}$ where $a = 2\pi R/L$ and k only taking discrete values shown in equation 4, resulting in

$$\epsilon_0 - t\left(e^{-i(ka+2\pi\phi/L)} + e^{i(ka+2\pi\phi/L)}\right) = E(k) \tag{17}$$

$$\epsilon_0 - 2t\cos(ka + 2\pi\phi/L) = E(k) \tag{18}$$

Assuming $ka + 2\pi\phi/L \ll \pi$, we Taylor expand the dispersion relation, and by choosing $\epsilon_0 = 2t$ the small argument expansion gives

$$E(k) \approx t\left(ka + 2\pi\phi/L\right)^2 \tag{19}$$

The new minimum of the dispersion relation does not occur at $k = 0$, but rather at $k = -2\pi\phi/(La)$ In fact, it is more natural to work with angular momentum m

$$E(m) \approx \frac{4\pi^2 t}{L^2}\left(m + \phi\right)^2 \tag{20}$$

Hence the integer m that is closest to $-\phi$ gives the ground state.

3.1 Probability current

Although the problem is stationary, *ie. the system is doing the same thing at all times, but there isn't time reversible symmetry due to the B field.*, we want to look at the probability current from each site.

We can consider the rate of change of occupation of site i by using Ehrenfest's Theorem. First we must define a positive circulation, we choose $i \to i+1$ to be a positive current. Units where $\hbar = c = 1$ are chosen and the Schrödinger picture is used.

$$\frac{d}{dt}\langle n_i\rangle = \frac{1}{i}\langle [n_i, H]\rangle \tag{21}$$

Only having nearest neighbor tunneling gives us the follow relation with the current $J_{i\to i+1}$

$$\frac{d}{dt}\langle n_i\rangle = J_{i-1\to i} - J_{i\to i+1} \tag{22}$$

Using the following commutation relations

$$[a_i, n_j] = a_i\delta_{ij}\ ,\ \left[a_i^\dagger, n_j\right] = -a_i^\dagger\delta_{ij}$$

We get [1]

$$\frac{d}{dt}\langle n_i\rangle = \frac{1}{i}\langle -te^{i2\pi\phi/L}c_i^\dagger c_{i+1} + te^{i2\pi\phi/L}c_{i+1}^\dagger c_i - te^{i2\pi\phi/L}c_i^\dagger c_{i-1} + te^{i2\pi\phi/L}c_{i-1}^\dagger c_i\rangle \tag{23}$$

[1]Full derivation of the probability current in the appendix

By comparing with equation 22, we can write down the current $J_{i\to i+1}$

$$\begin{aligned} J_{i\to i+1} &= i\langle -te^{i2\pi\phi/L}c_i^\dagger c_{i+1} + te^{-i2\pi\phi/L}c_{i+1}^\dagger c_i\rangle \\ &= -2t\,\mathrm{Im}\Big\{e^{-i2\pi\phi/L}\langle c_{i+1}^\dagger c_i\rangle\Big\} \end{aligned} \tag{24}$$

Considering a general state expressed in equation 16, we can find the expectation value

$$\begin{aligned} J_{i\to i+1} &\propto -2t\,\mathrm{Im}\{e^{-i2\pi\phi/L}e^{-ika}\} \\ &= 2t\sin(ka + 2\pi\phi/L) \end{aligned} \tag{25}$$

Writing in terms of angular momentum m and considering large L such that the small argument expansion for sin is a good approximation, we get

$$J_{i\to i+1} \approx \frac{4\pi t}{L}(m+\phi)$$

For the ground state current we get

$$J_{i\to i+1} \approx \frac{4\pi t}{L}([-\phi]+\phi) \tag{26}$$

where $[\phi]$ denotes the nearest integer to ϕ.

4 Initial Numerical Study

For the general many body case, we write down a Hubbard model corresponding to equation 14. The last term is the on-site Hubbard interaction term.

$$H = \sum_{i=1}^{L}\epsilon_0 n_i - t\sum_{i=1}^{L}\Big(e^{-i2\pi\phi/L}a_{i+1}^\dagger a_i + e^{i2\pi\phi/L}a_i^\dagger a_{i+1}\Big) + \frac{U}{2}\sum_{i=1}^{L}a_i^\dagger a_i^\dagger a_i a_i \tag{27}$$

We only want single occupation

$$\langle n_i\rangle = \{0,1\} \tag{28}$$

To do this, we take the limit $U\to\infty$ and ignore the Hubbard interaction term in equation 27 and thus giving a Hardcore Boson model. What changes is the basis states. Our local Fock states with the max single occupancy restriction allows us to map our Hamiltonian to a spin system.

The matrix representation of the local basis at site i is

$$|0_i\rangle = (1,0)^T \tag{29}$$

$$|1_i\rangle = (0,1)^T \tag{30}$$

In this representation, the matrices the local creation and annihilation operators are

$$a = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{31}$$

$$a^\dagger = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{32}$$

To get the whole Fock space, we take the tensor product of the local Fock spaces. We find the matrix representation of the basis states for the whole Foch space by taking every permutation of L Kronecker products of $(1,0)^T$ and $(0,1)^T$.

The matrix representation of the creation operator at site i is found by taking the appropriate number of Kronecker products with the identity matrix.

$$a_i^\dagger = \underbrace{\mathbb{1} \otimes \mathbb{1} ... \otimes \mathbb{1}}_{\text{i - 1 times}} \otimes a^\dagger \otimes \underbrace{\mathbb{1} \otimes \mathbb{1} ... \otimes \mathbb{1}}_{\text{L-i times}} \tag{33}$$

and likewise for the annihilation operator. The interpretation of equation 33 is that we apply the identity to all the other sites apart from site i, which we apply the local creation operator.

The single particle matrix elements of the creation and annihilation operators are all 0 because they do not conserve particle number.

$$\langle \Psi_{1,n} | a_j | \Psi_{1,m} \rangle = 0 \tag{34}$$

4.1 Numerical Dispersion Relation

The Hamiltonian matrix H can be thus be found by matrix multiplication and summing all the terms up in equation 27. The matrix size is $2^L \times 2^L$ and includes terms for single particle, two particles ... all the way up to L particles. Once the eigenvectors are found, we can find the k it corresponds to by finding the wavelength of the wavefunction.

$$\langle r | \Psi \rangle = \sum_m \psi_m \langle r | m \rangle \tag{35}$$

$$\Psi(r) = \sum_m \psi_m \xi_m(r) \tag{36}$$

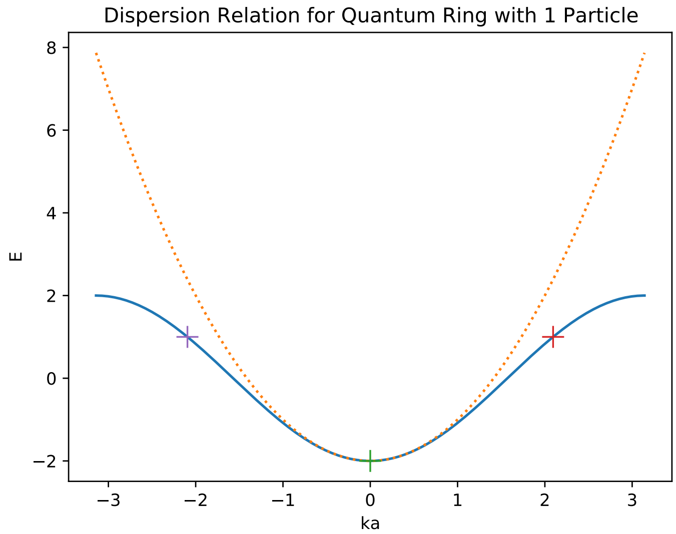

Figure 1: Plot of blue: exact dispersion relation for a single particle on a Quantum ring; orange: small momenta approximation for the dispersion relation. The three points are the eigenvalues for a single particle Hamiltonian for a Quantum ring with 3 sites. $\epsilon_0 = 0$, $a = 1$, $t = 1$, $\phi = 0$

I decided numerically that the sites are still labeled $1, 2, 3...$ even though python index starts at 0

4.2 Numerical Ground State Probability Current

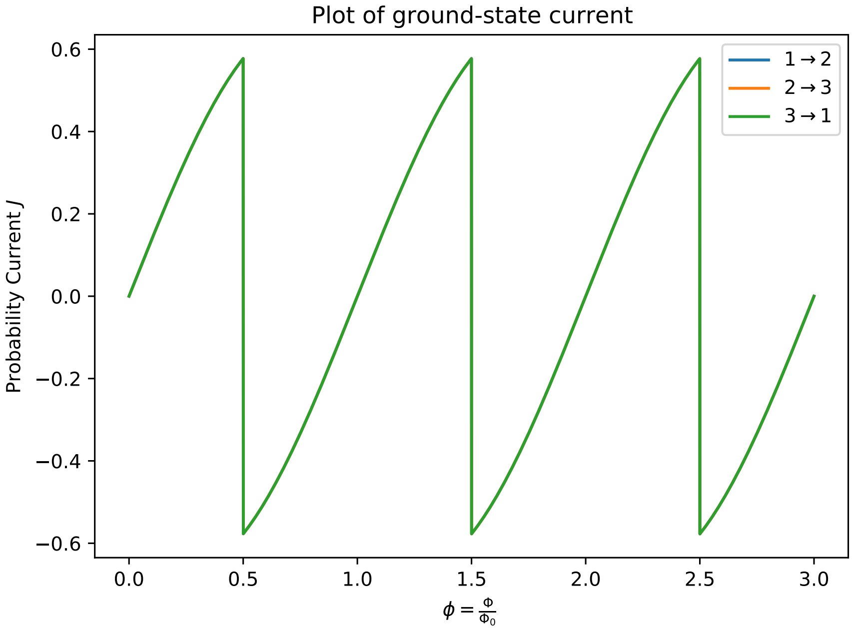

Figure 2: Plot of the probability current for the single particle ground state as a function of ϕ where $t = 1$. Note the current for different site hopping are all overlaid on each other, therefore all sites are equivalent. Another property of the relation to note is that it is periodic, with periodicity of 1. There is a maximum current at $0.5 - \epsilon$ (and its periodic repetitions) where $\epsilon > 0$ and is arbitrarily small, unlike for the classical car case where the cars there is no maximum speed for the cars.

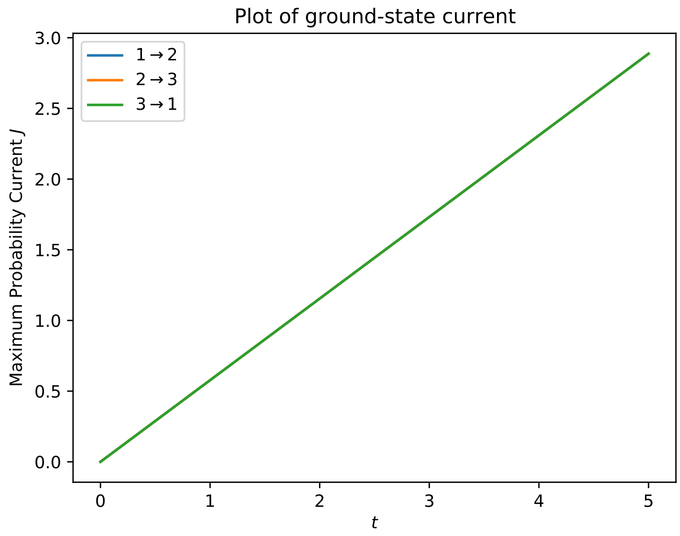

Figure 3: Plot of the maximum probability current for the single particle ground state as a function of t where $\phi = 0.49999999$.The relation is linear, with gradient 0.577350 and intercept of 0

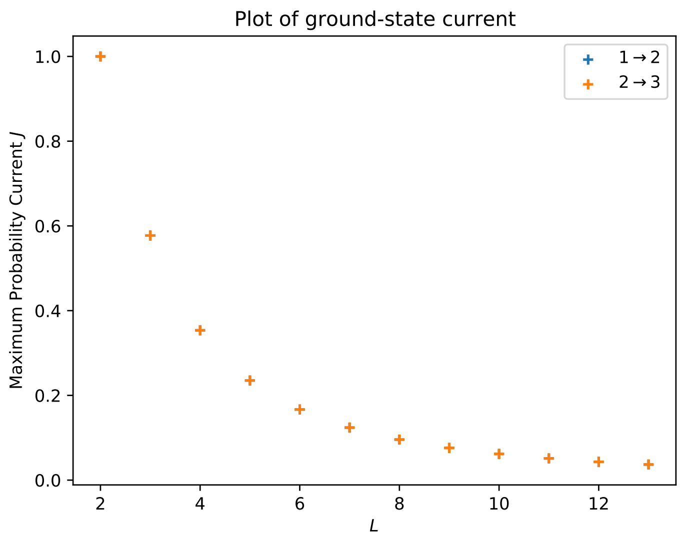

Figure 4: Plot of the maximum probability current for the single particle ground state as a discrete function of L where $\phi = 0.49999999$. As expected, the maximum current decays with increasing L as there is less probability per site to move.

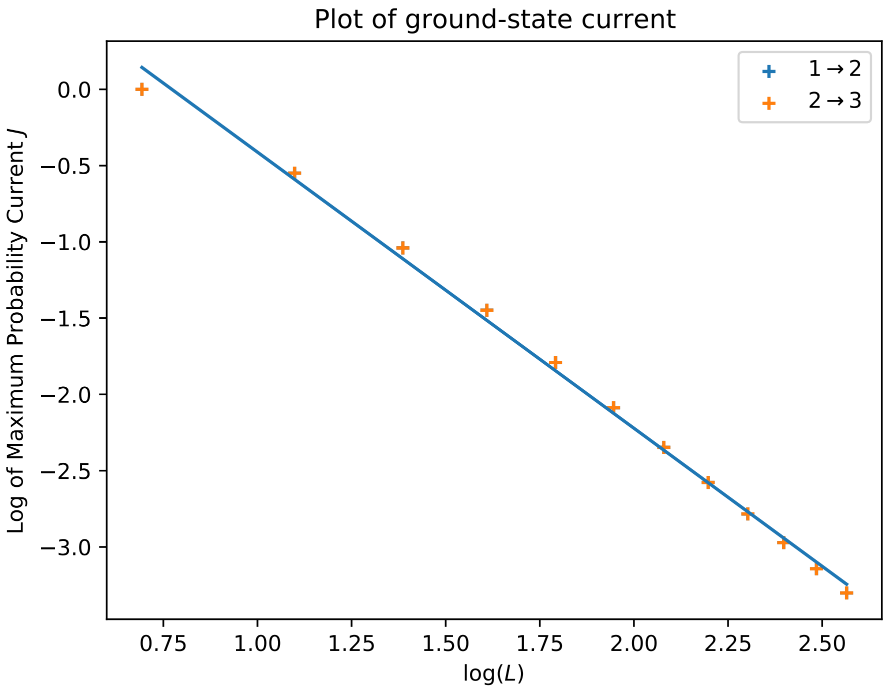

Figure 5: Plot of the log of the maximum probability current for the single particle ground state as a function of $\log(L)$ where $\phi = 0.49999999$ and $t = 1$. The linear fit gives the gradient: -1.8100496 and intercept: 1.3983348

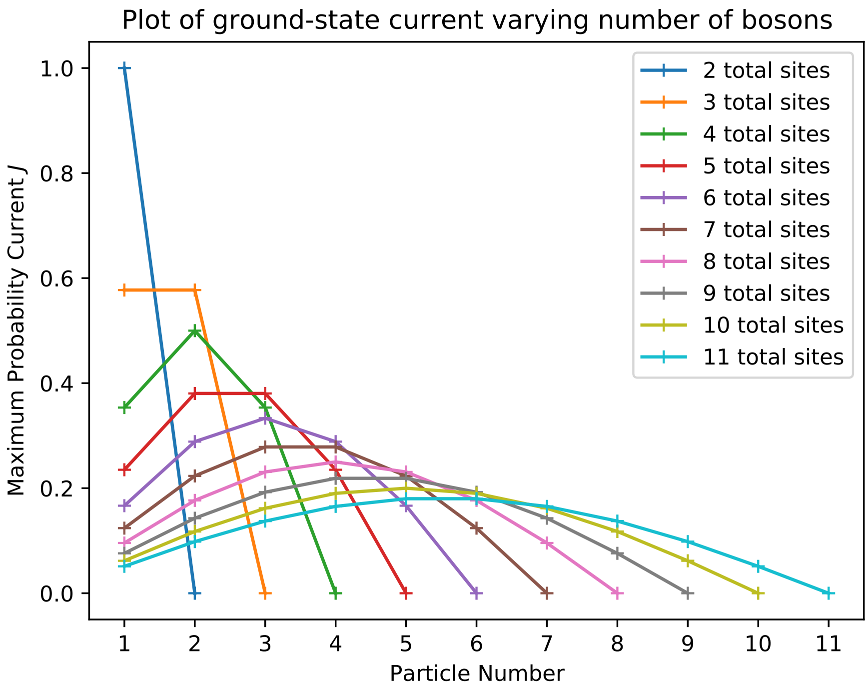

Figure 6: Plot of the maximum probability current for the ground state for different sized quantum rings, whilst varying the particle number of each from single particle to all sites occupied and where $\phi = 0.49999999$ and $t = 1$. We numerically see the maximum to the maximum probability current occurring at half occupation of the ring. Since particle number is discrete, for odd numbers of total sites, there are two particle occupations of the ring that lead to this maximum.

5 Quantum Quench

Now consider some different Hamiltonian at time t that is modeled after the classical traffic wave idea where one car stops. One can try a strong on site potential at site k

$$H_{perturb} = \sum_{i=1}^{L} \epsilon_0 n_i - t \sum_{i=1}^{L} \left(e^{-i2\pi\phi/L} a_{i+1}^{\dagger} a_i + e^{i2\pi\phi/L} a_i^{\dagger} a_{i+1} \right) + U a_k^{\dagger} a_k \tag{37}$$

We want to find the ground state for the Hamiltonian $H_{perturb}$ in equation 37, then we suddenly change the Hamiltonian back to H from equation 27. Using the ground state found, we can find the probability current at different sites then evolve the ground state by unitary transformation with the time independent H.

$$|\Psi(t)\rangle = U|\Psi_{g.s.}(0)\rangle = e^{-iHt}|\Psi_{g.s.}(0)\rangle \tag{38}$$

5.1 Investigation of the time evolution of the current

First thing to try is a delta potential for U. Numerically, however, an infinite value cannot be used within diagonalisation- so a large value for U was chosen.

Interestingly, with nonzero ϕ we get a resultant probability current with evolution. We see that the probability current reverses in sign with some sort of periodic fashion. There might be some sort of time delay between the evolution of the different currents, however it isn't clear. If we are thinking about cars, then the current wouldn't reverse in sign. I tested the perturbation at a different site, but plotting the same the current evolution of the site with the same relation, *i.e.* perturb at site $i+1$ and consider the evolution of the current at site i.

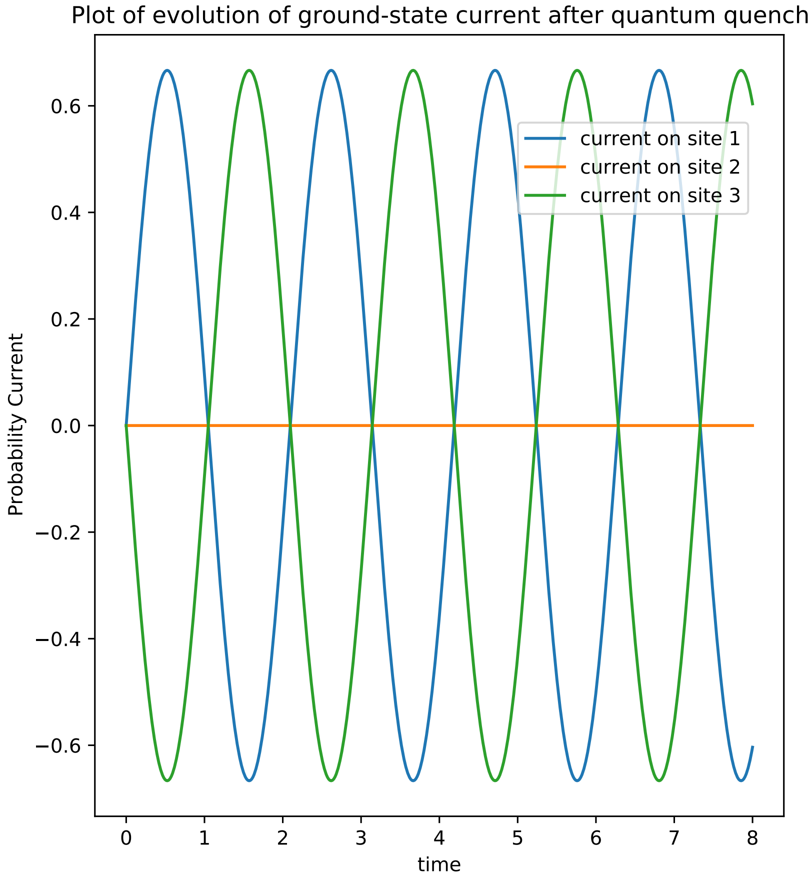

Figure 7: Plot of the evolution of the current after quantum quench for a single particle with the initial perturbation at site 1. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0$

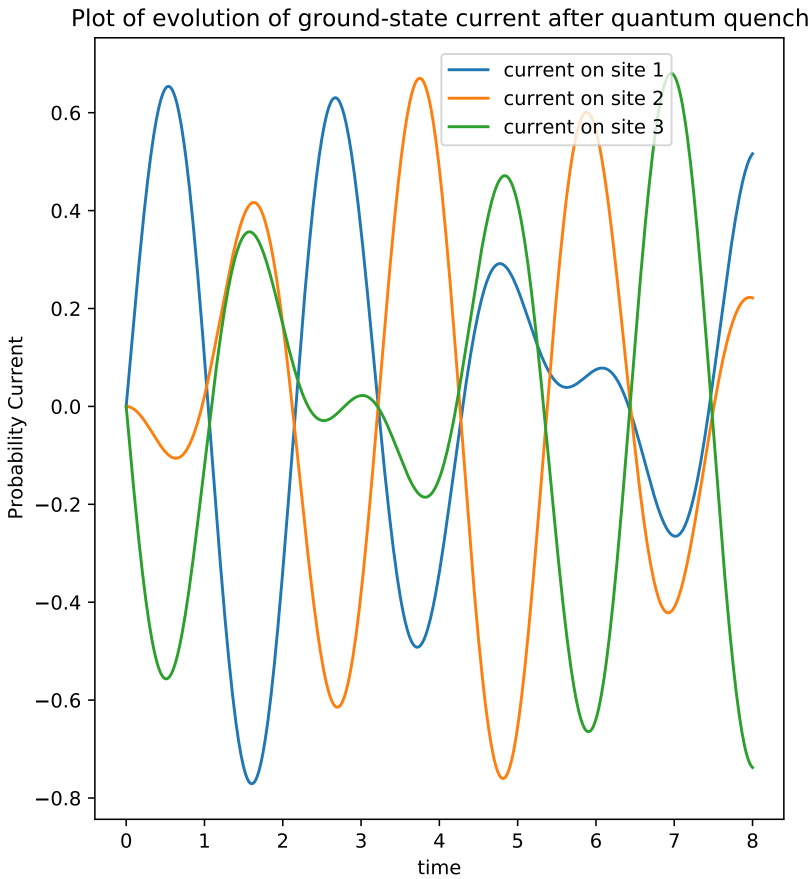

Figure 8: Plot of the evolution of the current after quantum quench for a single particle with the initial perturbation at site 1. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0.1$

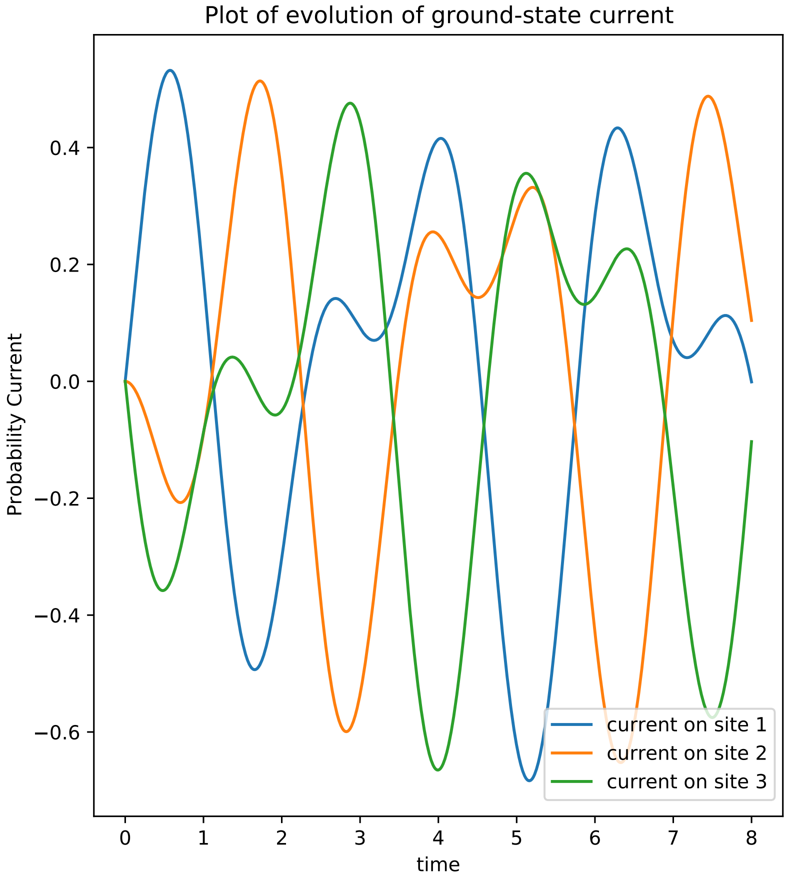

Figure 9: Plot of the evolution of the current after quantum quench for a single particle with the initial perturbation at site 1. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0.2$

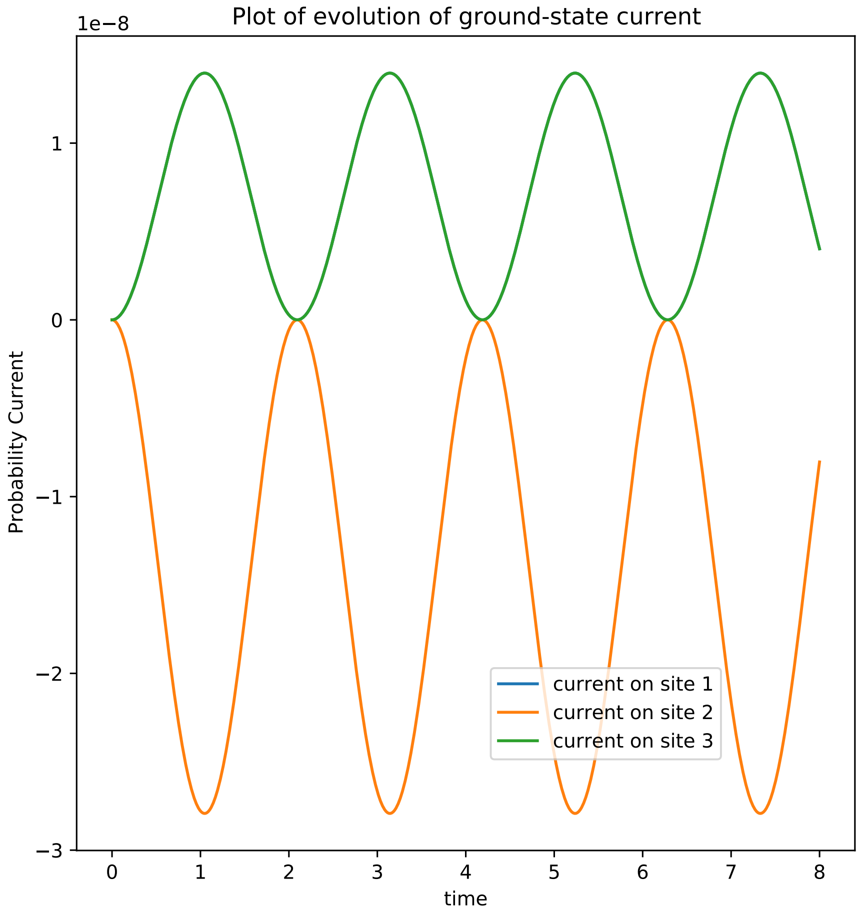

Figure 10: Plot of the evolution of the current after quantum quench for a single particle with the initial perturbation at site 1. Current on site 1 is overlaid on top of site 3. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0.49999999$

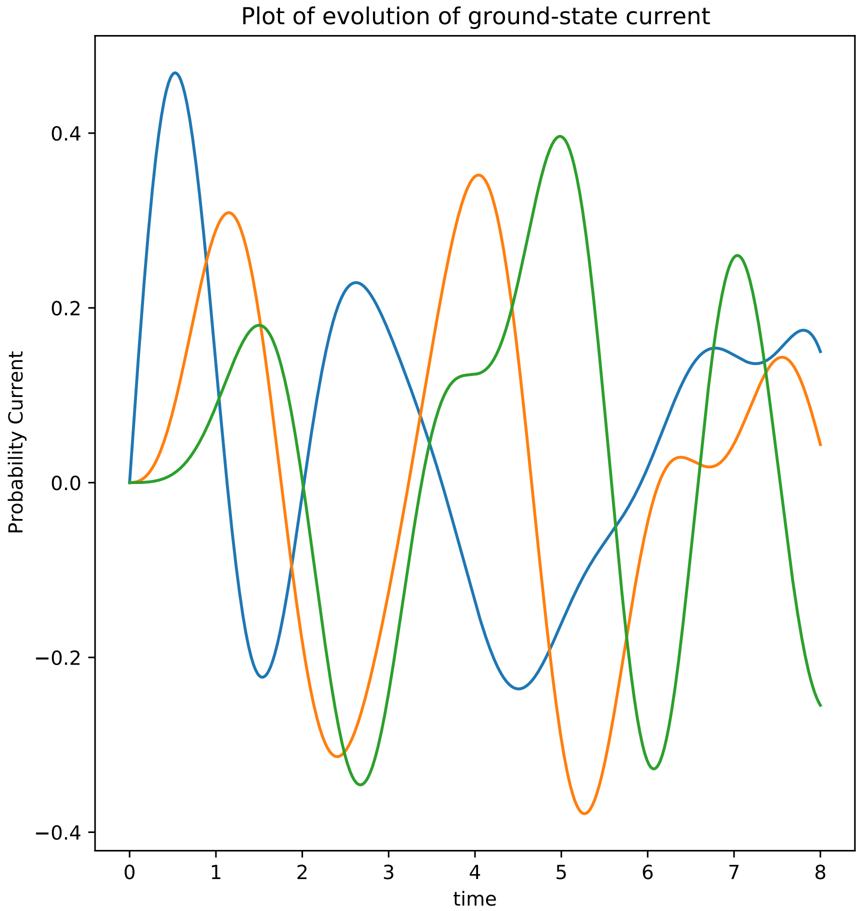

Figure 11: Plot of the evolution of the current after quantum quench for 3 particles with the initial perturbation at site 1. $L = 6$, $U = 10^5$, $t = 1$, $\phi = 0.2$

5.2 Investigation of the time evolution of the site occupation

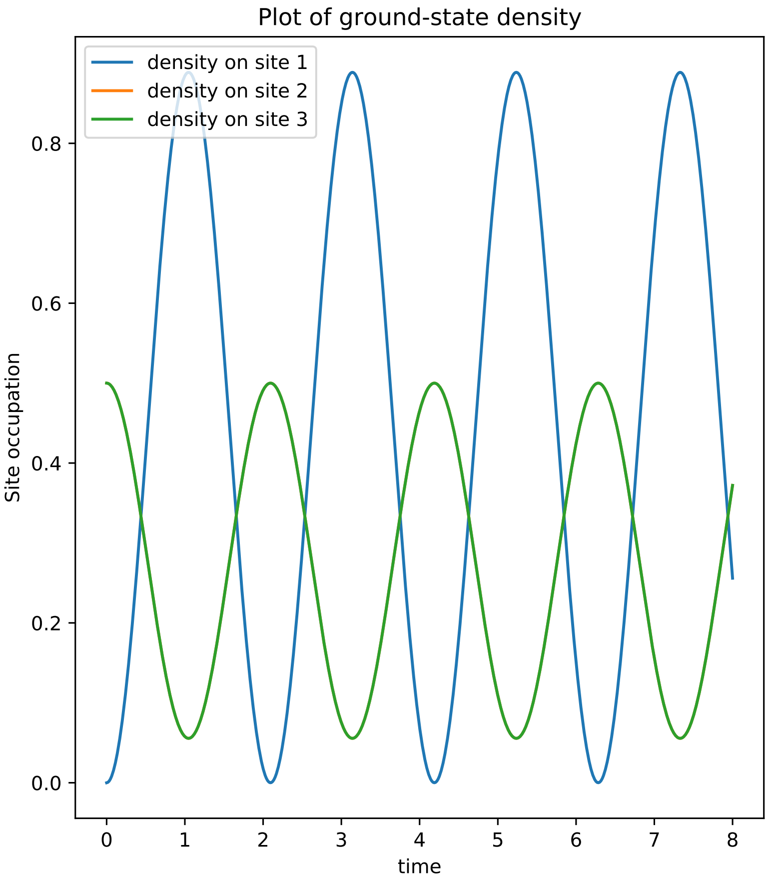

Figure 12: Plot of the evolution of the site occupation after quantum quench for 1 particle with the initial perturbation at site 1. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0$

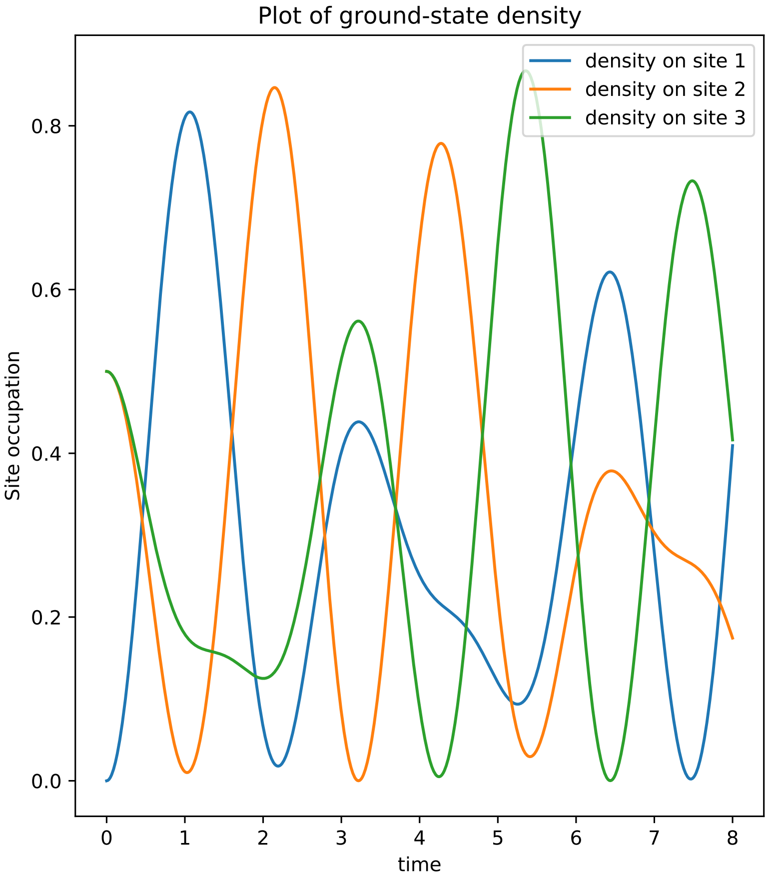

Figure 13: Plot of the evolution of the site occupation after quantum quench for 1 particle with the initial perturbation at site 1. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0.1$ Note how the oscillations seem to between the sites go between in phase and out of phase.

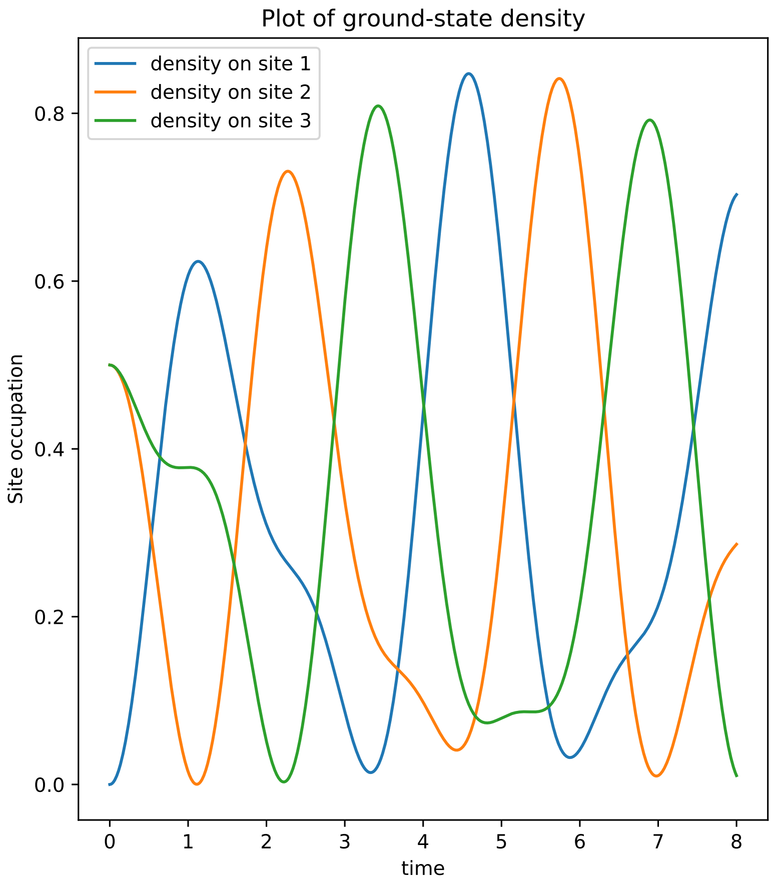

Figure 14: Plot of the evolution of the site occupation after quantum quench for 1 particle with the initial perturbation at site 1. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0.2$ Note how the peaks follow one after the other.

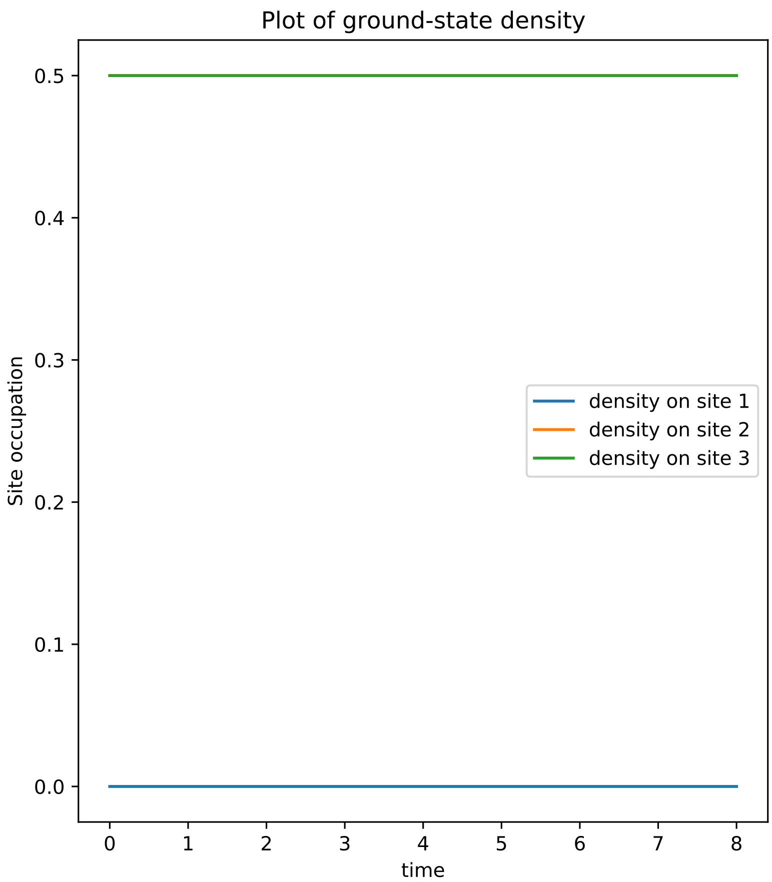

Figure 15: Plot of the evolution of the site occupation after quantum quench for 1 particle with the initial perturbation at site 1. $L = 3$, $U = 10^5$, $t = 1$, $\phi = 0.49999999$ Note how the particle only spreads out on sites 2 and 3.

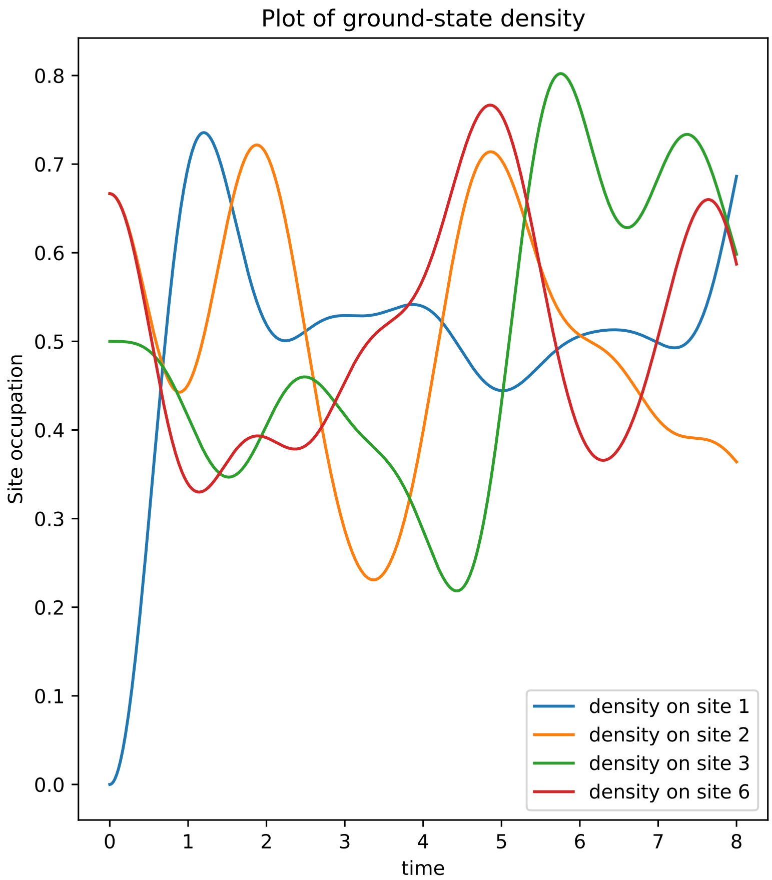

Figure 16: Plot of the evolution of the site occupation after quantum quench for 3 particle with the initial perturbation at site 1. $L = 6$, $U = 10^5$, $t = 1$, $\phi = 0.2$ I can't see any sort of structure here.

6 Mapping the Hard-Core Boson Model to a Free Fermion Model

In 1D, there is an exact mapping between the Hard-Core Boson Model with the Free Fermion Model, the transformation that takes from one to the other is the Jordan-Wigner transformation

$$f_j^\dagger = a_j^\dagger \tag{39}$$
$$f_j = a_j \tag{40}$$

We can do the above via a mapping to spin 1/2 Pauli operators, which we mentioned in section 4. Now we need to fix the anti-commutator relations for fermions with an extra transformation. For a 1D chain we have

$$c_j^\dagger = e^{\left(+i\pi \sum_{k=1}^{j-1} f_k^\dagger f_k\right)} \cdot f_j^\dagger \tag{41}$$
$$c_j = e^{\left(-i\pi \sum_{k=1}^{j-1} f_k^\dagger f_k\right)} \cdot f_j \tag{42}$$

Remembering $f_j^\dagger f_j \in \{0, 1\}$. For our ring case, we have to alter equations 41 and 42 slightly

$$c_j^\dagger = e^{\left(+i\pi \sum_{k\neq j} f_k^\dagger f_k\right)} \cdot f_j^\dagger \tag{43}$$
$$c_j = e^{\left(-i\pi \sum_{k\neq j} f_k^\dagger f_k\right)} \cdot f_j \tag{44}$$

The resulting fermionic operators are nonlocal with respect to the bosonic operators and have the following anticommutation relations

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \tag{45}$$
$$\{c_i, c_j^\dagger\} = \delta_{i,j} \tag{46}$$

The pairwise potential term in the hard-core boson model shown in equation 27 maps to 0