Fermion Transport for the Multi-site Model

Consider a one dimensional wire divided into three parts. The left part is a bath of length N_L which is held at temperature β_L and chemical potential μ_L. The middle part is the wire itself and has length N_W. The right part is a bath of length N_R which is held at temperature β_R and chemical potential μ_R. Each part is given by a decoupled Hamiltonian $H_0 = -w\sum_{x=1}^{n-1}(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x)$, and the different parts are coupled via terms like $-w'(c_{N_L}^\dagger c_{N_L+1} + c_{N_L+1}^\dagger c_{N_L})$. Therefore, the Hamiltonian of the system can be explicitly written as

$$
\begin{aligned}
H = -w\sum_{x=1}^{N_L-1}(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x) - w'(c_{N_L}^\dagger c_{N_L+1} + c_{N_L+1}^\dagger c_{N_L}) - w\sum_{x=N_L+1}^{N_L+N_W-1}(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x) \\
- w'(c_{N_L+N_W}^\dagger c_{N_L+N_W+1} + c_{N_L+N_W+1}^\dagger c_{N_L+N_W}) - w\sum_{x=N_L+N_W+1}^{N_L+N_W+N_R-1}(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x)
\end{aligned}
$$

Let $n = N_L + N_W + N_R$ be the total length of the system. Then we can define $2n$ Hermitian Majorana operators according to Eq. (5) in Prosen's paper:

$$w_{2m-1} = c_m + c_m^\dagger$$

$$w_{2m} = i(c_m - c_m^\dagger)$$

satisfying $\{w_j, w_k\} = 2\delta_{j,k}$. In terms of these operators, each term in the Hamiltonian becomes:

$$
\begin{aligned}
-w(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x) &= -\frac{w}{4}((w_{2x-1} + iw_{2x})(w_{2x+1} - iw_{2x+2}) + (w_{2x+1} + iw_{2x+2})(w_{2x-1} - iw_{2x})) \\
&= -\frac{w}{4}(w_{2x-1}w_{2x+1} + iw_{2x}w_{2x+1} - iw_{2x-1}w_{2x+2} + w_{2x}w_{2x+2} \\
&+ w_{2x+1}w_{2x-1} + iw_{2x+2}w_{2x-1} - iw_{2x+1}w_{2x} + w_{2x+2}w_{2x}) \\
&= \frac{iw}{4}(w_{2x-1}w_{2x+2} - w_{2x+2}w_{2x-1} + w_{2x+1}w_{2x} - w_{2x}w_{2x+1}) \\
&= \frac{iw}{2}(w_{2x-1}w_{2x+2} + w_{2x+1}w_{2x})
\end{aligned}
$$

One can use this to rewrite the whole Hamiltonian in the w basis. Define the $2n \times 2n$ matrix

$$
H_n = \begin{bmatrix}
0 & 0 & 0 & \frac{iw}{4} & 0 & 0 & \dots \\
0 & 0 & -\frac{iw}{4} & 0 & 0 & 0 & \dots \\
0 & \frac{iw}{4} & 0 & 0 & 0 & \frac{iw}{4} & \dots \\
-\frac{iw}{4} & 0 & 0 & 0 & -\frac{iw}{4} & 0 & \dots \\
0 & 0 & 0 & \frac{iw}{4} & 0 & 0 & \dots \\
0 & 0 & -\frac{iw}{4} & 0 & 0 & 0 & \dots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
$$

Then the Hamiltonian can be written in block matrix form

$$
H = \begin{bmatrix}
H_{N_L} & & & \frac{iw'}{4} & & \\
 & & -\frac{iw'}{4} & & & \\
 & \frac{iw'}{4} & H_{N_W} & & & \frac{iw'}{4} \\
-\frac{iw'}{4} & & & & -\frac{iw'}{4} & \\
 & & & \frac{iw'}{4} & H_{N_R} & \\
 & & -\frac{iw'}{4} & & &
\end{bmatrix}
$$

which is clearly Hermitian.

Next, we want to represent the bath operators. They are computed the same way for both the left and right baths. Therefore, in what follows, we describe the bath operators only for the left part. Let h_L be the single particle Hamiltonian for the left bath. In can be written as a $N_L \times N_L$ matrix in the c basis:

$$
h_L = \begin{bmatrix}
0 & -w & 0 & \dots \\
-w & 0 & -w & \dots \\
0 & -w & 0 & \dots \\
\vdots & \vdots & \vdots & \ddots
\end{bmatrix}
$$

Let ϵ_j and ψ_j be the eigenvalues and eigenvectors of this matrix, such that $h_L\psi_j = \epsilon_j\psi_j$ for all $j = 1, 2, \dots N_L$. The eigenvectors are also written in the c basis and can be viewed as functions of lattice site. There will be N_L in rates $v_{L,j} = \sqrt{\gamma_{in,j}}\psi_j$ and N_L out rates $u_{L,j} = \sqrt{\gamma_{in,j}}\psi_j^*$, where ψ_j is treated as a row vector. The only constraint on the rates is that

$$
\gamma_{in,j} e^{\beta_L(\epsilon_j - \mu_L)} = \gamma_{out,j}
$$

Since only the ratio of the two matters, we can set $\gamma_{in,j} = \gamma$ for all j. Therefore

$$u_{L,j} = \sqrt{\gamma e^{\beta_L(\epsilon_j - \mu_L)}}\psi_j^*$$

$$v_{L,j} = \sqrt{\gamma}\psi_j$$

Next, we need to write the rates in the w basis by expressing ψ_j in the w basis. This will allow us to write the jump operators in the form $u_{L,j} = l_{u,j} \cdot w$ and $v_{L,j} = l_{v,j} \cdot w$ with

$$l_{u,j,2i-1} = \frac{1}{2\sqrt{2}}\sqrt{\gamma e^{\beta_L(\epsilon_j - \mu_L)}}\psi_{j,i}^*$$

$$l_{u,j,2i} = -\frac{i}{2\sqrt{2}}\sqrt{\gamma e^{\beta_L(\epsilon_j - \mu_L)}}\psi_{j,i}^*$$

$$l_{v,j,2i-1} = \frac{1}{2\sqrt{2}}\sqrt{\gamma}\psi_{j,i}$$

$$l_{v,j,2i} = -\frac{i}{2\sqrt{2}}\sqrt{\gamma}\psi_{j,i}$$

for $i = 1, 2, \ldots N_L$, and $l_{u,j,2i-1} = l_{u,j,2i} = l_{v,j,2i-1} = l_{v,j,2i} = 0$ for all $i > N_L$. Similar computations are performed for the right bath. Note that the additional factor of $\frac{1}{\sqrt{2}}$ comes from the discrepancy in the Lindblad equation as defined in Prosen's paper and in the transport paper. The equation in Prosen's paper has an extra factor of 2, for which we compensate above.

Next, we proceed as in the two-site case. We compute the complex Hermitian $4n \times 4n$ matrix M given by $M_{jk} = \sum_\mu l_{\mu,j} l_{\mu,k}^*$ (Eq. (23)). Similarly, we compute the complex antisymmetric $4n \times 4n$ matrix A defined in Eq. (27) as

$$A_{2j-1,2k-1} = -2iH_{jk} - M_{jk} + M_{kj}$$

$$A_{2j-1,2k} = 2iM_{kj}$$

$$A_{2j,2k-1} = -2iM_{jk}$$

$$A_{2j,2k} = -2iH_{jk} + M_{jk} - M_{kj}$$

Since A is an antisymmetric matrix of even dimension, its eigenvalues come in pairs $(\beta, -\beta)$. Arrange the eigenvalues as $\beta_1, -\beta_1, ..., \beta_4, -\beta_4$, $Re(\beta_1) \geq ... \geq Re(\beta_4)$, and let $v_1, ..., v_8$ be the corresponding eigenvectors. We would like to normalize the eigenvectors such that they satisfy Eq. (30), $v_r \cdot v_s = J_{rs}$, where

$$J = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

The eigenvectors computed by MATLAB are such that $v_j \cdot v_j = 0$ and $v_{2j-1} \cdot v_{2j} = 1$. However, because the spectrum $\{\beta_j\}$ is degenerate, we are not guaranteed that $v_{2j} \cdot v_k = 0$ for all $k \neq 2j-1$. Therefore, we must consider a linear combination of v_js.

When we have multiple eigenvectors with the same eigenvalues, we put them next to each other in blocks $\beta_1, -\beta_1, \beta_1, -\beta_1, ...$ Let the corresponding eigenvectors in this block be $a_1, b_1, a_2, b_2, ...$, such that a_j is the eigenvector for the j^{th} positive eigenvalue β_1 and b_j is the eigenvector for the j^{th} negative eigenvalue $-\beta_1$. We are given that $a_i \cdot a_j = 0$ and $b_i \cdot b_j = 0$. Define linear combinations $c_i = \sum_j U_{ij} b_j$. Note that c_i is also an eigenvector with eigenvalue $-\beta_1$. We want c_js to satisfy $a_i \cdot c_j = \delta_{i,j}$. Hence

$$\sum_k U_{jk} a_i \cdot b_k = \delta_{i,j}$$

Define matrix T:

$$T_{ik} = a_i \cdot b_k = \sum_\alpha a_i^\alpha b_k^\alpha$$

$$\sum_k (U)^T_{kj} T_{ik} = (TU^T)_{ij} = \delta_{i,j}$$

Therefore $TU^T = I$ and $U = (T^{-1})^T$. Now we can use the matrix U to compute c_j as shown above. As a result of this procedure, we are left with eigenvectors $a_1, c_1, a_2, c_2, ...$

After applying these changes to all blocks of equal eigenvalues, we introduce the matrix V whose j^{th} row is the j^{th} eigenvector. This matrix is used to compute quadratic observables as described in Eq. (47) of Prosen's paper. Our observable is the current across two neighboring sites $(x, x+1)$, which is given by

$$
\begin{aligned}
I &=< -i(c_x^\dagger c_{x+1} - c_{x+1}^\dagger c_x) > \\
&=< \frac{1}{4i}((w_{2x-1} + iw_{2x})(w_{2x+1} - iw_{2x+2}) - (w_{2x+1} + iw_{2x+2})(w_{2x-1} - iw_{2x})) > \\
&=< \frac{1}{4i}(w_{2x-1}w_{2x+1} + iw_{2x}w_{2x+1} - iw_{2x-1}w_{2x+2} + w_{2x}w_{2x+2} \\
&- w_{2x+1}w_{2x-1} - iw_{2x+2}w_{2x-1} + iw_{2x+1}w_{2x} - w_{2x+2}w_{2x}) > \\
&= \frac{1}{2i}(< w_{2x-1}w_{2x+1} > + < w_{2x}w_{2x+2} >)
\end{aligned}
$$

where the expectation values are given by Eq. (47)

$$
< w_{2x-1}w_{2x+1} >= \frac{1}{2}\sum_{m=1}^{2n}(V_{2m,4x-3}V_{2m-1,4x+1} - V_{2m,4x-2}V_{2m-1,4x+2} - iV_{2m,4x-2}V_{2m-1,4x+1} - iV_{2m,4x-3}V_{2m-1,4x+2})
$$

$$
< w_{2x}w_{2x+2} >= \frac{1}{2}\sum_{m=1}^{2n}(V_{2m,4x-1}V_{2m-1,4x+3} - V_{2m,4x}V_{2m-1,4x+4} - iV_{2m,4x}V_{2m-1,4x+3} - iV_{2m,4x-1}V_{2m-1,4x+4})
$$

In my computations, I looked at the current in the middle of the wire, i.e. across the link $(N_L + \frac{N_W}{2}, N_L + \frac{N_W}{2} + 1)$.

Need to add derivations for electrical conductivity. Right now I'm computing σ exactly as in the Mathematica code.