

Generating Hubbard Model Solutions from Anderson Impurity Model Solutions

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1 Introduction

This is an attempt to obtain various quantities like Greens functions, self-energies, spectral functions and (if possible) energies and wavefunctions of the Hubbard model, using a cluster-bath approach. The cluster-bath system is taken to be a single-impurity Anderson model with a correlated bath. The correlation will be brought about in two ways: a self-energy $\Sigma(k, \omega)$ of the bath, and a double occupancy repulsion cost U_b . The Hubbard and the correlated single-impurity Anderson models are defined using the Hamiltonians

$$H_{\text{hubb}} = -t^H \sum_{\sigma, \langle i, j \rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + U^H \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu^H \sum_{i\sigma} \hat{n}_{i\sigma} \quad (1.1)$$

$$H_{\text{siam}} = \sum_{k\sigma} [\epsilon_k + \Sigma(k, \omega)] \hat{n}_{k\sigma} + \epsilon_d^A \sum_{\sigma} \hat{n}_{d\sigma} + U^A \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + U_b \sum_{kk'} \hat{n}_k \hat{n}_{k'} - t^A \sum_{k\sigma} \left(c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right) \quad (1.2)$$

Broadly speaking, the method involves first solving the SIAM using a unitary renormalisation group approach, to get the low energy effective theory, and then combining the low energy Hamiltonians in a symmetrized fashion to get the Hamiltonian for the Hubbard model lattice. It is reminiscent of dynamical mean-field theory (DMFT) - both involve an impurity-solver that solves an auxiliary system. The difference, however, lies in the following points:

- While DMFT primarily works with Greens functions and self-energies, this method involves Hamiltonians. The impurity-solver in DMFT provides an impurity Greens function (which is then equated with the local Greens function of the bath), while the impurity-solver in this method actually provides a low energy Hamiltonian.
- The final step of DMFT is the self-consistency equation, where the impurity and bath-local quantities are set equal. This ensures all sites, along with the impurity site, have the same self-energy, something which is required on grounds of translational invariance. The present method, however, brings about the translational invariance in a different way. It symmetrizes the Hamiltonians itself, such that all quantities then derived from the Hamiltonian are then guaranteed to have the symmetry.

The meaning of each of these statements will become clearer when we describe the method in more detail.

2 Philosophy of the method

The method is closely tied to the auxiliary system approach described in [1]. We can view the full Hamiltonian as a sum of two component Hamiltonians H_1, H_2 connected via the interaction term H_{12} .

$$H = \begin{pmatrix} H_1 & H_{12} \\ H_{12}^* & H_2 \end{pmatrix} = H_1 |1\rangle \langle 1| + H_2 |2\rangle \langle 2| + H_{12} |1\rangle \langle 2| + H_{12}^* |2\rangle \langle 1| \quad (2.1)$$

where $|1(2)\rangle$ actually represents a sum over all basis kets of the subsystem 1(2). As an example, we can split the the Hubbard model Hamiltonian between a particular site $i = p$ and the rest of the lattice as follows:

$$\begin{aligned} H_{\text{hubb}} = & \overbrace{U^H \hat{n}_{p\uparrow} \hat{n}_{p\downarrow} - \mu^H \sum_{\sigma} \hat{n}_{p\sigma}}^{H_1} \\ & + \underbrace{U^H \sum_{i \neq p} \hat{n}_{i\uparrow} \hat{n}_{p\downarrow} - \mu^H \sum_{i \neq p, \sigma} \hat{n}_{i\sigma} - t^H \sum_{\substack{\sigma, \langle i, j \rangle \\ i \neq p \neq j}} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.})}_{H_2} \\ & - \underbrace{t^H \sum_{\substack{\sigma, \\ i \in \text{N.N. of } p}} (c_{i\sigma}^\dagger c_{p\sigma} + \text{h.c.})}_{H_{12} + H_{12}^*} \end{aligned} \quad (2.2)$$

The Greens function of the full Hamiltonian can also be split in a similar fashion:

$$G(\omega) = \begin{pmatrix} G_1 & G_{12} \\ G_{12}^* & G_2 \end{pmatrix} \quad (2.3)$$

The subsystem 1 is usually taken to be the "smaller system", and consequently, subsystem 2 represents the "bath". The smaller system is typically chosen such that its eigenstates are known exactly. Progress is then made by choosing a simpler version of the bath H_2 and a simpler form also for its coupling H_{12} with the smaller system. This combination of the smaller system and the simpler bath is then called the *auxiliary system*. A typical auxiliary system for the Hubbard model would be the SIAM, where the impurity represents an arbitrary site p of the lattice, the bath represents the rest of the lattice sites and the hybridisation term between the impurity and the bath represents the coupling term H_{12} . Such a construction is shown in fig. 1. *It should be noted that any reasonable choice of the cluster and bath would break the translational symmetry of the full model. To allow computing quantities, one would need to make the bath (which is a much larger system) simpler than the cluster (which is a single site). This distinction breaks the translational symmetry of the Hubbard model. For eg., if one chooses eq. 1.2 as the auxiliary system, then the fact that the impurity has an onsite correlation while the bath only has a global capacitive cost ($\sim U_b N^2$) means we have broken the symmetry between the cluster and the bath.*

The algorithm of DMFT then involves starting with some local self-energy of the bath, $\Sigma(\omega)$, and using an impurity solver to calculate the impurity Greens function in the presence of this self-energy. This impurity Greens function is then used to calculate the impurity self-energy $\Sigma_d(\omega)$, and the self-energy of the bath is then set equal to this impurity self-energy: $\Sigma(\omega) = \Sigma_d(\omega)$, because we expect, on grounds of the lattice symmetry, that the impurity is the same as any other site in the bath. This is said to be the

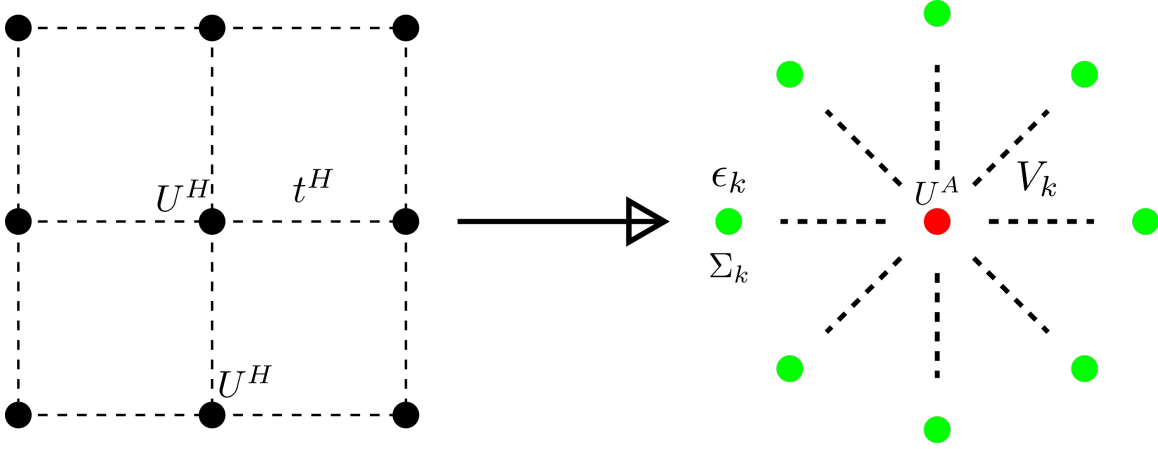


Figure 1: *Left*: Full Hubbard model lattice with onsite repulsion U^H on all sites and hopping between nearest neighbour sites with strength t^H . *Right*: Extraction of the auxiliary (cluster+bath) system from the full lattice. The central site on left becomes the impurity site (red) on the right (with an onsite repulsion ϵ_d), while the rest of the $N - 1$ sites on the left form a conduction bath (green circles) (with dispersion ϵ_k and correlation modelled by the self-energy $\Sigma_k(\omega)$) that hybridizes with the impurity through the coupling V .

self-consistency step, because the bath self-energy is completely determined only at the end. With this updated bath self-energy, one then repeats the entire process until there is no further change in the bath self-energy at the self-consistency step.

The present method intends to calculate the quantities in a different fashion. We start with a SIAM (with a correlated bath having a non-trivial self-energy), and solve it using the unitary renormalisation group approach to get to a fixed-point Hamiltonian. The fixed point Hamiltonian will in general involve the impurity site (with renormalised parameters ϵ_d^* , U^*) interacting with a smaller number of momentum states. Assuming the impurity-bath couplings are much larger than the dispersion of the bath, we can approximate the conduction bath part by a zero-mode of the kinetic energy part. The zero mode is defined as $c_0 = \frac{1}{\sqrt{N}} \sum_k c_k$, so it is just the zeroth site. What this means is that all the momentum states will then collapse to a single site (which we call the zero mode site, and represents the origin of the lattice). We will also pick out the zeroth site part of the onsite correlation part, and replace that with a single correlation coupling U_z^A . Such a model, shown in fig. 2 is exactly solvable.

$$H_{\text{corr}}^A = -t^A \sum_{\sigma} \left(c_{d\sigma}^\dagger c_{z\sigma} + \text{h.c.} \right) + U^A \tau_{d\uparrow} \tau_{d\downarrow} + U_z^A \tau_{z\uparrow} \tau_{z\downarrow} \quad (2.4)$$

The motivation for extracting the zero mode is that it leads to a very simple effective Hamiltonian (the asymmetric Anderson molecule) without losing much of the low energy physics.

We will then create the the entire Hubbard Hamiltonian by combining the zero-mode Hamiltonians according to a prescription which is guided by the symmetries of the problem. The impurity electron will be read off as an arbitrary site, p , of the lattice, while the zero-mode site becomes the site that is nearest to it. We will first demonstrate this explicitly for the Hubbard dimer. Then we will show how we can create a full Hubbard Hamiltonian by joining Anderson molecule Hamiltonians. At this point, we will assume that we have a Hubbard model in mind that has motivated a correlated SIAM as the auxiliary system, and we have performed renormalisation group analysis on this auxiliary system to get down to an effective Hamiltonian. We will also assume that the parameters of the auxiliary system have been chosen such that in the effective Hamiltonian, the impurity and zero mode have the same onsite repulsion: $U^A = U_z^A$ (this is required for translational invariance). What this all means is that the RG analysis of the auxiliary model

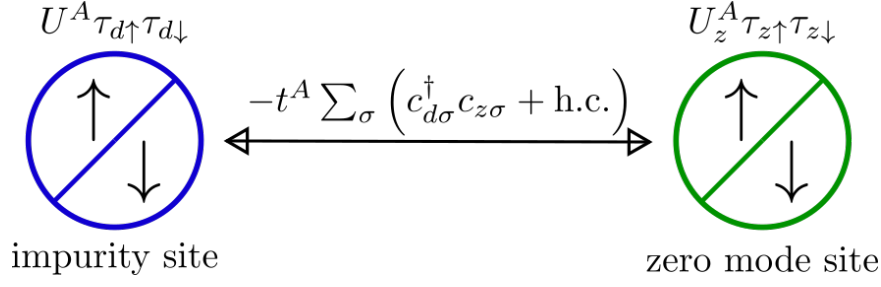


Figure 2: Correlated asymmetric Anderson molecule schematic version. It consists of two sites, impurity(blue) and zero mode(green). The impurity site has onsite repulsion, and there is inter-site hopping.

(appropriately chosen to model the bare Hubbard Hamiltonian) has led to a stable fixed point theory effective Hamiltonian described by a Hubbard dimer

$$H^D(U^D, t^D) \equiv -t^D \sum_{\sigma} (c_{0\sigma}^\dagger c_{1\sigma} + \text{h.c.}) + U^D (\tau_{0\uparrow} \tau_{0\downarrow} + \tau_{1\uparrow} \tau_{1\downarrow}) \quad (2.5)$$

This Hubbard dimer is shown in fig. 3.

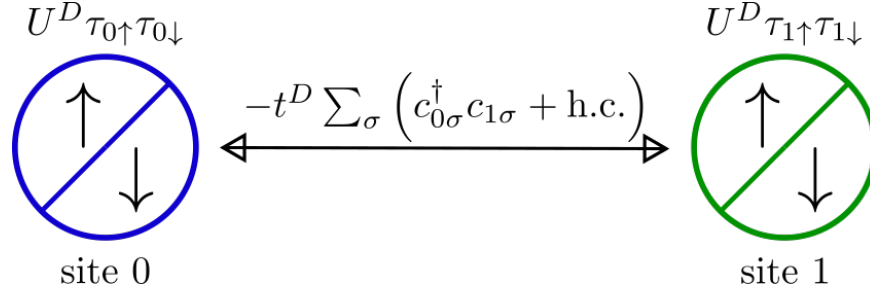


Figure 3: Hubbard dimer schematic version. It again consists of two sites, like the Anderson molecule, but now both sites have onsite repulsion, and there is again inter-site hopping.

The next step is to restore the lost translational invariance of the full system. We intend to do this by recreating a full Hubbard model, \tilde{H} , through the iterative real-space translation of the Hubbard dimer effective Hamiltonian obtained above. We will describe this process in detail below. However, we first specify the two approximations made along the entire journey from the original Hubbard model to the reconstructed one:

- We have replaced the full Hubbard model by an auxiliary system described by the SIAM Hamiltonian in eq. 1.2. The accuracy of this assumption is determined by the choice of the SIAM parameters, particularly the self-energy and repulsion of the bath. As discussed before, the very choice of the cluster and bath spoils the translational invariance of the parent model.
- We then perform a unitary RG on H^A . This leads to a fixed-point Hamiltonian $\mathcal{U}_A H^A \mathcal{U}_A^\dagger$. At this point, we extract a zero mode of this Hamiltonian to obtain the Hubbard dimer Hamiltonian: $H^D = Z [\mathcal{U}_A H^A \mathcal{U}_A^\dagger] Z^{-1}$, where Z defines the projection operator that extracts the zero mode from the effective stable fixed Hamiltonian $\mathcal{U}_A H^A \mathcal{U}_A^\dagger$. This constitutes the second approximation we make. This approximation further reduces the symmetry, because we have dropped all other lattice sites and kept just the zeroth lattice site (i.e., the site to which the impurity is coupled through single electron hybridisation).

We now tile the real-space lattice with this Hubbard dimer Hamiltonian to restore translational invariance (shown in a later section), and obtain a new Hubbard Hamiltonian, $\tilde{H} = T [H^D] T^{-1}$, where T denotes

the operator that performs the set of iterative real-space translations, and enables the dimer Hamiltonian to span the target real-space lattice. We quote the final form of \tilde{H} here to explain what the tiling means, but the explanation is given in a later section.

$$\tilde{H} = -\frac{2t^D}{Nw} \sum_{\sigma \langle ij \rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + \frac{2U^D}{N} \sum_i \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} = \frac{2}{Nw} \sum_{\langle ij \rangle} H^D(i, j, t^D, U^D) \quad (2.6)$$

What that means is that we have placed the Hubbard dimer at all nearest neighbour pairs to reconstruct a new Hubbard model. If we assume that the tiling mostly rectifies the explicit symmetry-breaking made while choosing the auxiliary system as well as taking the zero mode, we can write

$$\tilde{H} = \mathcal{U} H^H \mathcal{U}^{-1} = T Z \left[\mathcal{U}_A H^A \mathcal{U}_A^\dagger \right] Z^{-1} T^{-1}, \quad (2.7)$$

where $\mathcal{U} = T Z \mathcal{U}_A$ is some transformation that is either a unitary, or, at the very least, a similarity transformation that maps from the original to the reconstructed Hubbard Hamiltonian. The existence of \mathcal{U} is contingent on how good the approximations are, and strictly speaking needs to be verified.

3 Solution of the Hubbard dimer using the Anderson molecule

This section tries to see how far we can go if we just work with the Anderson molecule as the smallest unit of tiling. We will attempt to reproduce the entire spectrum of a Hubbard dimer by creating a new Hamiltonian made up purely of Anderson molecules. This will guide us in deciding how to generalize the "tiling method" for a general N -site Hubbard model, as well as give indications as to whether we need a different smallest unit for tiling.

The Hubbard dimer and Anderson molecules (zero-mode) are defined by the following respective Hamiltonians:

$$\begin{aligned} H^H &= -t^H \sum_{\sigma} \left(c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu^H \sum_{\sigma, i=1,2} \hat{n}_{i\sigma} \\ H^A &= -t^A \sum_{\sigma} \left(c_{d\sigma}^\dagger c_{z\sigma} + \text{h.c.} \right) + \epsilon_d^A \sum_{\sigma} \hat{n}_{d\sigma} + U^A \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \end{aligned} \quad (3.1)$$

In the first Hamiltonian, the indices $i = 1, 2$ refer to the two lattice sites that constitute the dimer. In the second Hamiltonian, the subscript d indicates the impurity site, while the subscript z indicates the zero-mode site. First, we will assume that the Hubbard dimer is at half-filling ($\frac{1}{2}U^H = \mu^H$):

$$\begin{aligned} H^H &= -t^H \sum_{\sigma} \left(c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} + \left(\frac{1}{2}U^H - \mu^H \right) \sum_{\sigma, i=1,2} \hat{n}_{i\sigma} + \text{constant} \\ &= -t^H \sum_{\sigma} \left(c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \end{aligned} \quad (3.2)$$

Since the Hubbard Hamiltonian is at half-filling, we will also place the impurity at half-filling by setting $\epsilon_d^A = -\frac{1}{2}U^A$:

$$\begin{aligned} H^A &= -t^A \sum_{\sigma} \left(c_{d\sigma}^\dagger c_{z\sigma} + \text{h.c.} \right) + \left(\epsilon_d^A + \frac{1}{2}U^A \right) \sum_{\sigma} \hat{\tau}_{d\sigma} + U^A \hat{\tau}_{d\uparrow} \hat{\tau}_{d\downarrow} + \text{constant} \\ &= -t^A \sum_{\sigma} \left(c_{d\sigma}^\dagger c_{z\sigma} + \text{h.c.} \right) + U^A \hat{\tau}_{d\uparrow} \hat{\tau}_{d\downarrow} \end{aligned} \quad (3.3)$$

The first step is to recreate the Hubbard dimer Hamiltonian eq. 3.2 using the Anderson molecule Hamiltonian eq. 3.3:

$$\begin{aligned}
H^H &= -t^H \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \\
&= \frac{1}{2} \left[-t^H \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + \text{h.c.} \right) + t^H \sum_{\sigma} \left(c_{2\sigma}^{\dagger} c_{1\sigma} + \text{h.c.} \right) \right] + \frac{1}{2} 2U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \\
&= \frac{1}{2} \left[-t^A \sum_{\sigma} \left(c_{d\sigma}^{\dagger} c_{z\sigma} + \text{h.c.} \right) \Big|_{\substack{z \rightarrow 2, d \rightarrow 1 \\ t^A \rightarrow t^H}} + t^A \sum_{\sigma} \left(c_{2\sigma}^{\dagger} c_{1\sigma} + \text{h.c.} \right) \Big|_{\substack{d \rightarrow 2, z \rightarrow 1 \\ t^A \rightarrow t^H}} \right] \\
&\quad + \frac{1}{2} \left(U^A \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \Big|_{U^A \rightarrow 2U^H}^{d \rightarrow 1} + U^A \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \Big|_{U^A \rightarrow 2U^H}^{d \rightarrow 2} \right) \\
&= \frac{1}{2} \left[H^A \left(t^A \rightarrow t^H, U^A \rightarrow 2U^H, d \rightarrow 1, z \rightarrow 2 \right) + H^A \left(t^A \rightarrow t^H, U^A \rightarrow 2U^H, d \rightarrow 2, z \rightarrow 1 \right) \right]
\end{aligned} \tag{3.4}$$

The conclusion we can draw from this is that the Hubbard dimer Hamiltonian can be obtained from the Anderson dimer Hamiltonian in the following fashion:

- The essential idea is that we have to create a local Hubbard Hamiltonian for each site of the Hubbard lattice by replacing the impurity label d in the Anderson dimer with the label of the particular site. So if there are two sites, we will get two local Hamiltonians obtained by replacing d with 1 and 2 respectively. For each local Hamiltonian, the zero-mode label z is replaced by the site that is nearest to the one that d is being replaced by. So, if $d \rightarrow 1(2)$, then $z \rightarrow 2(1)$.
- This, however, is not the only change that we must make, in order to get the local Hamiltonian for a particular site. Along with d and z , we must also make the transformations $t^A \rightarrow t^H, U^A \rightarrow 2U^H$.
- Finally, once we have the local Hamiltonians for sites 1 and 2, we average them to get the total Hubbard Hamiltonian.

Note that we expect most of these "rules" to be specific for the dimer, and there will be generalizations to most of them for a general N -site Hubbard Hamiltonian.

The wavefunctions for the $N = 2$ sector can also be connected through these transformations. Since both the Hamiltonians are analytically solvable, we can write down their groundstate wavefunctions [2]:

$$\begin{aligned}
|\Psi_{\text{GS}}^H\rangle &= a_1(U^H, t^H) \frac{1}{\sqrt{2}} (|\uparrow_1, \downarrow_2\rangle - |\downarrow_1, \uparrow_2\rangle) - a_2(U^H, t^H) \sqrt{2} (|\uparrow_1 \downarrow_1, \rangle - |\uparrow_2 \downarrow_2\rangle) \\
|\Psi_{\text{GS}}^A\rangle &= a_1\left(\frac{1}{2}U^A, t^A\right) \frac{1}{\sqrt{2}} (|\uparrow_d, \downarrow_z\rangle - |\downarrow_d, \uparrow_z\rangle) - a_2\left(\frac{1}{2}U^A, t^A\right) \sqrt{2} (|\uparrow_d \downarrow_d, \rangle - |\uparrow_z \downarrow_z\rangle) \\
E_{\text{GS}}^H &= -\frac{1}{2}\Delta(U^H, t^H), E_{\text{GS}}^A = -\frac{1}{2}\Delta\left(\frac{1}{2}U^A, t^A\right)
\end{aligned} \tag{3.5}$$

where

$$a_1(U, t) \equiv \frac{4t}{\sqrt{2\Delta(U, t) (\Delta(U, t) - U)}}, \quad a_2(U, t) \equiv \sqrt{\frac{\Delta(U, t) - U}{2\Delta(U, t)}}, \quad \Delta(U, t) \equiv \sqrt{U^2 + 16t^2} \tag{3.6}$$

a_1, a_2 satisfy $a_1(-U, t) = -a_2(U, t)$ and $a_1(U, t)a_2(U, t) = \frac{2t}{\Delta(U, t)}$. From the forms of the wavefunctions and eigenenergies, we can immediately write down

$$|\Psi_{\text{GS}}^H\rangle = \frac{1}{2} \left[|\Psi_{\text{GS}}^A\rangle (t^A, U^A \rightarrow t^H, 2U^H, d \rightarrow 1, z \rightarrow 2) + |\Psi_{\text{GS}}^A\rangle (t^A, U^A \rightarrow t^H, 2U^H, d \rightarrow 2, z \rightarrow 1) \right] \quad (3.7)$$

$$E_{\text{GS}}^H = E_{\text{GS}}^A (t^A, U^A \rightarrow t^H, 2U^H)$$

This shows that the rules laid out before work for the Hamiltonians, as well as the wavefunctions and energy eigenvalues of the $N = 2, 0, 4$ sector. These sectors specifically work because it is only in these sectors can we ensure that $n_d = n_z$, which is required for the Hubbard Hamiltonian because $n_1 = n_2$. In the other sectors ($N = 1, 3$), the impurity site and the zero-mode sites have to be singly-occupied in some part, and since the impurity site incurs a single-occupation cost of $-\frac{U^H}{2}$ which is not borne by the zero-mode site, there is an intrinsic dissimilarity between the two sites of the Anderson molecule in this regime. This dissimilarity does not exist for the Hubbard model, so we cannot hope to connect the two models in this regime. Going forward, we will switch to using Hubbard dimers as the smallest tiling unit for a general Hubbard model.

4 Creating General N -site Hubbard Hamiltonian from Hubbard dimers

We will follow the strategy outlined in the previous section. For concreteness, we will consider a lattice of N lattice sites and w nearest neighbours for each site. Note that a uniform number of nearest neighbours means that there is perfect translational invariance on the lattice, which means there cannot be any edge sites. This is achieved by applying periodic boundary conditions on the edges of the lattice. A square 2d lattice is thus placed on a 2-torus.

For each site i out of the N sites (having nearest neighbours $\{i_j, j \in [1, w]\}$), we will create w local Hamiltonians $\{H_{i,i_j}^H, i \in [1, N], j \in [1, w]\}$ out of the Hubbard dimer Hamiltonians, by setting the impurity index d to i and the zero-mode index z to i_j . We will also need to suitably transform the Hamiltonian parameters U^A, t^A , but we will figure those out as we go along. All N sites will then produce Nw local Hamiltonians in total, and the general Hubbard Hamiltonian should be the average of these local Hamiltonians.

The local Hamiltonians look like

$$H_{i,i_j}^D = -t^D \sum_{\sigma} \left(c_{i\sigma}^{\dagger} c_{i_j\sigma} + \text{h.c.} \right) + U^D \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} + U^D \hat{\tau}_{i_j\uparrow} \hat{\tau}_{i_j\downarrow} \quad (4.1)$$

We havent transformed the dimer parameters U^D, t^D to the Hubbard parameters yet. The sum of all local Hamiltonians for a particular site i then gives the total Hamiltonian for that site:

$$H_i^D = \sum_{j \in [1, w]} H_{i,i_j}^D = \sum_{\substack{\sigma \\ j \in \text{N.N. of } i}} -t^D \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + w U^D \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} + U^D \sum_{j \in \text{N.N. of } i} \hat{\tau}_{j\uparrow} \hat{\tau}_{j\downarrow} \quad (4.2)$$

If we now sum over all the lattice sites and take the average of all the Hamiltonians (Nw in number), we get

$$\begin{aligned}
\tilde{H} &= \frac{1}{Nw} \sum_{i=1}^N H_i^D \\
&= \frac{1}{Nw} \left[\sum_{\sigma, i=1}^N \sum_{j \in \text{NN of } i} -t^D \left(c_{\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + wU^D \sum_{i=1}^N \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} + U^D \sum_{i=1}^N \sum_{j \in \text{N.N. of } i} \hat{\tau}_{j\uparrow} \hat{\tau}_{j\downarrow} \right] \\
&= \frac{1}{Nw} \left[-t^D 2 \sum_{\sigma, \langle ij \rangle} \left(c_{\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + 2U^D \sum_{\langle ij \rangle} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} + 2U^D \sum_{\langle ij \rangle} \hat{\tau}_{j\uparrow} \hat{\tau}_{j\downarrow} \right] \\
&= \frac{2}{Nw} \sum_{\langle ij \rangle} \left[-t^D \sum_{\sigma} \left(c_{\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + U^D \left(\hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} + \hat{\tau}_{j\uparrow} \hat{\tau}_{j\downarrow} \right) \right] \\
&= \frac{2}{Nw} \sum_{\langle ij \rangle} H^D(i, j, t^D, U^D)
\end{aligned} \tag{4.3}$$

There we used the identity

$$\sum_{i=1}^N \sum_{j \in \text{NN of } i} = 2 \sum_{\langle ij \rangle} \tag{4.4}$$

The sum $\langle ij \rangle$ is over all nearest-neighbour pairs. Thus, \tilde{H} can be written as

$$\tilde{H} = -\frac{2t^D}{Nw} \sum_{\sigma, \langle ij \rangle} \left(c_{\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + \frac{2U^D}{N} \sum_i \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} = \frac{2}{Nw} \sum_{\langle ij \rangle} H^D(i, j, t^D, U^D) \tag{4.5}$$

The conclusion is that on tiling the Hubbard dimer Hamiltonians into all the nearest neighbour pairs, we end up with a new Hubbard model Hamiltonian with "renormalised parameters" given by

$$\tilde{t} = \frac{2t^D}{Nw} \quad , \quad \tilde{U} = \frac{2U^D}{N} . \tag{4.6}$$

It is thus apparent that translating the Hubbard dimers throughout the lattice has restored translational invariance, and generated correlations on all sites.

The claim made in a previous section was that this Hamiltonian is very close to a similarity transformed Hubbard Hamiltonian:

$$\tilde{H} = \frac{2}{Nw} \sum_{\langle ij \rangle} H^D(i, j, t^D, U^D) \equiv \mathcal{U} H^H \mathcal{U}^{-1} , \tag{4.7}$$

where \mathcal{U} is in general distinct from the unitary transformation that completes the URG starting from the bare cluster+bath Anderson model up to the fixed-point Hamiltonian. As shown earlier, U transformation that involves three steps: the URG transformations \mathcal{U}_A , the extracting of the zero mode Z and the tiling procedure outline in this section, T

$$\mathcal{U} = T Z \mathcal{U}_A . \tag{4.8}$$

With some knowledge of the RG procedure, one can even write down the relation between the Hubbard dimer couplings t^D, U^D and the parent Hubbard model parameters t^H, U^H . We have seen previously in another work that in the absence of any explicit spin or charge isospin exchange couplings, the impurity-bath

hybridisation coupling t^A does not flow under the RG. In going from the Hubbard model to the auxiliary model, we replace the non-local operator c_i with the local operator c_d . If we define the normalization of the Fourier transform such that both spaces have $\frac{1}{\sqrt{N}}$, then the auxiliary model coupling can be written as $t^A = \sqrt{N}t^H$. When we write the fixed-point hopping purely in terms of zero mode, another such factor appears: $\sum_k c_k = \sqrt{N}c_0$, such that $t^D = \sqrt{N}(t^A)^*$. Combining these, we get

$$t^D = \sqrt{N} \times (t^A)^* = \sqrt{N} \times t^A = N \times t^H$$

As for the on-site repulsion U^H , we will constrain the RG flows such that the fixed-point value of the impurity on-site repulsion U^A is identical to that of the on-site repulsion of the bath, U_b . A sensible choice for the bath on-site repulsion is simply $U^H \times N$. The factor of N maintains the extensivity of the bath correlation term. We can therefore write

$$U^D \equiv (U^A)^* = U_b = N \times U^H$$

5 Formal expressions for single particle Greens functions and other related many-body quantities

5.1 Expressing matrix elements of the inverse single particle Greens function in terms of Hubbard dimer counterparts

Since the two Hamiltonians H^H and \tilde{H} are connected via a similarity transformation \mathcal{U} , their ground states are also connected by the same transformation. That is, if the ground states are $|\Phi_0\rangle$ and $|\tilde{\Phi}_0\rangle$ respectively, then $|\tilde{\Phi}_0\rangle = \mathcal{U}|\Phi_0\rangle$. This means that matrix elements of the type in eq. 9.19 will also be connected. The matrix elements are of the inverse Greens function operator defined in eq. 9.18:

$$\mathcal{G}(\omega, H) = \frac{1}{\omega - (H - E_{\text{GS}})} \quad (5.1)$$

Its easy to see that the matrix elements of the original and renormalised versions of this operator, between the original and renormalised states, are equal:

$$\begin{aligned} \left[\mathcal{G}_H^{-1} \right]_{\nu\nu'} &= \langle \nu | \omega - H^H + E_{\text{GS}} | \nu' \rangle = \langle \nu | \mathcal{U}^{-1} \left(\omega - \mathcal{U} H^H \mathcal{U}^{-1} + E_{\text{GS}} \right) \mathcal{U} | \nu' \rangle = \langle \tilde{\nu} | \left(\omega - \tilde{H} + E_{\text{GS}} \right) | \tilde{\nu}' \rangle \\ &= \left[\tilde{\mathcal{G}}^{-1} \right]_{\tilde{\nu}, \tilde{\nu}'} \end{aligned} \quad (5.2)$$

where we have defined the renormalised excitation $|\tilde{\nu}'\rangle \equiv \tilde{c}_{\nu'}^\dagger |\tilde{\Phi}_0\rangle \equiv \left(\mathcal{U} c_{\nu'}^\dagger \mathcal{U}^{-1} \right) \mathcal{U} |\Phi_0\rangle = \mathcal{U} |\nu'\rangle$. These equalities are important because they allows us to calculate these matrix elements for \tilde{H} and then equate them to those of H^H , and once we have the matrix elements of \mathcal{G} , we can use them to obtain the single-particle Greens functions using eq. 9.19. More specifically, to calculate the real space single-particle Greens function between the lattice sites i and j , both with spin σ , we will use the relation:

$$G(i\sigma, j\sigma, \omega) = \langle i\sigma | \mathcal{G}(\omega, H) | j\sigma \rangle - \langle \bar{i}\sigma | \mathcal{G}(-\omega, H) | \bar{j}\sigma \rangle = \mathcal{G}(\omega, H)_{i\sigma, j\sigma} - \mathcal{G}(-\omega, H)_{\bar{i}\sigma, \bar{j}\sigma} \quad (5.3)$$

where $|i\sigma\rangle = c_{i\sigma}^\dagger |\Phi_0\rangle$ and $|\bar{i}\sigma\rangle = c_{i\sigma} |\Phi_0\rangle$. We can see from the relation that we will need two types of matrix elements, one that propagates a particle excitation ($|i\sigma\rangle$) and the one that propagates a hole excitation ($|\bar{i}\sigma\rangle$).

To this end, we rewrite eq. 4.5 in terms of inverse Greens function operators for the new (symmetrized) Hubbard model and the Hubbard dimer respectively:

$$\tilde{\mathcal{G}}(\omega) = \frac{1}{\omega - (\tilde{H} - E_{\text{GS}})}, \quad \mathcal{G}_D(\omega) = \frac{1}{\omega - (H^D - E_{\text{GS}})} \quad (5.4)$$

These are the same operators that appear in the appendix. However, before proceeding, we should note that even though eq. 4.5 used the indices i , the correct indices are actually \tilde{i}, \tilde{j} , in light of the fact that operators get renormalised as $c_i \rightarrow \tilde{c}_i \equiv U c_i$. With this in mind, we can write

$$\omega - \tilde{\mathcal{G}}^{-1}(\omega) = \frac{2}{Nw} \sum_{\langle \tilde{i}, \tilde{j} \rangle} \left[\omega - \mathcal{G}_D^{-1}(\tilde{i}, \tilde{j}) \right] \quad (5.5)$$

where $\mathcal{G}_D^{-1}(\tilde{i}, \tilde{j})$ is the Greens function inverse matrix of the Hubbard dimer Hamiltonian with \tilde{i}, \tilde{j} as the two sites. Since the ω on the RHS of eq. 5.5 is independent of the summation indices, they can be pulled out along with a factor. The factor is just the total number of nearest neighbour pairs, which is $\frac{Nw}{2}$. This allows it to cancel the ω on the LHS. The equation then simplifies to

$$\tilde{\mathcal{G}}^{-1}(\omega) = \frac{2}{Nw} \sum_{\langle \tilde{i}, \tilde{j} \rangle} \mathcal{G}_D^{-1}(\omega, \tilde{i}, \tilde{j}) \quad (5.6)$$

We will now calculate the site-diagonal and site-off-diagonal matrix elements for particle propagation. The site-diagonal matrix element is calculated between the state $|\tilde{i}, \sigma\rangle = \mathcal{U} c_{i\sigma}^\dagger |\Phi_0\rangle$ and its bra, while the off-diagonal one is between $|\tilde{j}\sigma\rangle$ and $\langle \tilde{i}\sigma|$. Since it has already been shown that the matrix elements of the renormalised Hamiltonian are the same as those of the original Hamiltonian, we will directly replace the former with the latter.

First lets consider the diagonal matrix element at \tilde{i}^{th} site. The only terms that will contribute on the RHS of eq. 5.6 are those that have \tilde{i} in one of the indices. There will be w such terms, because \tilde{i} has w nearest neighbours. Thus, the right hand side will be a sum of w terms, each term being the inverse Greens function of a Hubbard dimer. Each term will be a real space local Greens function, and because of translational invariance, it will be the same on both sites. The entire thing is thus w times this local Greens function.

$$\left(\mathcal{G}_H^{-1}(\omega) \right)_{ii}^\sigma = \frac{2}{Nw} \langle \tilde{\Phi}_0 | c_{0\sigma} \mathcal{G}_D^{-1}(\omega) c_{0\sigma}^\dagger | \tilde{\Phi}_0 \rangle \times w = \frac{2}{N} \langle \tilde{\Phi}_0 | c_{0\sigma} \mathcal{G}_D^{-1}(\omega) c_{0\sigma}^\dagger | \tilde{\Phi}_0 \rangle \quad (5.7)$$

We can expand the state $c_{0\sigma}^\dagger |\tilde{\Phi}_0\rangle$ and $c_{1\sigma}^\dagger |\tilde{\Phi}_0\rangle$ in terms of a complete set of orthogonal states:

$$c_{0\sigma}^\dagger |\tilde{\Phi}_0\rangle = \sum_n C_n^0 |n\rangle, \quad c_{1\sigma}^\dagger |\tilde{\Phi}_0\rangle = \sum_n C_n^1 |n\rangle \quad (5.8)$$

where C^0 and C^1 are coefficients of the linear superposition defined by

$$C_n^0 = \langle n | c_{0\sigma}^\dagger | \tilde{\Phi}_0 \rangle, \quad C_n^1 = \langle n | c_{1\sigma}^\dagger | \tilde{\Phi}_0 \rangle. \quad (5.9)$$

Due to the translation invariance, the coefficients C_n^0 and C_n^1 are independent of the site indices. The index n actually defines a set of quantum numbers that characterize the state $|n\rangle$. For example it might be a combination of number of particles, parity and total spin angular momentum ($n \equiv n, P, S^z$). One simple way of choosing the orthogonal basis $\{|n\rangle\}$ is to take them from the eigenstates of a system comprising a Hubbard dimer and a conduction bath, decoupled from each other. The dimer will of course have 2 sites,

which means the conduction bath will have $N - 2$ sites, or $N - 2$ momentum states. The set of eigenstates that have the total number of particles (combining the dimer and the bath) equal to $N + 1$ will then form the basis in question. Since the dimer is decoupled from the bath, the total wavefunction will be a direct product of a Hubbard dimer wavefunction and a bath wavefunction.

$$|m, \alpha, \beta\rangle = \Phi_{m,\alpha}^D \otimes \Psi_{N-m+1,\beta}^B \quad (5.10)$$

α is an internal quantum number of the Hubbard dimer while β is that for the bath. The subscripts m and $N - m + 1$ label the total number of particles in each part of the wavefunction. These two labels have to add to $N + 1$. Our choice of the $|n\rangle$ is motivated by noting that the effective auxiliary model we are invoking here is that of a Hubbard dimer connected to a bath via single-particle hybridisation; the eigenstates of the isolated dimer and bath subsystems then act as the natural choices of the orthogonal bases in which to expand the wavefunction for the single-particle excitation of the interacting system $c_{0\sigma}^\dagger |\tilde{\Phi}_0\rangle$. Further, while the eigenstates ($\Phi_{m,\alpha}^D$) of the Hubbard dimer are known analytically, we can safely assume the eigenstates of the bath ($\Psi_{N-m+1,\beta}^B$) to be a simple direct product of various single-particle Fock states in k -space. We then compute the matrix element of eq.(5.7) for site i and its immediate neighbours (i.e., a given realisation of a auxiliary model). Then, using translation invariance, we demand that this matrix element is independent of the site index i . The correctness of this auxiliary model approach hinges on how close the state $|\tilde{\Phi}_0\rangle$ is to the 2-site local nature of the exact ground state of the target model (here the Hubbard model on a given lattice). Further improvement can be made by improving (i) the state $|\tilde{\Phi}_0\rangle$ for the present auxiliary model (involving a Hubbard dimer), or (ii) choosing a better auxiliary model with an "impurity" system that has more sites than two (i.e., a Bethe-Peierls improvement of the dimer auxiliary model).

Using this expansion, the matrix element of \mathcal{G} can be written as

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ii}^\sigma = \frac{2}{N} \sum_{nn'} \left(C_{n'}^0\right)^* \langle n' | \mathcal{G}_D^{-1}(\omega) | n \rangle C_n^0 \quad (5.11)$$

Since the Hubbard dimer of the ket $|n\rangle$ is an actual eigenstate, $\mathcal{G}_D^{-1}(\omega)$ will be diagonal in that basis:

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ii}^\sigma = \frac{2}{N} \sum_n |C_n^0|^2 \left(\mathcal{G}_D^{-1}(\omega)\right)_{nn} \quad (5.12)$$

Now we come to the off-diagonal Greens function for the nearest neighbour sites i and j . We will extract this using the definition. This will receive contribution from only one nearest neighbour pair in the summation of the RHS of eq. 5.6, namely that of (i, j) . This will not be a diagonal Greens function. Instead, it involves two nearest neighbour sites.

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ij}^\sigma = \frac{2}{Nw} \langle \tilde{\Phi}_0 | c_{0\sigma} \mathcal{G}_D^{-1}(\omega) c_{1\sigma}^\dagger | \tilde{\Phi}_0 \rangle = \frac{2}{Nw} \sum_n \left(C_n^0\right)^* C_n^1 \left(\mathcal{G}_D^{-1}(\omega)\right)_{nn} \quad (5.13)$$

For convenience, we define $g_n = \left(\mathcal{G}_D^{-1}(\omega)\right)_{nn}$.

The matrix elements for hole propagation are obtained similarly. Here the relevant excitations are $|\bar{i}\sigma\rangle \equiv c_{i\sigma} |\tilde{\Phi}_0\rangle$, at frequency $-\omega$. To expand these states, we choose the eigenstates with $N - 1$ total particles as the orthonormal basis:

$$c_{0\sigma} |\tilde{\Phi}_0\rangle = \sum_n \bar{C}_n^0 |\bar{n}\rangle, \quad c_{1\sigma} |\tilde{\Phi}_0\rangle = \sum_n \bar{C}_n^1 |\bar{n}\rangle \quad (5.14)$$

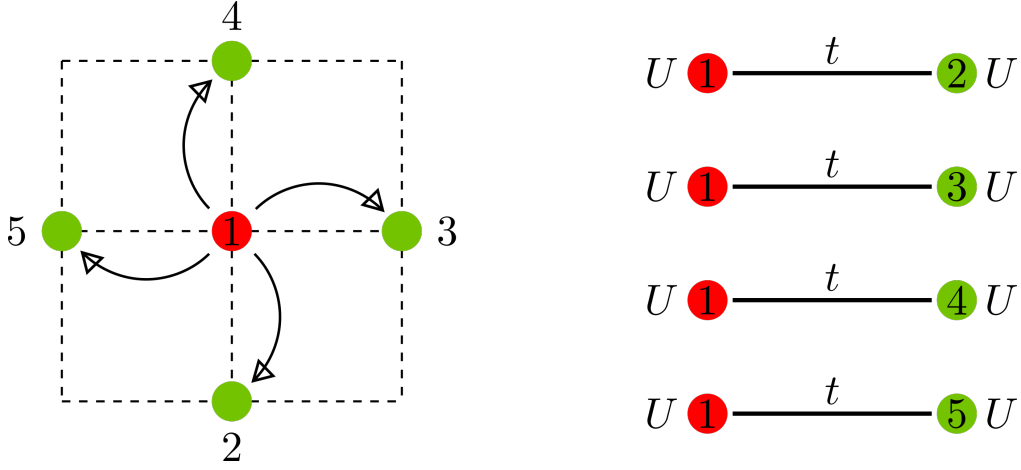


Figure 4: *Left:* Part of the lattice that is picked out by the Greens function on the LHS of eq. 5.7. *Right:* Hamiltonian whose Greens functions appear on the right hand side of same equation. The two submodels are identical.

and the counterpart for g_n , here, is

$$\overline{g}_n = \langle \overline{n} | \mathcal{G}_D^{-1}(-\omega) | \overline{n} \rangle \quad (5.15)$$

By suitably replacing the symbols, we can write down the matrix elements of $\mathcal{G}_H^{-1}(-\omega)$ for hole propagation:

$$\begin{aligned} \left(\mathcal{G}_H^{-1}(-\omega) \right)_{\overline{ii}}^{\sigma} &= \frac{2}{N} \sum_n |\overline{C}_n^0|^2 \overline{g}_n \\ \left(\mathcal{G}_H^{-1}(-\omega) \right)_{ij}^{\sigma} &= \frac{2}{Nw} \sum_n \left(\overline{C}_n^0 \right)^* \overline{C}_n^1 \overline{g}_n \end{aligned} \quad (5.16)$$

5.2 Constructing full Greens function matrix from the inverse matrix

The matrix elements $\left(\mathcal{G}_H^{-1}(\omega) \right)_{ii}^{\sigma}$ and its nearest neighbour partner can be obtained simply by inverting the internal matrix \mathcal{G}_D^{-1} . This is because,

$$A_{ij} = \sum_{mn} \langle i|n \rangle A_{nm} \langle m|j \rangle \implies A_{ij}^{-1} = \sum_{mn} \langle i|n \rangle A_{nm}^{-1} \langle m|j \rangle \quad (5.17)$$

The spectral weights remain unchanged; only the matrix element changes from A_{nm} to $(A^{-1})_{nm}$. Inverting the matrix \mathcal{G}_D is actually simple because it is diagonal in the chosen basis:

$$\left(\mathcal{G}_D^{-1} \right)_{nn} = \begin{pmatrix} g_0 & 0 & \dots & 0 \\ 0 & g_1 & & \\ & & \ddots & \\ 0 & & & g_M \end{pmatrix} \implies (\mathcal{G}_D)_{nn} = \begin{pmatrix} \frac{1}{g_0} & 0 & \dots & 0 \\ 0 & \frac{1}{g_1} & & \\ & & \ddots & \\ 0 & & & \frac{1}{g_M} \end{pmatrix} \quad (5.18)$$

This allows us to write

$$(\mathcal{G}_H(\omega))_{ii}^{\sigma} = \frac{2}{N} \sum_n |C_n^0|^2 \frac{1}{g_n}, \quad (\mathcal{G}_H(-\omega))_{ii}^{\sigma} = \frac{2}{N} \sum_n |\overline{C}_n^0|^2 \frac{1}{g_n} \quad (5.19)$$

and

$$(\mathcal{G}_H(\omega))_{ij}^\sigma = \frac{2}{Nw} \sum_n C_n^{0*} C_n^1 \frac{1}{g_n}, \quad (\mathcal{G}_H(-\omega))_{\bar{i}\bar{j}}^\sigma = \frac{2}{Nw} \sum_n \bar{C}_n^{0*} \bar{C}_n^1 \frac{1}{g_n} \quad (5.20)$$

These two expressions can be used to obtain an expression for the real space local and nearest-neighbour Greens functions:

$$\begin{aligned} G_H(\omega)_{\text{loc}} &= (\mathcal{G}_H(\omega))_{ii} - (\mathcal{G}_H(-\omega))_{\bar{i}\bar{i}} = \frac{2}{N} \sum_n \left(|C_n^0|^2 \frac{1}{g_n} - |\bar{C}_n^0|^2 \frac{1}{g_n} \right) \\ G_H(\omega)_{\text{nn}} &= (\mathcal{G}_H(\omega))_{ij} - (\mathcal{G}_H(-\omega))_{\bar{j}\bar{i}} = \frac{2}{Nw} \sum_n \left(C_n^{0*} C_n^1 \frac{1}{g_n} - C_n^{0*} \bar{C}_n^1 \frac{1}{g_n} \right) \end{aligned} \quad (5.21)$$

The momentum space Greens function can be expressed as a Fourier transform of the real space Greens functions:

$$G_H(\vec{k}, \omega) = \frac{1}{N} \sum_{\vec{r}_i, \vec{r}_j} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} G_H(|\vec{r}_i - \vec{r}_j|, \omega) \quad (5.22)$$

where \vec{r}_i is the position vector of a particular lattice site. Because of translation invariance, the real space Greens function depends only on the relative vector between any two sites. As a result, $\vec{r} = 0$ gives the local Greens function, $|\vec{r}| = a$ gives the nearest-neighbour Greens function and so on (a being the lattice spacing). As we do not have real space Greens function that are more non-local than nearest neighbour, we will attempt to obtain momentum space Greens function from these two contributions:

$$G_H(\vec{k}, \omega) \simeq \frac{1}{N} \sum_{\vec{r}_i = \vec{r}_j} G_H(\omega)_{\text{loc}} + \frac{1}{N} \sum_{|\vec{r}_i - \vec{r}_j| = a} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} G_H(\omega)_{\text{nn}} \quad (5.23)$$

The first summation produces a factor of N , while the second summation can be factorized into a sum over all sites (which again returns N) and a sum over all the primitive vectors connecting any single site with all its nearest neighbours, $\{\vec{a}_i : i \in [1, w]\}$.

$$\begin{aligned} G_H(\vec{k}, \omega) &\simeq G_H(\omega)_{\text{loc}} + G_H(\omega)_{\text{nn}} \sum_{i=1}^w e^{i\vec{k} \cdot \vec{a}_i} \\ &= G_H(\omega)_{\text{loc}} + G_H(\omega)_{\text{nn}} \xi_{\vec{k}} \\ &= \frac{2}{N} \sum_n \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} \bar{C}_n^1 \right) \frac{1}{g_n} \right] \end{aligned} \quad (5.24)$$

where we defined $\xi_{\vec{k}} \equiv \sum_{i=1}^w e^{i\vec{k} \cdot \vec{a}_i}$. For example, on a d -dimensional hypercubic lattice, we obtain

$$\xi_{\vec{k}} = \sum_{i=1}^d \left(e^{ik_i a_i} + e^{-ik_i a_i} \right) = 2 \sum_{i=1}^d \cos k_i a_i \quad (5.25)$$

On a 2D square lattice with lattice spacing a , this simplifies to

$$\begin{aligned} \xi_{\vec{q}} &= 2(\cos q_x a + \cos q_y a) \equiv \frac{-\epsilon_{\vec{q}}}{tH}, \\ \epsilon_{\vec{q}} &= -2t^H (\cos q_x a_x + \cos q_y a_y) \end{aligned} \quad (5.26)$$

where $\epsilon_{\vec{q}}$ is the tight-binding dispersion.

We can now compute the k -space spectral function $A_H(\vec{k}, \omega)$ and the real-space local spectral function $A_H(\vec{r}=0, \omega)$ as

$$\begin{aligned} A_H(\vec{k}, \omega) &= -\frac{1}{\pi} \text{Im}(G_H(\vec{k}, \omega)) = -\frac{2}{N\pi} \text{Im} \sum_n \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \\ A_H(\vec{r}=0, \omega) &= -\frac{1}{\pi} \text{Im}(G_H(\vec{r}=0, \omega)) = \frac{1}{N} \sum_{\vec{k}} A_H(\vec{k}, \omega) \end{aligned} \quad (5.27)$$

We can again use eqs.(5.26), (5.7) and (5.13) to obtain the spectral functions $A_H(\vec{k}, \omega)$ and $A_H(\vec{r}=0, \omega)$ for the Hubbard model on the 2D square lattice.

5.3 Calculation of self energy matrix from the Dyson equation

With the knowledge of the momentum-space Greens function $G_H(\vec{k}, \omega)$, we can now use Dyson's equation to calculate the self-energy for propagation of momentum excitations:

$$\Sigma(\vec{k}, \omega) = G_0(\vec{k}, \omega)^{-1} - G(\vec{k}, \omega)^{-1} \quad (5.28)$$

where the $G_0(\vec{k}, \omega)^{-1} = \omega - \epsilon_k = \omega + t^H \xi_k$ is the inverse k -space Greens function for the appropriate non-interacting tight-binding system. Substituting this as well as the full Greens function $G_H(\vec{k}, \omega)$ into Dyson's equation gives

$$\Sigma_H(\vec{k}, \omega) = \omega + t^H \xi_{\vec{k}} - \frac{N}{2} \left\{ \sum_n \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \right\}^{-1} \quad (5.29)$$

Thus, we can use eqs.(5.26), (5.7) and (5.13) to obtain the full self-energy $\Sigma(\vec{k}, \omega)$ for the Hubbard model on the 2D square lattice.

6 Some comments on writing down the orthonormal basis $\{|n\rangle\}$

As mentioned previously, for a parent model of N sites, the orthonormal basis is constructed out of those eigenstates of a decoupled dimer+bath system that have total number of particles equal to $\mathcal{N}_{\text{tot}} = \mathcal{N}_{\text{dim}} + \mathcal{N}_{\text{bath}} = N + 1$. The condition on the total number is necessary because that is also the total particle number of the state we are expanding $(c_{i\sigma}^\dagger |\tilde{\Phi}_0\rangle)$. The dimer will have 2 sites, while the rest $N - 2$ sites go into the bath.

If we are solving the trivial example of $H^H = H^D$ (that is, if we take the Hubbard dimer itself as the full Hubbard model that we are trying to solve), the bath is non-existent. The entire set of $|n\rangle$ for expanding $c_{i\sigma}^\dagger |\tilde{\Phi}_0\rangle$ is then made up by the $\mathcal{N} = N + 1 = 3, S^z = \frac{1}{2}\sigma$ eigenstates of H^D . There are two of those; these two make up the entire orthonormal basis in which we can expand the single-particle excitations:

$$\{|n\rangle\} = |3 \pm \sigma\rangle \quad (6.1)$$

Similarly, for expanding the hole excitations $c_{i\sigma} |\tilde{\Phi}_0\rangle$, we will instead choose the $\mathcal{N} = N - 1 = 1, S^z = -\frac{1}{2}\sigma$ eigenstates of H^D . There are again two of those:

$$\{|\bar{n}\rangle\} = |1 \pm -\sigma\rangle \quad (6.2)$$

For a more general $N(> 2)$ -site model, there will be a bath of $N - 2$ momentum states. These momentum states are labelled as k_1, k_2, \dots, k_{N-2} . Let us designate the set of eigenstates of the Hubbard dimer as $\{|\Phi_i^D\rangle\}$ and those of the bath as $\{|\Psi_{j,\nu^j}^B\rangle\}$. Since the bath is non-interacting, those eigenstates can be written down easily:

$$\{|\Psi_{j,\nu^j}^B\rangle\} = \left\{ \bigotimes_{i=1}^j \hat{n}_{\nu_i^j} = 1 : \begin{array}{l} j \in [0, 2N - 4] \\ \nu^j \in \text{all subsets of length } j \text{ of the set } [k_1 \uparrow, k_1 \downarrow, k_2 \uparrow, \dots, k_{N-2} \uparrow, k_{N-2} \downarrow] \end{array} \right\} \quad (6.3)$$

j defines the number of occupied states in a particular eigenstate of the conduction bath. The string ν^j runs over all possible set of quantum numbers of a particular length j . For example, if we have 3 momentum states in the bath k_1, k_2, k_3 , then ν^2 would take the values

$$\begin{aligned} \{\nu^2\} = & (k_1 \uparrow, k_1 \downarrow), (k_1 \uparrow, k_2 \uparrow), (k_1 \uparrow, k_2 \downarrow), (k_1 \uparrow, k_3 \uparrow), (k_1 \uparrow, k_3 \downarrow), (k_1 \downarrow, k_2 \uparrow), (k_1 \downarrow, k_2 \downarrow), \\ & (k_1 \downarrow, k_3 \uparrow), (k_1 \downarrow, k_3 \downarrow), (k_2 \uparrow, k_2 \downarrow), (k_2 \uparrow, k_3 \uparrow), (k_2 \uparrow, k_3 \downarrow), (k_2 \downarrow, k_3 \uparrow), (k_2 \downarrow, k_3 \downarrow), \\ & (k_3 \uparrow, k_3 \downarrow) \end{aligned} \quad (6.4)$$

The $j = 0$ case means the bath is empty. The general complete set of orthonormal kets is given by

$$\{|n\rangle\} = \sum_{i=1}^{16} \sum_{j=0}^{N-2} \sum_{\nu^j} |\Phi_i^D\rangle \otimes |\Psi_{j,\nu^j}^B\rangle \quad (6.5)$$

The first twp sums are unconstrained. The index i runs through all 16 eigenstates of the Hubbard dimer, the index j runs through all the possible total number of particles the eigenstate of the bath can have. For each value of j , the string ν^j runs through all possible combinations of length j from the complete set of quantum numbers $\{k\sigma\}$.

7 Calculating the coefficients $C_n^{0,1}$ and $\bar{C}_n^{0,1}$ in practice

The expressions for $C_n^{0,1}$ and $\bar{C}_n^{0,1}$, as mentioned above, involve taking the projection of the exact ground state of the full Hubbard model, $|\tilde{\Phi}_0\rangle$, against the chosen orthogonal basis $|n\rangle$.

1. Since the full Hubbard model ground state wavefunctions are not readily available, one can, as the simplest approximation, assume the ground state has the form

$$|\tilde{\Phi}_0\rangle = \sum_{\langle \hat{i}\hat{j} \rangle} |\Phi_{\hat{i}\hat{j}}^D\rangle \otimes |\Psi_{\hat{i},\hat{j}}^{\hat{z},\hat{z}}\rangle \quad (7.1)$$

$|\Phi_{\hat{i}\hat{j}}^D\rangle$ would be the ground state of the Hubbard dimer with i, j creating the two sites of the dimer, while $|\Psi_{\hat{i},\hat{j}}^{\hat{z},\hat{z}}\rangle$ would be the wavefunction involving the rest of the sites. This of course assumes that the two sets (i, j) and $(a, b, \dots, h, k, \dots)$ are not entangled, and is not true in general. With this assumption, g_0 and g_1 become related to the inverse Greens functions of the Hubbard dimer. Such a choice of the wavefunction is motivated by the fact that in the auxiliary system we chose, the bath had only a diagonal interaction; there was no off-diagonal two particle scattering term. It is further enforced when we extract the zero mode of the entire bath (i.e., we keep just the zeroth site). The zeroth site, along with the impurity, then forms the $|\Phi\rangle$ part of the wavefunction. This will allow for analytic insight, but at the cost of accuracy as discussed above.

2. Another way of approaching the problem is to obtain the ground state wavefunction of a Hubbard model numerically for several values of U^H and t^H , and then computing the matrix elements of H^D against this wavefunction to obtain a family of (g_0, g_1) . This brings the numerical accuracy for a given finite-sized lattice realisation of the Hubbard model. However, this also means we lose any analytical insight into the structure of g_0 and g_1 .
3. The most promising approach of calculating g_0 and g_1 is by systematically improving the required ground state wavefunctions as follows. We obtain numerically the ground state wavefunction of a Hamiltonian that has not just the Hubbard dimer, but also a bath (with dispersion) that connects to both the sites of the dimer:

$$H_{\text{bath}}^D(\tilde{i}, \tilde{j}) = \underbrace{U \left(\tau_{\tilde{i}\uparrow} \tau_{\tilde{i}\downarrow} + \tau_{\tilde{j}\uparrow} \tau_{\tilde{j}\downarrow} \right)}_{\text{Hubbard dimer}} - t \sum_{\sigma} \left(c_{i\sigma}^{\dagger} c_{\tilde{j}\sigma} + \text{h.c.} \right) + \underbrace{\sum_{k\sigma} \epsilon_{k\sigma} \tau_{k\sigma}}_{\text{bath}} - t \underbrace{\sum_{k\sigma} \left(c_{i\sigma}^{\dagger} c_{k\sigma} + c_{\tilde{j}\sigma}^{\dagger} c_{k\sigma} + \text{h.c.} \right)}_{\text{bath-dimer hybridisation}} \quad (7.2)$$

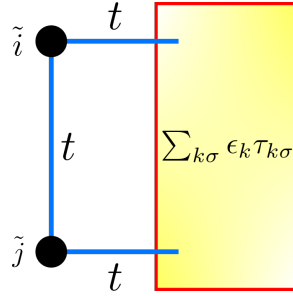


Figure 5: Hubbard dimer with dispersion that connects to both sites

By systematically increasing the number of momentum states in the bath dispersion, we can systematically improve the numerical computation of the ground state wavefunction. From here, we can compute matrix elements of H^D , and hence the functions g_0 and g_1 . The presence of the bath can be understood as follow. In the absence of a bath, i.e., we have just a Hubbard dimer, an electron can at most hop between the two sites and lead to the wavefunction in eq. 7.1. However, with a single particle hopping term connecting the dimer to a bath, an electron can also journey between the two sites of the bath via the bath. This leads to entanglement between the dimer's sites and those in the bath; this was clearly ignored in the ground state wavefunction eq. 7.1. The introduction of the bath dispersion offers the possibility that we can capture a site diagonal spectral function of the three peak form, because we have previously seen such a spectral function in the fixed point of the URG analysis of the SIAM (where the fixed point effective Hamiltonian was an Anderson molecule with dispersion). If this can be found, then a metal-insulator transition of the full Hubbard model can perhaps be captured by studying the spectral functions of the bath-coupled Hubbard dimer.

4. Another improvement can be made by introducing a self-energy $\Sigma(k, \omega)$ into the bath dispersion. This introduces correlation within the bath. The Hamiltonian that we would need to solve would be the same as eq. 7.2, but with ϵ_k replaced by $\tilde{\epsilon}_k \equiv \epsilon_k + \Sigma(k, \omega)$. The self-energy $\Sigma(k, \omega)$ will have to be chosen depending on the phase we want to look at (e.g., metal, insulator etc.). With a Σ that is singular near the Fermi surface at $\omega \rightarrow 0$, the dispersion will become gapped and the phase will be insulating. In such a situation, there are no low-energy bath excitations within a given energy window proximate to its putative Fermi energy. This will localise the bath electrons, as well as confine all journeys between the two sites of the dimer to only the direct path. This is an indication of the localisation of electrons in the Hubbard model to holon-doublon excitations on

nearest neighbour sites. In such a circumstance, eq. 7.1 will be a very good approximation to the actual insulating ground state of the Hubbard model. On the other hand, if we use a self energy that vanishes near the Fermi surface ($\Sigma(\omega) \sim \omega^2$, i.e., a Fermi liquid bath), then we expect to end up in a metallic phase of the Hubbard model. This is simply due to the possibility of holons and doublons now dispersing throughout the lattice, and be concomitant with the presence of a pole in the single-particle Greens function $G(k, \omega)$ of the Hubbard model. Introducing the self energy therefore gives us a larger variety of wavefunctions and features to work with. Further, this appears to be in line with the original proposals offered by Mott and Kohn for the Mott metal insulator transition as the localisation-delocalisation transition of holon-doublon pairs. With regards to the transition itself, the precise form of the bath $\Sigma(k, \omega)$ (or spectral function) remains to be determined.

Once we have chosen a test Hamiltonian whose wavefunction we can calculate, we can use that to obtain the ground state energy of this state. The wavefunction will act as our $|0\rangle$ and the ground state energy will be our E_{GS} . We can then substitute these into the Lehmann representation form of the Greens function, and calculate the matrix elements $\mathcal{G}_D(\omega)_{\nu\nu'}$ and $\mathcal{G}_D(-\omega)_{\bar{\nu}\bar{\nu}'}$ for the Hubbard dimer Hamiltonian. Each set will form a 2×2 matrix, and we can invert them to obtain $\mathcal{G}_D(\omega)$, and then the matrix elements of this inverted matrix will give all the parameters g_0 through \bar{g}_1 .

8 Analytic consistency checks

8.1 Single-particle Greens function and self energy for the Hubbard dimer

The simplest test involves choosing $H^H = H^D$ and then calculating the momentum space Greens function at $k = 0$, $G(k = 0, \uparrow)$, for the Hubbard dimer ($N = 2, w = 1$). The discrete set of momenta are $\{\vec{k}_n\} = 0, \frac{\pi}{a}$. For $k = 0$, we have

$$\xi_{\vec{k}=0} = e^{i\vec{k}r} = 1 \quad (8.1)$$

Substituting this into eq. 5.24 gives

$$G(k = 0, \uparrow) = \sum_n \left[\left(|C_n^0|^2 + C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + C_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \quad (8.2)$$

The expansion in terms of the exact eigenstates takes the form:

$$\begin{aligned} c_{0\uparrow}^\dagger |\tilde{\Phi}_0\rangle &= x |3+ \uparrow\rangle + y |3- \uparrow\rangle, \quad c_{1\uparrow}^\dagger |\tilde{\Phi}_0\rangle = x |3+ \uparrow\rangle - y |3- \uparrow\rangle \\ c_{0\uparrow} |\tilde{\Phi}_0\rangle &= y |1+ \downarrow\rangle + x |1- \downarrow\rangle, \quad c_{1\uparrow} |\tilde{\Phi}_0\rangle = y |1+ \downarrow\rangle - x |1- \downarrow\rangle \end{aligned} \quad (8.3)$$

where $|(3, 1) \pm (\uparrow, \downarrow)\rangle$ are the $N = (3, 1), S^z = (+\frac{1}{2}, -\frac{1}{2})$ eigenstates of even (+) and odd (-) parity:

$$\begin{aligned} H^D |3\pm \uparrow\rangle &= \pm t |3\pm \uparrow\rangle \\ H^D |1\pm \downarrow\rangle &= \mp t |1\pm \downarrow\rangle \end{aligned} \quad (8.4)$$

and $x = \frac{a_2 - a_1}{2}, y = \frac{a_2 + a_1}{2}$. The orthogonal basis is therefore

$$\begin{aligned} \{|n\rangle\} &= |3+ \uparrow\rangle, |3- \uparrow\rangle \\ \{|\bar{n}\rangle\} &= |1+ \downarrow\rangle, |1- \downarrow\rangle \end{aligned} \quad (8.5)$$

The coefficients can thus be determined:

$$C_\pm^0 = \langle 3\pm \uparrow | c_{0\uparrow}^\dagger | \tilde{\Phi}_0 \rangle = x, y$$

$$\begin{aligned}
C_{\pm}^1 &= \langle 3\pm \uparrow | c_{1\uparrow}^\dagger | \tilde{\Phi}_0 \rangle = x, -y \\
\bar{C}_{\pm}^0 &= \langle 1\pm \downarrow | c_{0\uparrow} | \tilde{\Phi}_0 \rangle = y, x \\
\bar{C}_{\pm}^1 &= \langle 1\pm \downarrow | c_{1\uparrow} | \tilde{\Phi}_0 \rangle = y, -x \\
g_{\pm} &= \langle 3\pm \uparrow | (\omega + E_{GS} - H^D) | 3\pm \uparrow \rangle = \omega + E_{GS} \mp t \\
\bar{g}_{\pm} &= \langle 1\pm \downarrow | (-\omega + E_{GS} - H^D) | 1\pm \downarrow \rangle = -\omega + E_{GS} \pm t
\end{aligned}$$

We can see that $|C_-^0|^2 + C_-^{0*} C_-^1 = y^2 - y^2 = 0$ and $|\bar{C}_-^0|^2 + \bar{C}_-^{0*} \bar{C}_-^1 = x^2 - x^2 = 0$. So we do not need to consider those terms. With this preparation, we can now calculate the Greens function:

$$G(k=0, \omega) = \left(|C_+^0|^2 + C_+^{0*} C_+^1 \right) \frac{1}{g_+} - \left(|\bar{C}_+^0|^2 + \bar{C}_+^{0*} \bar{C}_+^1 \right) \frac{1}{\bar{g}_+} = \frac{2x^2}{\omega + E_{GS} - t} - \frac{2y^2}{-\omega + E_{GS} + t} \quad (8.6)$$

The final step is to recognize that $2x^2 = \frac{a_1^2 + a_2^2 - 2a_1 a_2}{2} = \frac{1}{2} - \frac{2t}{\Delta}$, $2y^2 = \frac{a_1^2 + a_2^2 + 2a_1 a_2}{2} = \frac{1}{2} + \frac{2t}{\Delta}$ and $E_{GS} = -\frac{\Delta}{2}$. Then,

$$G(k=0, \omega) = \frac{\frac{1}{2} - \frac{2t}{\Delta}}{\omega - \frac{\Delta}{2} - t} - \frac{\frac{1}{2} + \frac{2t}{\Delta}}{-\omega - \frac{\Delta}{2} + t} = \frac{\frac{1}{2} - \frac{2t}{\Delta}}{\omega - \frac{\Delta}{2} - t} + \frac{\frac{1}{2} + \frac{2t}{\Delta}}{\omega + \frac{\Delta}{2} - t} \quad (8.7)$$

8.2 On the Bethe lattice

Another test involves considering the case of infinite number of nearest neighbours $w \rightarrow \infty$ (the coordination number, and effectively the dimensionality). Here, as has been argued in the DMFT literature, the correct scaling of the t^H hopping parameter is $t^H \rightarrow t^H / \sqrt{w}$ such that the kinetic energy of the associated tight-binding lattice model is finite. This allows for the competition between the kinetic and potential terms of the Hamiltonian to drive a metal-insulator transition in the limit of $w \rightarrow \infty$ as well. Further, it has been argued in the DMFT literature that the Greens function matrix of the Hubbard model on the Bethe lattice with $w \rightarrow \infty$ becomes purely local (i.e., it has vanishing inter-site matrix elements). We can also see this from eqs.(5.20)- the nearest-neighbour inverse Greens function vanishes in the limit of $w \rightarrow \infty$:

$$(\mathcal{G}_H(\omega))_{ij}^\sigma = \frac{2}{Nw} \sum_n \bar{C}_n^{0*} \bar{C}_n^1 \frac{1}{g_n} \implies \lim_{w \rightarrow \infty} (\mathcal{G}_H(\omega))_{ij}^\sigma \rightarrow 0 \quad (8.8)$$

There we used the fact since at half-filling on an $SU(2)$ symmetric mode, we expect $\langle \hat{n}_{i\uparrow} \rangle = \frac{1}{2}$, the orthonormal expansion of $c_{i\sigma}^\dagger | \tilde{\Phi}_0 \rangle = \sum_n C_n^i | n \rangle$ to be constrained to $\sum_n |C_n^i|^2 = \frac{1}{2}$, such that the only term that scales with w is w itself. This result then implies that G^H matrix has no k dependence.

In this limit, the self-energy also simplifies:

$$\begin{aligned}
\lim_{w \rightarrow \infty} \Sigma_H(\vec{k}, \omega) &= \omega + t^H \xi_{\vec{k}} - \frac{N}{2} \left\{ \sum_n \lim_{w \rightarrow \infty} \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \frac{1}{g_n} \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} \bar{C}_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \right\}^{-1} \\
&= \omega + t^H \xi_{\vec{k}} - \frac{N}{2} \frac{1}{\sum_n \left[\frac{|C_n^0|^2}{g_n} - \frac{|\bar{C}_n^0|^2}{\bar{g}_n} \right]}
\end{aligned} \quad (8.9)$$

We can now see that even in the limit of $w \rightarrow \infty$, the competition between g_0 (the on-site repulsion) and the hopping related kinetic energy ($t^H \xi_{\vec{k}}$) can lead to a metal-insulator transition.

9 Future goals

1. Obtain the metal insulator transition of the 2D Hubbard model on the square lattice from our formalism. Compare with what is obtained from DMFT and its improvements. Also, determine the nature of the bath $\Sigma(k, \omega)$ for the transition point.
2. Once the zero temperature Mott metal-insulator transition is observed, we will investigate its nature.
3. While we have provided expressions for the single particle Greens functions of the N -site Hubbard model from their equivalent single particle Greens functions of the Hubbard dimer, we expect that eq.(5.6) holds quite generally for the two-particle Greens function sector as well. We will provide these expressions at a later point in time. More specifically, we will calculate the Greens functions for holon-doublon and spinon-spinon excitations as they are likely to contain more information regarding the ground state.
4. It is also important to benchmark the ground state energy and double occupancy obtained from this method against the ground state wavefunction obtained from exact diagonalisation of small lattices and finite size scaling.
5. It should also prove instructive to investigate the nature of many-particle entanglement in the ground state wavefunction of various phases, and look for signs of a quantum liquid.
6. Once we have a handle on the zero temperature features, we intend to compute Greens functions at non zero temperatures.
7. This method can also be extended to various other models of strong correlation:
 - (a) Heisenberg model, by starting from a Kondo model effective Hamiltonian
 - (b) Periodic Anderson model, by starting from a SIAM with a dispersive bath
 - (c) Periodic Kondo model, by starting from a Kondo model with a dispersive bath
 - (d) Hubbard-Heisenberg model, by starting from a generalized Anderson molecule (Anderson molecule with two-particle spin and charge interactions between the two sites)

Appendix: Spectra of Hubbard dimer

Here we document the spectrum of the Hamiltonian in eqs. 3.2.

eigenstate	symbol	eigenvalue
$ 0, 0\rangle$	$ 0\rangle$	$\frac{U^H}{2}$
$\frac{1}{\sqrt{2}} (\sigma, 0\rangle \pm 0, \sigma\rangle)$	$ 0\sigma_{\pm}\rangle$	$\mp t^H$
$ \sigma, \sigma\rangle$	$ \sigma\sigma\rangle$	$-\frac{U^H}{2}$
$\frac{1}{\sqrt{2}} (\uparrow, \downarrow\rangle + \downarrow, \uparrow\rangle)$	$ ST\rangle$	$-\frac{U^H}{2}$
$\frac{1}{\sqrt{2}} (2, 0\rangle - 0, 2\rangle)$	$ CS\rangle$	$\frac{U^H}{2}$
$a_1(U^H, t^H) \frac{1}{\sqrt{2}} (\uparrow, \downarrow\rangle - \downarrow, \uparrow\rangle) + a_2(U^H, t^H) \frac{1}{\sqrt{2}} (2, 0\rangle + 0, 2\rangle)$	$ -\rangle$	$-\frac{1}{2}\Delta(U^H, t^H)$
$-a_2(U^H, t^H) \frac{1}{\sqrt{2}} (\uparrow, \downarrow\rangle - \downarrow, \uparrow\rangle) + a_1(U^H, t^H) \frac{1}{\sqrt{2}} (2, 0\rangle + 0, 2\rangle)$	$ +\rangle$	$\frac{1}{2}\Delta(U^H, t^H)$
$\frac{1}{\sqrt{2}} (\sigma, 2\rangle \pm 2, \sigma\rangle)$	$ 2\sigma_{\pm}\rangle$	$\pm t^H$
$ 2, 2\rangle$	$ 4\rangle$	$\frac{U^H}{2}$

Table 1: Spectrum of Hubbard dimer at half-filling

Appendix: Local Greens function for the Hubbard dimer

From the spectral representation, we have the following expression for the local Greens function for the Hubbard dimer at site 0:

$$G_{D,00}^{\sigma}(\omega) = \frac{1}{Z} \sum_{m,n} ||\langle m| c_{i\sigma} |n\rangle||^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \frac{1}{\omega + E_m - E_n} \quad (9.1)$$

m, n sum over the exact eigenstates. E_m, E_n are the corresponding energies. We are interested in the $T \rightarrow 0$ Greens function. In that limit, all exponentials except that for the ground state E_{gs} will die out. The exponential inside the summation will then cancel the exponential in the partition function.

$$\begin{aligned} G_{D,00}^{\sigma}(\omega, T \rightarrow 0) &= \sum_n \left[||\langle GS| c_{i\sigma} |n\rangle||^2 \frac{1}{\omega + E_{GS} - E_n} + ||\langle n| c_{i\sigma} |GS\rangle||^2 \frac{1}{\omega + E_n - E_{GS}} \right] \\ &= \sum_n \left[||\langle n| c_{i\sigma}^{\dagger} |GS\rangle||^2 \frac{1}{\omega + E_{GS} - E_n} + ||\langle n| c_{i\sigma} |GS\rangle||^2 \frac{1}{\omega + E_n - E_{GS}} \right] \end{aligned} \quad (9.2)$$

The ground state $|GS\rangle$ is just the state $|-\rangle$ in the table 1. We will choose to look at $\sigma = \uparrow$. Then,

$$\begin{aligned} c_{1\uparrow} |-\rangle &= \frac{a_1}{\sqrt{2}} |0, \downarrow\rangle + \frac{a_2}{\sqrt{2}} |\downarrow, 0\rangle \\ c_{1\uparrow}^{\dagger} |-\rangle &= -\frac{a_1}{\sqrt{2}} |2, \uparrow\rangle + \frac{a_2}{\sqrt{2}} |\uparrow, 2\rangle \end{aligned} \quad (9.3)$$

The set of states $|n\rangle$ that give non-zero inner product $|GS\rangle$ are therefore

$$\begin{aligned}\{|n\rangle\} &= |0 \downarrow_{\pm}\rangle \\ ||\langle n| c_{\uparrow\sigma} |GS\rangle||^2 &= \frac{1}{4} (a_2 \pm a_1)^2 = \frac{1}{4} (1 \pm 2a_1 a_2) \\ \{E_n\} &= \mp t\end{aligned}\tag{9.4}$$

for the second inner product, and

$$\begin{aligned}\{|n\rangle\} &= |2 \uparrow_{\pm}\rangle \\ ||\langle n| c_{\uparrow\sigma}^\dagger |GS\rangle||^2 &= \frac{1}{4} (a_2 \mp a_1)^2 = \frac{1}{4} (1 \mp 2a_1 a_2) \\ \{E_n\} &= \pm t\end{aligned}\tag{9.5}$$

for the first. The Greens function is therefore

$$G_{D,00}^\uparrow(\omega, T \rightarrow 0) = \left(\frac{1}{2} + \frac{2t}{\Delta}\right) \frac{\omega}{\omega^2 - \left(t - \frac{\Delta}{2}\right)^2} + \left(\frac{1}{2} - \frac{2t}{\Delta}\right) \frac{\omega}{\omega^2 - \left(t + \frac{\Delta}{2}\right)^2} = G_{D,00}^\downarrow(\omega, T \rightarrow 0) .\tag{9.6}$$

In the atomic limit ($t = 0$), the Greens function simplifies to

$$G_{D,00}^\uparrow(\omega, T \rightarrow 0) \Big|_{\text{atomic}} = \frac{\omega}{\omega^2 - \frac{1}{4}U^2}\tag{9.7}$$

In the atomic limit, the singly-occupied state has zero energy:

$$E_1(t = 0) = \langle 1, 0 | \left(U\tau_{0\uparrow}\tau_{0\downarrow} + U\tau_{1\uparrow}\tau_{1\downarrow} \right) | 1, 0 \rangle = 0\tag{9.8}$$

We can write the atomic limit Greens function in terms of this energy and the self energy:

$$G_{D,00}^\uparrow(\omega, T \rightarrow 0) \Big|_{\text{atomic}} = \frac{1}{\omega - E_1(t = 0) - \Sigma(t = 0)} = \frac{1}{\omega - 0 - \frac{U^2}{4\omega}}\tag{9.9}$$

The self energy in the atomic limit can be read off as

$$\Sigma(t = 0) = \frac{U^2}{4\omega}\tag{9.10}$$

The site local spectral function can also be calculated from the local Greens function:

$$\begin{aligned}A(0 \uparrow, \omega) &= -\frac{1}{\pi} \text{Im } G_{D,00}^\uparrow(\omega) \\ &= \left(\frac{1}{4} - \frac{t}{\Delta}\right) \left[\delta\left(\omega - \frac{1}{2}\Delta - t\right) + \delta\left(\omega + \frac{1}{2}\Delta + t\right) \right] \\ &\quad + \left(\frac{1}{4} + \frac{t}{\Delta}\right) \left[\delta\left(\omega - \frac{1}{2}\Delta + t\right) + \delta\left(\omega + \frac{1}{2}\Delta - t\right) \right] \\ &= A(0 \downarrow, \omega) .\end{aligned}\tag{9.11}$$

Finally, the inter-site Greens function for the Hubbard dimer is given by

$$G_{D,01}^\uparrow(\omega, T \rightarrow 0) = \left(\frac{1}{2} + \frac{2t}{\Delta}\right) \frac{t - \frac{\Delta}{2}}{\omega^2 - \left(t - \frac{\Delta}{2}\right)^2} + \left(\frac{1}{2} - \frac{2t}{\Delta}\right) \frac{t + \frac{\Delta}{2}}{\omega^2 - \left(t + \frac{\Delta}{2}\right)^2} = G_{D,01}^\downarrow(\omega, T \rightarrow 0) .\tag{9.12}$$

Using the diagonal and off-diagonal real space Greens functions, we can now compute the momentum-space Greens functions. The two momentum states are $ka = 0, \pi$. By Fourier transforming, these two Greens functions can be written as

$$\begin{aligned} G(k=0, \sigma) &= \sum_r e^{ikr} G(r, \sigma) = G(r=0, \sigma) + G(r=a, \sigma) = \frac{1/2 + 2t/\Delta}{\omega - t + \Delta/2} + \frac{1/2 - 2t/\Delta}{\omega - t - \Delta/2} \\ G(k=\pi, \sigma) &= \sum_r e^{ikr} G(r, \sigma) = G(r=0, \sigma) - G(r=a, \sigma) = \frac{1/2 + 2t/\Delta}{\omega + t - \Delta/2} + \frac{1/2 - 2t/\Delta}{\omega + t + \Delta/2} \end{aligned} \quad (9.13)$$

Appendix: Relation between single-particle Greens function and the Greens function operator ($T = 0$)

The single-particle Greens function is defined as the solution of the equation:

$$(i\partial_t - H(\vec{r})) G(\vec{r}, \vec{r}', t) = \delta(\vec{r} - \vec{r}') \quad (9.14)$$

and is given by the expression

$$G(\vec{r}, \vec{r}', t) = -i\theta(t) \left\langle \left\{ c(\vec{r}, t) c^\dagger(\vec{r}', 0) \right\} \right\rangle \quad (9.15)$$

This solution can be written in the Lehmann representation and at $T = 0$ as

$$G(\vec{r}\sigma, \vec{r}'\sigma, \omega) = \sum_n \left[\frac{\langle GS | c(\vec{r}, \sigma) | n \rangle \langle n | c^\dagger(\vec{r}', \sigma) | GS \rangle}{\omega + E_{GS} - E_n} + \frac{\langle GS | c^\dagger(\vec{r}', \sigma) | n \rangle \langle n | c(\vec{r}, \sigma) | GS \rangle}{\omega + E_n - E_{GS}} \right] \quad (9.16)$$

The sum is over the exact eigenstates of the Hamiltonian. In what follows, we will represent $\vec{r}, \sigma \equiv \nu$ and $\vec{r}', \sigma \equiv \nu'$.

$$\begin{aligned} G(\nu, \nu', \omega) &= \sum_n \left[\frac{\langle GS | c(\nu) | n \rangle \langle n | c^\dagger(\nu') | GS \rangle}{\omega + E_{GS} - E_n} + \frac{\langle GS | c^\dagger(\nu') | n \rangle \langle n | c(\nu) | GS \rangle}{\omega + E_n - E_{GS}} \right] \\ &= \langle GS | c(\nu) \frac{1}{\omega + E_{GS} - H} c^\dagger(\nu') | GS \rangle + \langle GS | c^\dagger(\nu') \frac{1}{\omega + H - E_{GS}} c(\nu) | GS \rangle \end{aligned} \quad (9.17)$$

If we now define a Greens function operator

$$\mathcal{G}(\omega, H) = \frac{1}{\omega - (H - E_{GS})} \quad (9.18)$$

we can write the single-particle Greens function as a sum of the matrix elements of this operator:

$$G(\nu, \nu', \omega) = \langle \nu | \mathcal{G}(\omega, H) | \nu' \rangle - \langle \bar{\nu}' | \mathcal{G}(-\omega, H) | \bar{\nu} \rangle = \mathcal{G}(\omega, H)_{\nu, \nu'} - \mathcal{G}(-\omega, H)_{\bar{\nu}', \bar{\nu}} \quad (9.19)$$

where we have defined the states $|\nu\rangle \equiv c^\dagger(\nu) | GS \rangle$ and $|\bar{\nu}\rangle \equiv c(\nu) | GS \rangle$. The two matrix elements can also be represented in their individual spectral representations:

$$\begin{aligned} \mathcal{G}(\omega, H)_{\nu, \nu'} &= \sum_n \frac{\langle GS | c(\nu) | n \rangle \langle n | c^\dagger(\nu') | GS \rangle}{\omega + E_{GS} - E_n} \\ \mathcal{G}(\omega, H)_{\bar{\nu}', \bar{\nu}} &= \sum_n \frac{\langle GS | c^\dagger(\nu') | n \rangle \langle n | c(\nu) | GS \rangle}{\omega + E_{GS} - E_n} \end{aligned} \quad (9.20)$$

10 Appendix: Writing single-particle excitations of ground state in terms of $N = 3, S^z = \frac{1}{2}$ eigenstates

The excited state $c_{0\uparrow}^\dagger |\text{GS}\rangle$ can actually be written in terms of the $N = 3, S^z = +\frac{1}{2}$ eigenstates $|3\pm \uparrow\rangle$ defined in table 1.

$$|3\pm \uparrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow, 2\rangle \pm |2, \uparrow\rangle), \quad H^D |3\pm \uparrow\rangle = \pm t |3\pm \uparrow\rangle \quad (10.1)$$

In terms of these eigenstates, we can write

$$\begin{aligned} c_{0\uparrow}^\dagger |\text{GS}\rangle &= c_{0\uparrow}^\dagger [a_1 |SS\rangle + a_2 |CT\rangle] \\ &= a_2 \frac{1}{\sqrt{2}} |\uparrow, 2\rangle - a_1 \frac{1}{\sqrt{2}} |2, \uparrow\rangle \\ &= (x + y) \frac{1}{\sqrt{2}} |\uparrow, 2\rangle + (x - y) \frac{1}{\sqrt{2}} |2, \uparrow\rangle \\ &= x |3+ \uparrow\rangle + y |3- \uparrow\rangle \end{aligned} \quad (10.2)$$

where $x + y \equiv a_2$ and $x - y \equiv -a_1$. Similarly, for the other site excitation, we can write

$$\begin{aligned} c_{1\uparrow}^\dagger |\text{GS}\rangle &= c_{1\uparrow}^\dagger [a_1 |SS\rangle + a_2 |CT\rangle] \\ &= a_2 \frac{1}{\sqrt{2}} |2, \uparrow\rangle - a_1 \frac{1}{\sqrt{2}} |\uparrow, 2\rangle \\ &= (x + y) \frac{1}{\sqrt{2}} |2, \uparrow\rangle + (x - y) \frac{1}{\sqrt{2}} |\uparrow, 2\rangle \\ &= x |3+ \uparrow\rangle - y |3- \uparrow\rangle \end{aligned} \quad (10.3)$$

Solving for x and y gives

$$x = \frac{a_2 - a_1}{2}, \quad y = \frac{a_2 + a_1}{2} \quad (10.4)$$

Similarly, we can also write the single-hole excitation $c_{0\uparrow} |\text{GS}\rangle$ in terms of the $N = 1, S^z = -\frac{1}{2}$ eigenstates, $|1\pm \downarrow\rangle$:

$$|1\pm \downarrow\rangle = \frac{1}{\sqrt{2}} (|\downarrow, 0\rangle \pm |0, \downarrow\rangle), \quad H^D |1\pm \downarrow\rangle = \mp t |1\pm \downarrow\rangle \quad (10.5)$$

$$\begin{aligned} c_{0\uparrow} |\text{GS}\rangle &= a_1 \frac{1}{\sqrt{2}} |0, \downarrow\rangle + a_2 \frac{1}{\sqrt{2}} |\downarrow, 0\rangle = y |1+ \downarrow\rangle + x |1- \downarrow\rangle \\ c_{1\uparrow} |\text{GS}\rangle &= a_1 \frac{1}{\sqrt{2}} |\downarrow, 0\rangle + a_2 \frac{1}{\sqrt{2}} |0, \downarrow\rangle = y |1+ \downarrow\rangle - x |1- \downarrow\rangle \end{aligned} \quad (10.6)$$

11 Appendix: Matrix elements of G^{-1} between single-particle momentum excitations, for the Hubbard dimer

$$G^{-1} \equiv \omega + E_{\text{GS}} - H_D \quad (11.1)$$

The particle excitation momentum space kets are $|k_0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$, $|k_\pi\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$. Therefore,

$$\begin{aligned} \left(G^{-1}\right)_{k_0 k_0} &= \frac{1}{2} (\langle 0| + \langle 1|) (\omega + E_{\text{GS}} - H_D) (|0\rangle + |1\rangle) \\ &= \frac{1}{2} (2x \langle +|) (\omega + E_{\text{GS}} - H_D) (2x |+\rangle) \\ &= 2x^2 (\omega + E_{\text{GS}} - t) \end{aligned} \quad (11.2)$$

At the final step, we used $\langle +, +\rangle = 1$ and $\langle +|H_D|+\rangle = t$.

References

- [1] Lucia Reining Richard M. Martin and David M. Ceperley. *Interacting Electrons-Theory and Computational Approaches*. Cambridge University Press, 2016.
- [2] Eva Pavarini. Dynamical mean-field theory for materials, September 2019.