Exact Diagonalization

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2 Review of Second Quantization

Before delving into correlated electron models, we will briefly review the formalism of second quantization. Second quantization provides a convenient way to describe N-particle states in many-body quantum physics.

2.1 Single particle Hilbert space

Suppose he have a Hilbert space $\mathcal{H}_1$ describing a single-particle subject to a Hamiltonian $\hat{\mathcal{H}}$. The time-independent Schrödinger equation for this system is:

$$\hat{\mathcal{H}} |\lambda\rangle = E_\lambda |\lambda\rangle . \tag{2.1}$$

Here, $|\lambda\rangle$ denotes an eigenstate of the Hamiltonian and λ is a short hand notation which specifies the full set of quantum numbers that identify the eigenstate. For example, if the system was a single spin 1/2 electron moving in a 3D box, the quantum numbers would be the wavector $\mathbf{k}$ and the spin σ: $|\lambda\rangle = |\mathbf{k}, \sigma\rangle$. If the was system was a positively charged particle subject to a Coulomb potential, the good quantum numbers would be $|n, l, m_l\rangle$. We refer to such a set of quantum numbers as a single-particle state.

Since $\hat{\mathcal{H}}$ is Hermitian, its eigenvectors form an orthonormal basis of $\mathcal{H}_1$, such that $\langle\lambda|\lambda'\rangle = \delta_{\lambda\lambda'}$. The wavefunction $\phi_\lambda(\mathbf{r})$ associated to a state $|\lambda\rangle$ is its projection on the eigenbasis of the position operator $\hat{\mathbf{r}}$:

$$\phi_\lambda(\mathbf{r}) = \langle\mathbf{r}|\lambda\rangle . \tag{2.2}$$

2.2 Many-particle Hilbert space

There are two types of particles in quantum mechanics: Bosons and Fermions. Bosons have integer spin and a many-body bosonic wavefunction doesn't change sign if we swap the coordinates of two particles. Fermions have half-integer spin and a many-fermion wavefunction changes sign if we swap the coordinates of two particles. We restrict our discussion to Fermions only. Consequently, an N body wavefunction satisfies:

$$\Psi_{\lambda_1 \ldots \lambda_N}(\mathbf{r}_1, \ldots \mathbf{r}_i, \ldots \mathbf{r}_j, \ldots \mathbf{r}_N) = -\Psi_{\lambda_1 \ldots \lambda_N}(\mathbf{r}_1, \ldots \mathbf{r}_j, \ldots \mathbf{r}_i, \ldots \mathbf{r}_N). \tag{2.3}$$

For example, a two particle wavefunction with fermions in single particle states $|\lambda_1\rangle$ and $|\lambda_2\rangle$ would be written as:

$$\Psi_{\lambda_1\lambda_2}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left(\phi_{\lambda_1}(\mathbf{r}_1)\phi_{\lambda_2}(\mathbf{r}_2) - \phi_{\lambda_1}(\mathbf{r}_2)\phi_{\lambda_2}(\mathbf{r}_1)\right). \tag{2.4}$$

More generally, if we have N fermions, than the many-body wavefunction can be written as a Slater determinant:

$$\Psi_{\lambda_1 \ldots \lambda_N}(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\lambda_1}(\mathbf{r}_1) & \phi_{\lambda_2}(\mathbf{r}_1) & \ldots & \phi_{\lambda_N}(\mathbf{r}_1) \\ \phi_{\lambda_1}(\mathbf{r}_2) & \phi_{\lambda_2}(\mathbf{r}_2) & \ldots & \phi_{\lambda_N}(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\lambda_1}(\mathbf{r}_N) & \phi_{\lambda_2}(\mathbf{r}_N) & \ldots & \phi_{\lambda_N}(\mathbf{r}_N) \end{vmatrix} . \tag{2.5}$$

These wavefunctions form an orthonormal basis of the N fermion Hilbert space.

2.3 Second quantization

We know that to represent many-body Fermion states, we need to use Slater determinants which guarantee the right statistics for Fermions. Instead of working with antisymmetric wavefunctions in the position basis, we work with Dirac kets of the so called *Fock basis*. We describe and N fermion state by specifying the occupancies of each single particle state (either 0 or 1 due to the Pauli exclusion principle). A Fock state can be written as:

$$|n\rangle = |\overset{\lambda_1}{n_1}, \overset{\lambda_2}{n_2}, \ldots\rangle \,. \tag{2.6}$$

Starting from the Fock vacuum, $|0\rangle$, which is the state with no particles that is noramlized, we introduce the creation $\hat{c}^\dagger_\lambda$ operator which adds a fermion to the single particle state, such that $\hat{c}^\dagger_\lambda |0\rangle = |\lambda\rangle$. We also define the annihilation $\hat{c}_\lambda$ operator, which is the Hermitian adjoint of the creation operator. This operator removes a fermion from a single particle state, such that $|0\rangle = \hat{c}_\lambda |\lambda\rangle$. We want our states to be antisymmetric: $|n_1, n_2\rangle = -|n_2, n_1\rangle \Rightarrow \hat{c}^\dagger_{\lambda_1}\hat{c}^\dagger_{\lambda_2} = -c^\dagger_{\lambda_2}\hat{c}^\dagger_{\lambda_1}$. This puts constraints on the creation operators, namely that they must anticommute: $\hat{c}^\dagger_\lambda \hat{c}^\dagger_{\lambda'} + \hat{c}^\dagger_{\lambda'}\hat{c}^\dagger_\lambda = \{\hat{c}^\dagger_\lambda, \hat{c}^\dagger_{\lambda'}\} = 0$. Finally, from the fact the the single particle basis states are orthonormal we get the anticommutation relations between the annihilation and creation operator: $\langle\lambda|\lambda'\rangle = \delta_{\lambda\lambda'} \Rightarrow \langle 0|\hat{c}_\lambda \hat{c}^\dagger_{\lambda'}|0\rangle = \delta_{\lambda\lambda'} \Rightarrow \langle 0|\{\hat{c}_\lambda, \hat{c}^\dagger_{\lambda'}\} - \hat{c}^\dagger_{\lambda'}\hat{c}_\lambda|0\rangle \Rightarrow \{\hat{c}_\lambda, \hat{c}^\dagger_{\lambda'}\} = \delta_{\lambda\lambda'}$. To recap, here are the definitions of the objects we've introduced:

$$\begin{aligned} \hat{c}_\lambda |0\rangle = 0, \quad & \{\hat{c}_\lambda, \hat{c}_{\lambda'}\} = \{\hat{c}^\dagger_\lambda, \hat{c}^\dagger_{\lambda'}\} = 0 \\ \langle 0|0\rangle = 1, \quad & \{\hat{c}_\lambda, \hat{c}^\dagger_{\lambda'}\} = \delta_{\lambda\lambda'}. \end{aligned} \tag{2.7}$$

3 Correlated Fermion models

3.1 The Heisenberg model

The Heisenberg model

The Heisenberg Hamiltonian is given by:

$$\hat{\mathcal{H}} = J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j = J \sum_{\langle ij \rangle} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z), \tag{3.1}$$

where J is the magnetic exchange coupling for the distinct pairs of first neighbor sites, labelled i and j, $(i < j)$ and $\hat{\mathbf{S}}_i$ is the total spin operator for site i. The spin operator can be written in terms of the Pauli matrices: $\hat{\mathbf{S}}_i = \frac{1}{2}\hat{\boldsymbol{\sigma}}_i$, where $\hat{\boldsymbol{\sigma}}_i = (\hat{\sigma}_i^x, \hat{\sigma}_i^y, \hat{\sigma}_i^z)$. In the down-up basis, $\{|\downarrow\rangle, |\uparrow\rangle\}$, the Pauli matrices can be represented as:

$$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.2}$$

We also recall that the components of the spin operator satisfy the commutation relations:

$$[\hat{S}_j^\alpha, \hat{S}_k^\beta] = i\delta_{jk}\epsilon^{\alpha\beta\gamma} S_k^\gamma. \tag{3.3}$$

The Heisenberg model describes spin 1/2 electrons interacting on a crystal. In equation 3.1 the range of interactions is limited to first neighbours (closest sites) but in principle, one could include longer range interactions by specifying the entries of an interaction matrix J_{ij}.

The Heisenberg model is quantum spin model. It describes spins interacting

3.2 The Fermi-Hubbard model

The Fermi-Hubbard model

The Fermi-Hubbard Hamiltonian is given by:

$$\hat{\mathcal{H}} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \tag{3.4}$$

The sum runs over the site indices i and j and the spin $\sigma = \{\uparrow, \downarrow\}$, t_{ij} is the hopping integral from sites i to j, $\hat{c}_{i\sigma}^\dagger$ creates an electron of spin σ at site i and $\hat{c}_{i\sigma}$ annihilates an electron of spin σ from site i. The second sum runs over all the sites and U is the on-site repulsion term. Finally, $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ is the number operator for site i.

The Hubbard Hamiltonian is a simple toy model which contains two competing terms. The first sum represents electrons hopping to different sites. This is captured by the non-zero hopping matrix elements t_{ij}. In many cases, only first neighbor hoppings $\langle ij \rangle$ are considered. The second sum represents the on site repulsion that electrons of opposite spin experience when they are on the same site.

The Hubbard model was originally proposed in 1963 by John Hubbard [1] to study the metal-insulator transition in transition metal monoxides [2]. Despite its simplicity, the Hubbard model exhibits a wide range of phases at different

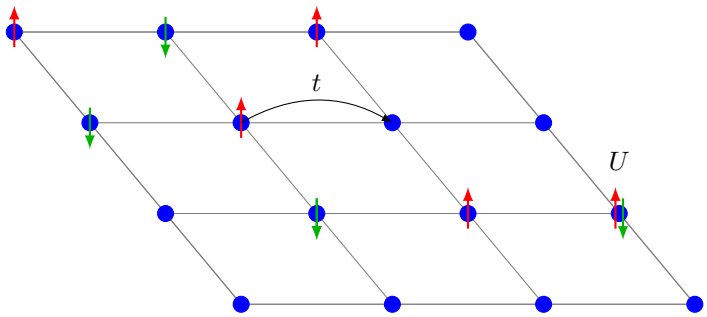

Figure 1: Schematics of the Hubbard model. The figure shows s orbitals (blue balls) on a crystal lattice that can be empty, occupied by one electron of spin up (red arrows), occupied by one electron of spin down (green arrows) or doubly occupied by electrons of opposite spins. The electrons can hop to nearby sites represented by t and experience a repulsion when they are on the same site (U).

regimes and is use to study correlated phenomena in condensed matter, such has magnetism and high-temperature superconductivity [3]. A detailed review of the Hubbard model can be found in [4].

3.3 The tJ model

The tJ model

The tJ Hamiltonian is given by:

$$\hat{\mathcal{H}} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} + \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{1}{4} \hat{n}_i \hat{n}_j. \tag{3.5}$$

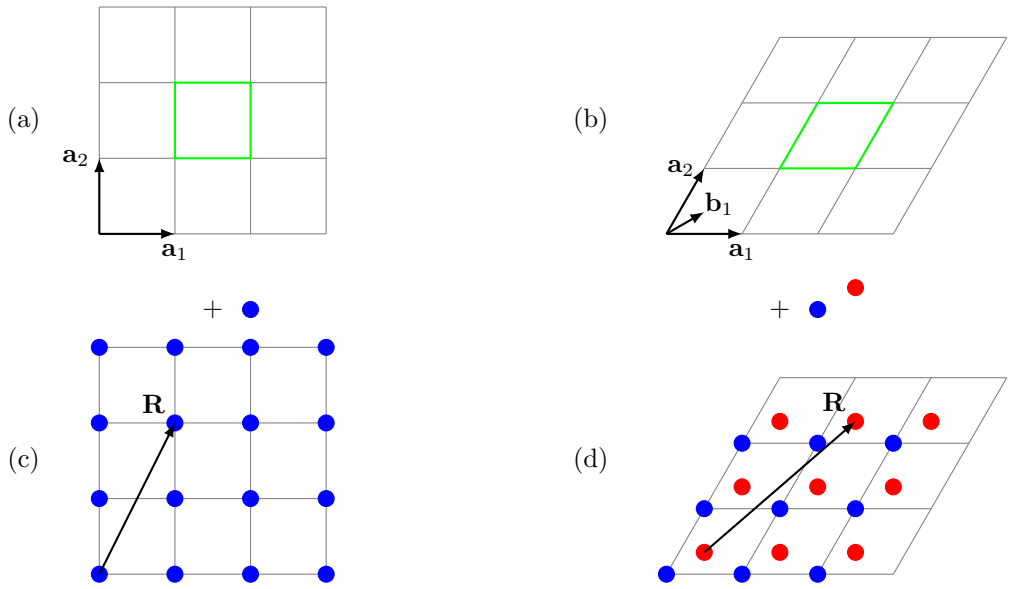

Figure 2: Crystal structure. Panels (a) and (b) show two different lattices (square and triangular respectively). For the square lattice, the primitive lattice vectors are $\mathbf{a}_1 = (a, 0)$ and $\mathbf{a}_2 = (0, a)$ and for the triangular lattice, they are $\mathbf{a}_1 = (a, 0)$ and $\mathbf{a}_2 = \frac{a}{2}(1, \sqrt{3})$. The primitive unit cells are the green shapes. Panels (c) and (d) show square and honeycomb crystal structures. The square crystal is constructed from the square lattice with a blue atom at each site. The honeycomb crystal is constructed from the triangular lattice with a two atom basis, one blue atom at each lattice site and a red one offset from the blue ones by $\mathbf{b}_1 = \frac{\mathbf{a}_1+\mathbf{a}_2}{3}$. Both (c) and (d) show a lattice vector $\mathbf{R} = \mathbf{a}_1 + 2\mathbf{a}_2$.

4 Lattices

The correlated electron models discussed in the previous section are used to describe the properties of materials. In many materials, the atoms are arranged in regular patterns, forming what is known as a crystal structure [5]. In this section, we provide an elementary introduction to crystal structure and explain how to properly define the lattice which will be used for computations in the ED code. We restrict our discussion to 1D and 2D crystals only.

4.1 Crystal structure

A crystal structure can be described by specifying the lattice and the basis. The lattice is a regular periodic array of points in space. The basis is the set of atoms or molecules that constitute the crystal see 2. It is also useful to define the primitive unit cell [5] (PUC), which can be defined as the minimal repeating unit to specify the lattice. It contains exactly one lattice point. In 1D, the PUC is specified by one primitive lattice vector $\mathbf{a}_1$. For a 2D crystal, we need to specify two primitive lattice vectors to define a unit cell $\{\mathbf{a}_1, \mathbf{a}_2\}$, such that the PUC is the parallelogram spanned by the primitive lattice vectors. Starting from a point, the exact same point in a different PUC can be reached by a translation by a lattice vector:

$$\mathbf{R} = m\mathbf{a}_1 + n\mathbf{a}_2, \quad m, n \text{ integers.} \tag{4.1}$$

The environment seen by the particles at a point $\mathbf{r}$ of the crystal is exactly the same at the point $\mathbf{r} + \mathbf{R}$, where $\mathbf{R}$ is a lattice vector. This is known as translational invariance.

4.2 Finite supercell with periodic boundary conditions

Computers have limited memory which constrains us to work on finite lattices and use periodic boundary conditions. We call such finite lattices *supercells*. The supercell is specified by the supercell lattice vectors $\{\mathbf{A}_1, \mathbf{A}_2\}$, which are linear combinations of the primitive lattice vectors, $\{\mathbf{a}_1, \mathbf{a}_2\}$. It contains a fixed number of primitive unit cells and thus a finite number of sites. For a 1D system, $\mathbf{A}_1 = m\mathbf{a}_1$ where m is an integer. For a 2D crystal, the supercell vectors are defined by a transformation matrix $\mathbf{M}$ in the following way:

$$\begin{pmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \end{pmatrix} = \begin{pmatrix} m_1 & n_1 \\ m_2 & n_2 \end{pmatrix} \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \end{pmatrix} = \mathbf{M}\mathbf{a}. \tag{4.2}$$

The use of periodic boundary conditions has the effect of mapping the 1D chain to a circle and the 2D crystal to a torus. The number of unit cells contained in the supercell is given by $N_c = \det \mathbf{M} = m_1 n_2 - m_2 n_1$ and the number of lattice sites is $M = N_a \det \mathbf{M}$ where N_a is the number of atoms in the PUC.

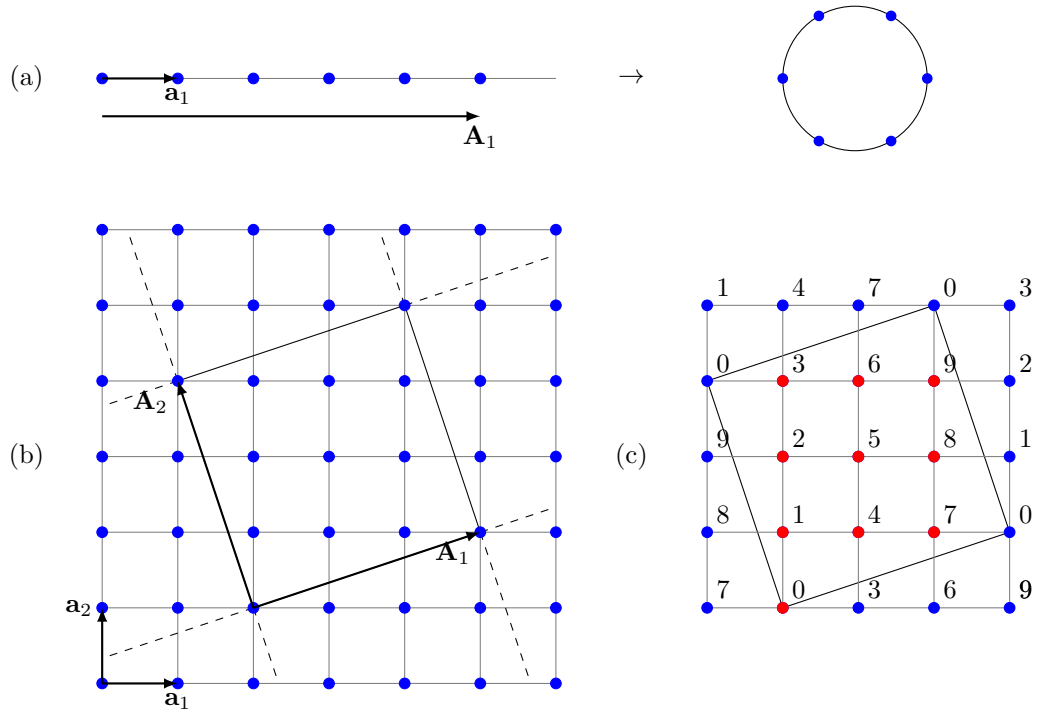

Figure 3: Supercells. Panel (a) shows a 1D supercell, where $\mathbf{A}_1 = 6\mathbf{a}_1$ and how it is mapped to a circle when using periodic boundary conditions. Panel (b) shows a square crystal structure. A supercell with vectors $\mathbf{A}_1 = 3\mathbf{a}_1 + \mathbf{a}_2$ and $\mathbf{A}_2 = -\mathbf{a}_1 + 3\mathbf{a}_2$ is shows in the middle. Panel (c) show the smallest diagonal cell which encloses the $\{\mathbf{A}_1, \mathbf{A}_2\}$ supercell from panel (b). The red balls indicate sites that lie in the supercell and they are labelled with numbers to show the periodic boundary conditions.

The first step is to find the coordinates of the sites that are in the supercell. The case where the supercell is diagonal, $n_1, m_2 = 0$ is trivial since the boundaries of the supercell will coincide with the boundaries of the primitive unit cells. The case $n_1, m_2 \neq 0$ implies that we are trying to find the set of sites:

$$\mathbf{r} = x\mathbf{a}_1 + y\mathbf{a}_2 \tag{4.3}$$

such that $\mathbf{r}$ lies in the parallelogram spanned by $\{\mathbf{A}_1, \mathbf{A}_2\}$. Note that if there is more than one atom in the primitive unit cell, x and y are not necessarily integers. Points in the parallelogram have the property that their position can be written as a linear combination of the supercell vectors, with coefficients that satisfy:

$$\mathbf{r} = \mu\mathbf{A}_1 + \lambda\mathbf{A}_2, \quad \mu, \lambda \in [0, 1). \tag{4.4}$$

We can thus pick the real numbers x, y and find the supercell expansion coefficients using $\mathbf{a} = \mathbf{M}^{-1}\mathbf{A}$, which means that:

$$\begin{pmatrix} x\mathbf{a}_1 \\ y\mathbf{a}_2 \end{pmatrix} = \begin{pmatrix} x & 0 \\ 0 & y \end{pmatrix} \mathbf{M}^{-1} \begin{pmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \end{pmatrix} \Rightarrow N_c\mu = xn_2 - ym_2, \quad N_c\lambda = ym_1 - xn_1. \tag{4.5}$$

A method for finding the valid sites starting from the supercell coefficients is to start from a diagonal supercell that contains the the 'target supercell' and for every point in the diagonal supercell, find those meet both the conditions: $0 \leq \mu < 1$ and $0 \leq \lambda < 1$. The schematics of this are explained in figure 3. Finding the smallest diagonal cell which encloses the target supercell can be done by finding the supercell's maximal and minimal extent in the $\mathbf{a}_1$ and $\mathbf{a}_2$ directions, such that the coefficients of the cell whose points we check are $\max(m_1, m_2, m_1 + m_2)$ and $\max(n_1, n_2, n_1 + n_2)$.

4.3 Pairs of equidistant points

The Fermion models that we have discussed so far include interactions between neighbors on the lattice, or equidistant points. Given a supercell, we need to construct a $M \times M$ distance matrix $\mathbf{D}$ such that D_{ij} is the neighbor distance between the sites labelled i and j. Obviously, $D_{ii} = 0$ and $D_{ij} = D_{ij}$. For example, the distance matrix for the supercell in panel (c) of figure 3 would be:

$$\mathbf{D} = \begin{pmatrix} 0 & 1 & 2 & 1 & 2 & 4 & 2 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 & 1 & 2 & 4 & 2 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 1 & 2 & 4 & 2 & 1 \\ 1 & 2 & 1 & 0 & 1 & 2 & 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 1 & 0 & 1 & 2 & 1 & 2 & 4 \\ 4 & 2 & 1 & 2 & 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 & 2 & 1 & 0 & 1 & 2 & 1 \\ 1 & 2 & 4 & 2 & 1 & 2 & 1 & 0 & 1 & 2 \\ 2 & 1 & 2 & 4 & 2 & 1 & 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 2 & 4 & 2 & 1 & 2 & 1 & 0 \end{pmatrix} \tag{4.6}$$

For example, the first-neighbors of site 1 in the figure are $(2, 4, 8, 10)$. To construct such a matrix for a general 2D crystal, we compute the distance between all the sites $i < j$ using the minimum image convention. That is, we calculate $\min |\mathbf{r}_i + \boldsymbol{\delta} - \mathbf{r}_j|$ where $\boldsymbol{\delta} = \{\pm\mathbf{A}_1, \pm\mathbf{A}_2, \pm\mathbf{A}_1 \pm \mathbf{A}_2\}$. This computes the euclidean distance in all replicas of the supercell. Once this has been done we sort the possible distances supported by the supercell and assign a unique integer to each distance. This is the *neighbor distance.*

4.4 Reciprocal space

4.5 Python package

5 Encoding the Problem

With the background from the previous sections, we are ready to see how a numerical scheme to encode the problem can be devised. We explain how to generate and store the basis as well as how to construct a matrix representation for the Hamiltonian in the case of the Heisenberg, Hubbard and tJ model. We assume that we're working on an M site crystal.

5.1 Basis

Heisenberg model

In the Heisenberg model, each site is occupied in two different ways. We can expresse the occupancies in second quantization using the the Fock vaccuum and the creation operators:

1. There is a spin down on site i: $|\downarrow\rangle = \hat{c}^\dagger_{i\downarrow} |0\rangle$.
2. Or there is a spin up on site i: $|\uparrow\rangle = \hat{c}^\dagger_{i\uparrow} |0\rangle$.

This gives a total Hilbert space dimension of 2^M. The space is spanned by the kets specfiying the nature $\uparrow, \downarrow$ of the spin occupying each of the M sites. A general basis state can be written in second quantized form as:

$$|n\rangle = \prod_{i=0}^{M-1} \hat{c}^\dagger_{i\sigma} |0\rangle . \tag{5.1}$$

The occupations of each state are ordered by site index. Because of the anticommutation relations of the Fermionic creation and annihilation operators, it is important to define a convention for ordering them and then to maintain it during the computations. The spin at each site can be specified using a number: $n_i = 0$ for spin down or $n_i = 1$ for spin up. This allows us to associate a unique bit-string to each basis state and store it as a binary number:

$$|n\rangle \to n = \sum_{i=0}^{M-1} n_i 2^i. \tag{5.2}$$

For example, the following 6 site state can be encoded in the following way:

$$|\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow\rangle = \hat{c}^\dagger_{5\downarrow}\hat{c}^\dagger_{4\downarrow}\hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{0\uparrow} |0\rangle = [0_6 0_4 1_3 1_2 0_1 1_0] = 2^0 + 2^2 + 2^3 = 13. \tag{5.3}$$

The indices in the bit string representation are used to label the site index. The full basis is the set of numbers from 0 to $2^M - 1$. The following pseudocode shows how to construct the basis for the Heisenberg model on an M site system.

Algorithm 1 Heisenberg model basis construction

```
basis = list
M = number of sites
for n ∈ {0, 1, ..2^{M-1}} do
    basis[n] ← n
end for
```

Fermi-Hubbard model

In the Fermi-Hubbard model, each site can be occupied in four different ways:

1. The site i is unoccupied: $|0\rangle$.
2. The site i is occupied by one spin down electron: $|\downarrow\rangle = \hat{c}^\dagger_{i\downarrow}|0\rangle$.
3. The site i is occupied by one spin up electron: $|\uparrow\rangle = \hat{c}^\dagger_{i\uparrow}|0\rangle$.
4. Or, the site is doubly occupied by two electrons of opposite spin: $|\downarrow\uparrow\rangle = \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}|0\rangle$.

Note the order in which the creation operators appear: we will order them first by spin and then site index. For an M site lattice this gives a total Hilbert space dimension of 4^M. A general Fock state $|n\rangle$ of this space is given by:

$$|n\rangle = \prod_{i=0}^{M-1} \hat{c}^{\dagger n_{i\uparrow}}_{i\uparrow} \prod_{i=0}^{M-1} \hat{c}^{\dagger n_{i\downarrow}}_{i\downarrow} |0\rangle, \tag{5.4}$$

where $n_{i\sigma} = 0$ or 1. To give a concrete example, the following basis state of a 6 site model can be written as:

$$|\downarrow\uparrow, 0\uparrow, \downarrow, 0, \downarrow\uparrow\rangle = \hat{c}^\dagger_{5\uparrow}\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{0\uparrow}\hat{c}^\dagger_{5\downarrow}\hat{c}^\dagger_{3\downarrow}\hat{c}^\dagger_{0\downarrow}|0\rangle. \tag{5.5}$$

Following the encoding scheme we used for the Heisenberg model, basis states of the Hubbard model can be encoded using bit-strings of size $2M$, where the first M entries correspond to the spin down occupancies and the last M entries correspond to the spin up occupancies. Given a state $|n\rangle$, we can encode its spin-up bit string as an integer $n_\uparrow$ and its spin-down bit string as $n_\downarrow$ and construct the corresponding integer from the two:

$$|n\rangle \to n = 2^M n_\uparrow + n_\downarrow. \tag{5.6}$$

Going back to our example from equation 5.5, the state can be encoded as

$$|\downarrow\uparrow, 0\uparrow, \downarrow, 0, \downarrow\uparrow\rangle = [1_5 0_4 0_3 1_2 0_1 1_0 | 1_5 0_4 1_3 0_2 0_1 1_0] = [37|41] = 37 \times 2^6 + 41 = 2409. \tag{5.7}$$

5.2 Operators

Our binary number representation not only provides a very convenient method of storing the basis elements of the Hilbert space but can also be used to construct the Hamiltonian using bitwise operations. Using the tools we've previously developed, we explain how to implement the action of various operators on Fock basis states.

Creation and annihilation operators

In this section, we discuss the implementation of the terms that contain creation and annihilation operators in the Hubbard model.

Lets start by getting a feeling for the U term of the Hubbard model, which involves the quartic operator $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}$. Using equation 5.4, we can write its action on a general state of the basis as:

$$\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}|n\rangle = \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\hat{c}^{\dagger n_{M\uparrow}}_{M\uparrow}\ldots\hat{c}^{\dagger n_{1\uparrow}}_{1\uparrow}\hat{c}^{\dagger n_{M\downarrow}}_{M\downarrow}\ldots\hat{c}^{\dagger n_{1\downarrow}}_{1\downarrow}|0\rangle. \tag{5.8}$$

To find the new Fock state, we need to anticommute the creation and annhilation operators as many times as it takes to get to $i,\downarrow$ and then $i,\uparrow$. Since we have pairs of operators that act on the same site the same spin index, we immeadiately see that there will be no phase picked up when anticommuting them. This gives:

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}|n\rangle = |n\rangle \text{ if } n_{i\uparrow} - n_{i\downarrow} = 0, \text{ 0 otherwise.} \tag{5.9}$$

Let's now look at the hopping terms: $\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}$. First, we notice that the phase is not impacted by the nature of the spin that the operator is acting on. For example, with our convention, acting $\hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}$ would require us to first anticommute both operators as many times as it takes to get to the spin down sector, resulting in no phase. To act a hopping operator on a state, we first anticommute $\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}$ to get them behind $\hat{c}^{\dagger n_{j\uparrow}}_{j\uparrow}$, which doesn't induce any phase:

$$\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow}|n\rangle = \hat{c}^{\dagger n_{M\uparrow}}_{M\uparrow}\dots\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow}\hat{c}^{\dagger n_{j\uparrow}}_{j\uparrow}\dots\hat{c}^{\dagger n_{i\uparrow}}_{i\uparrow}\dots|0\rangle\,.$$

We notice that if $n_{j\uparrow} = 0$, the annihilation operator will kill the state. Assuming $n_{j\uparrow} = 1$, the annihilation operator will remove the spin, so we are left with:

$$\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow}|n\rangle = \hat{c}^{\dagger n_{M-1\uparrow}}_{M-1\uparrow}\dots\hat{c}^\dagger_{i\uparrow}\hat{c}^{\dagger n_{j-1\uparrow}}_{j-1\uparrow}\dots\hat{c}^{\dagger n_{i\uparrow}}_{i\uparrow}\dots|0\rangle\,.$$

Now we need to anticommute $\hat{c}^\dagger_{i\uparrow}$ all the way to behind $\hat{c}^{\dagger n_{i\uparrow}}_{i\uparrow}$, which corresponds to $\sum_{l=i+1}^{j-1} n_{l\uparrow}$ times. This leaves us with:

$$\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow}|n\rangle = (-1)^{\sum_{l=i+1}^{j-1} n_{l\uparrow}}\hat{c}^{\dagger n_{M-1\uparrow}}_{M-1\uparrow}\dots\hat{c}^{\dagger n_{j\uparrow}}_{j\uparrow}\dots\hat{c}^\dagger_{i\uparrow}\hat{c}^{\dagger n_{i\uparrow}}_{i\uparrow}\dots|0\rangle\,.$$

Finally we see that if $n_{i\uparrow} = 1$, the product of two creation operators will also kill the state. To summarize, we can write down the expression for a general hopping term for the Hubbard model:

$$\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}|n\rangle = (-1)^{\sum_{l=i+1}^{j-1} n_{l\sigma}}|n'\rangle \text{ if } n_{j\sigma} - n_{i\sigma} = 0, \text{ 0 otherwise.} \tag{5.10}$$

Here $|n'\rangle$ is the new state obtained from removing a spin σ at site j and adding a spin σ at site i. Again, these operators can be easily implemented using bitwise operations.

5.3 Spin operators

Now we look at the implementation of the spin operators that appear in the Heisenberg and tJ models. We first discuss their implementation in the Heisenberg model. The dot product of spin operators contains three terms:

$$\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j = \hat{S}^x_i\hat{S}^x_j + \hat{S}^y_i\hat{S}^y_j + \hat{S}^z_i\hat{S}^z_j. \tag{5.11}$$

The first terms, involving the x components flips the spins on sites i and j. The last term, which involves the z components is diagonal in the Fock basis. When it acts on one of our binary encoded states, it returns the eigenvalue $(2\sigma_i - 1)(2\sigma_j - 1)$ where σ_i and $\sigma_j = \{0, 1\} = \{\downarrow, \uparrow\}$ are the ith and jth bits of the state. Finally, the y term flips the spin and also returns the same phase than the z term. These operations can be easily implemented with bitwise arithmetic.

When working with spin operators in the Heisenberg model, we don't need to worry about the sign structure. This is because the total spin operator for site i can be expressed in terms of the creation and annihilation operator in the following way:

$$\hat{\mathbf{S}}_i = \sum_{\alpha\alpha'}\hat{c}^\dagger_{i\alpha}\frac{\boldsymbol{\sigma}_{\alpha\alpha'}}{2}\hat{c}_{i\alpha'}, \tag{5.12}$$

where $\alpha = \{\downarrow, \uparrow\}$ is the spin index. We see that it contains pairs of creation and annhilation operators that act on the same site, so when we compute something like $\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$, we have to anticommute the pairs of creation and annihilation the same number of times, resulting in no phase picked up. The following pseudocode snippet shows a way to act the product of spin operators on a basis state:

Algorithm 2 Acting spin operators on basis states in the Heisenberg model

function $\mathrm{S}_z S_z$(N,I,J)

5.4 Hamiltonian construction

We now have the necessary tools to construct the matrix representation for the Hamiltonian. The main idea is to calculate the matrix elements $\langle m|\hat{\mathcal{H}}|n\rangle$ for all the states in the basis. It is convenient to decompose $\hat{\mathcal{H}}$ into a sum of operators that map basis states to other basis states or 0, such that:

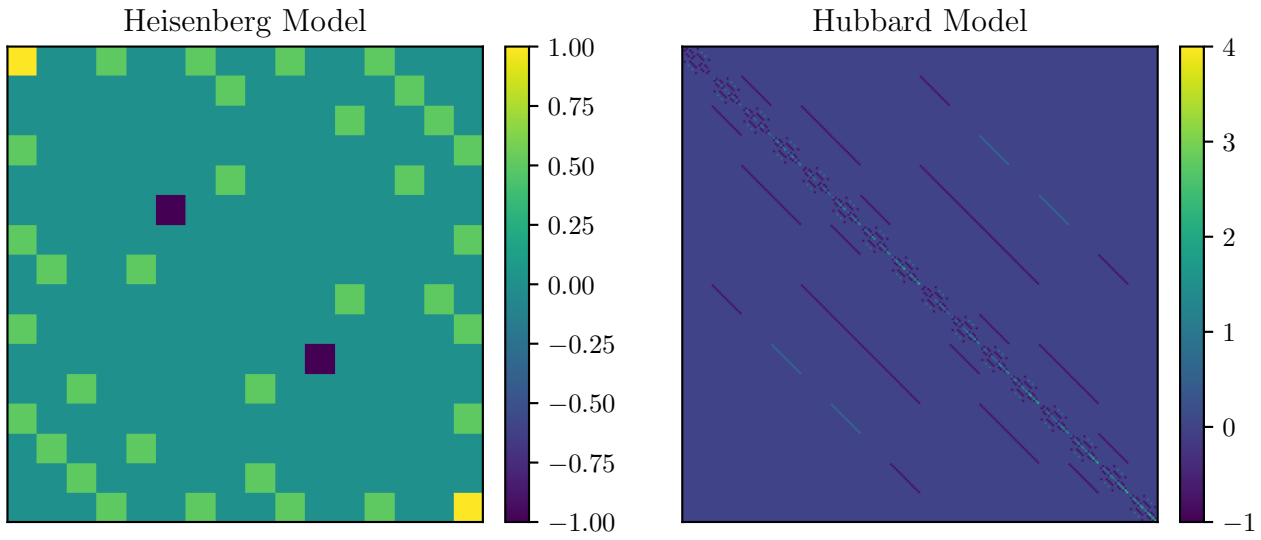

Figure 4: Hamiltonian sparsity patterns for the isotropic Heisenberg model, Hubbard model and tJ model on a 1D four site chain with periodic boundary conditions. The operators that mix sites only act on first-neighbors. The Hilbert space dimensions are 16, 256 and 81 respectively.

$$\hat{\mathcal{H}} = \sum_j \hat{\mathcal{H}}^{(j)}, \quad \hat{\mathcal{H}}^{(j)}\,|n\rangle = \mathcal{H}^{(j)}_{nn'}\,|n'\rangle\,. \tag{5.13}$$

To construct the full matrix, we first recall the decomposition of the Hamiltonian in the Fock basis:

$$\hat{\mathcal{H}} = \sum_{n,n'} |n\rangle\ \langle n|\hat{\mathcal{H}}|n'\rangle\ \langle n'|\,. \tag{5.14}$$

By decomposing the Hamiltonian like in equation 5.13 and taking the scalar product with the vector $|n\rangle$, we get the expression for the nth column of the matrix:

$$\hat{\mathcal{H}}\,|n\rangle = \sum_{j,n'} \langle n'|\hat{\mathcal{H}}^{(j)}|n\rangle\,|n'\rangle = \sum_{j,n'} \mathcal{H}^{(j)}_{n'n}\,|n'\rangle\,. \tag{5.15}$$

Heatmaps of the $\hat{\mathcal{H}}$ for the Heisenberg, Hubbard and tJ models on a 1D chain can be found in figure 4. The Hamiltonian matrix is very sparse, meaning it has a lot of zero entries. Instead of storing the full d^2, entries where d

is the dimension of the Hilbert space, one can only store three lists, one for the matrix element, one for the row and one for the column of these non-zero values.

The following pseudo-code snippet shows how one can calculate and store the Hamiltonian matrix in sparse format.

Algorithm 3 Constructing and storing the matrix

```
rows, cols, vals = empty lists        ▷ empty lists for storing row, column indices and the matrix elements.
for |n⟩ in basis do
    for all j do
        element, n′ = actHj(n)
        rows ← n
        cols ← n′
        vals ← element
    end for
end for=0
```

6 Symmetries

So far in our discussion of tackling correlated electron models, we haven't included the use of symmetries and how they can be exploited to reduce the dimensionality of the problem at hand. By finding a set observables that commute with each other and the Hamiltonian (complete set of commuting observables, CSCO) we can make the problem slightly more tractable for exact diagonalization, allowing us to probe larger systems. In this section, we will discuss some of the symmetries that are present in the Heisenberg, Hubbard and tJ model as well as how to implement them in an ED code. Apart from translational invariance, we will omit other spatial symmetries that depend on the crystal structure being studied.

6.1 Spin and particle number conservation

The three models that we've discussed conserve the number of particles and the total component of spin along a quantization axis (usually taken to be the z axis). These quantities are captured by the following operators:

$$\hat{S}^z = \frac{1}{2}\sum_i \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}, \quad \hat{n} = \sum_i \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}. \tag{6.1}$$

This means that the Hamiltonian commutes with these two. Moreover, it is easy to see that $[\hat{S}^z, \hat{n}] = 0$. This means that the eigenstates of $\hat{\mathcal{H}}$ are simultaneous eigenstates of these operators. Hence, we can fix the number of particles in each spin sector $n_\uparrow, n_\downarrow$ and work in the subspace of the full Hilbert space which has a fixed number of particles and fixed S^z. Essentially, the Hamiltonian is block diagonal when the basis states are ordered from increasing number of particles and increasing total S^z. This is captured in figure 5. Exploiting these symmetries reduces the dimension of the Hilbert space. For the case of the Heisenberg model, the dimension of the reduced basis will be given by the number of ways $N_\uparrow$ electrons of spin up and be distributed of M sites:

$$d = \frac{M!}{N_\uparrow! N_\downarrow!}. \tag{6.2}$$

For the Hubbard model this is given by the number of ways $N_\uparrow$ particles can be distributed over M sites times the number of ways $N_\downarrow$ particles can be distributed over M sites:

$$d = \binom{M}{N_\uparrow}\binom{M}{N_\downarrow}. \tag{6.3}$$

To exploit these symmetries, we need to slightly change the scheme for generating the basis. In the case of the Heisenberg model, instead of generating all the numbers from 0 to $2^M - 1$, the basis can be constructed by generating all distinct permutations of an array of size M with $N_\uparrow$ ones. For the Hubbard model, we generate all the arrays of size M with $N_\uparrow$ ones and then all the arrays of size M with $N_\downarrow$ ones, this gives us all the possible number $N_\uparrow$ and $N_\downarrow$, allowing us to construct the basis using equation 5.6.

We also need to modify our method for identifying the row corresponding to a new state when constructing the Hamiltonian. When generating each number in the reduced basis, we can assign a unique integer from 0 to $d - 1$ where d is the dimension of the basis and store these in a hash table. Another approach would be to generate each basis element and compute the corresponding row of the matrix by using lexicographic indices to identify the new states. This saves memory but slows the speed of the code.

6.2 Translational symmetry

This section follows derivations from [**?**] As we previously discussed, when considering periodic boundary conditions, the crystal lattice is a translationally invariant system. The Hamiltonian inherits this symmetry, it commutes with

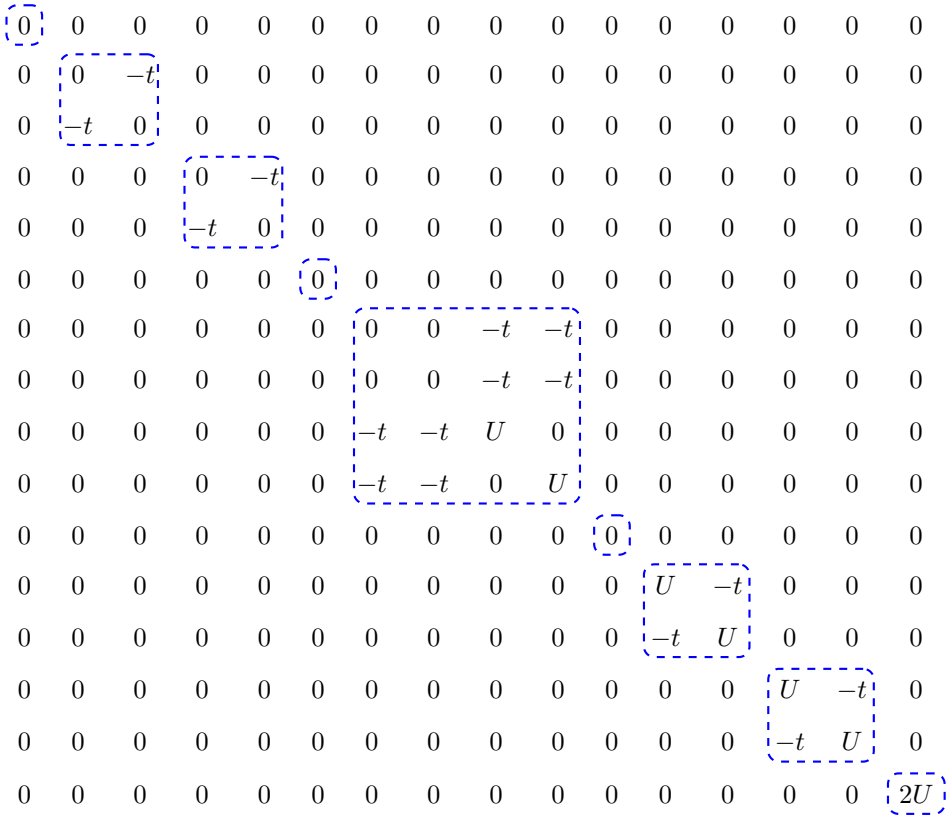

Figure 5: Matrix representation of the Hubbard dimer, two sites connected with periodic boundary conditions. When the basis is ordered by particle number and then total $\hat{S}^z$, it assumes block diagonal form. This is a consequence of the vanishing commutators $[\hat{\mathcal{H}}, \hat{n}]$ and $[\hat{\mathcal{H}}, \hat{S}^z]$. Of interest is the central 4×4 block which corresponds to 0 S^z and a half filling.

Fock state	Number	Index
$\|\downarrow,\uparrow\rangle$	9	0
$\|\uparrow,\downarrow\rangle$	6	1
$\|\downarrow\uparrow,0\rangle$	5	2
$\|0,\downarrow\uparrow\rangle$	10	3

Table 1: Hash table for the Hubbard dimer in the $S^z = 0$ sector at half-filling (central 4×4 block on figure 5). Each state of this sector is associated to a unique integer between 0 and $d-1$, where d is the dimension of the sector. By storing the number as the key and the index as the value, one can find off-diagonal matrix elements by querying the hash table.

the translation operator $\hat{T}(\mathbf{R})$ that shifts states by a lattice vector $\mathbf{R}$. For a more detailed discussion of the translation operator, We can define its action on a basis Fock state in the following way:

$$\hat{T}\,|n\rangle = |T(n)\rangle\,, \tag{6.4}$$

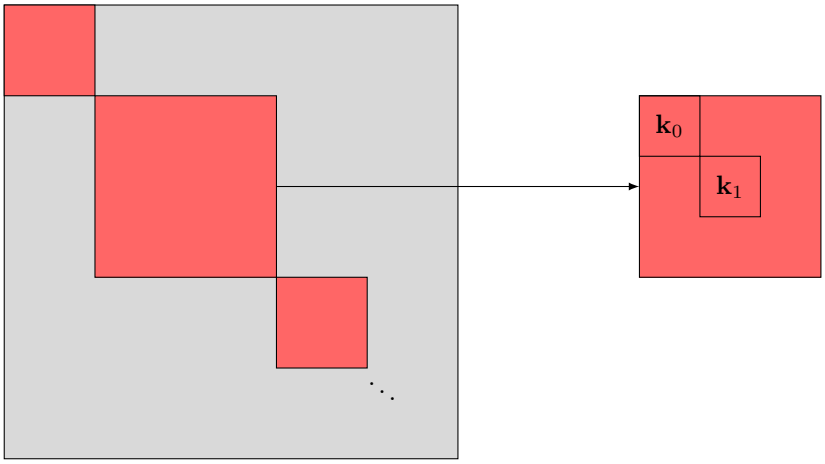

Figure 6: Translational symmetry. The panel on the left shows the full Hamiltonian taking a block diagonal form in the occupation number and $\hat{S}^z$ basis. Since the translation operator commutes with both $\hat{n}$ and $\hat{S}^z$, it can be block diagonalized again where each sub-block is characterized by the quantum number $\mathbf{k}$.

where $T(n)$ is the new integer obtained from shifting the spins in the configuration n by a lattice vector $\mathbf{R}$. It is best to choose the translation vector to be the smallest allowed translation on the lattice, which corresponds to a primitive lattice vector.

The Hamiltonian commutes with $\hat{T}$ so its eigenstates $|\psi\rangle$ are also simultaneous eigenvectors of $\hat{T}$. The eigenvalues of the translation operator are $e^{i\mathbf{k}\cdot\mathbf{R}}$. This means that in general, eigenstates satisfy:

$$\hat{T}\,|\psi\rangle = e^{i\mathbf{k}\cdot\mathbf{R}}\,|\psi\rangle \tag{6.5}$$

On an infinite lattice, the values of $\mathbf{k}$ form a continuum. However, here we're working on a finite cell with periodic boundary conditions which means that if we translate $|\psi\rangle$ by a supercell vector $\mathbf{A}$, we must get $e^{i\mathbf{k}\cdot\mathbf{A}}\,|\psi\rangle = |\psi\rangle$, which means that $\mathbf{k}\cdot\mathbf{A}$ is an integer mutliple of 2π, so $\mathbf{k}$ is a reciprocal supercell vector. Suppose we have the expansion coefficient ψ_n for a certain Fock state, then the expansion coefficient of $\psi_{n'}$ where $n' = T(n)$ is immediately known since:

$$\psi_{n'} = \langle n|\hat{T}^\dagger|\psi\rangle = e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_n. \tag{6.6}$$

which means that knowing one of the expansion coefficient for a state allows us to determine the expansion coefficient for all the states that are translations of $|n\rangle$. This motivates us to work in a reduced basis, spanned by the different eigenstates of $\hat{T}$. Given a state $|n\rangle$, we find the states that can be reached from it by applying powers of $\hat{T}$, which we call a *cycle*: $\mathcal{C}_n = \{|n\rangle, \hat{T}\,|n\rangle, \hat{T}^2\,|n\rangle, \ldots\}$. Each cycle can be completely specified by storing only one state, which we call the group representative. The group representative $\bar{n}$ of $\mathcal{C}_n$ is the element of the cycle with the smallest integer representation. We can now construct properly symmetrized eigenstates of the translation operator with eigenvalue $e^{i\mathbf{k}\cdot\mathbf{R}}$:

$$|\bar{n}(\mathbf{k})\rangle = \frac{1}{\sqrt{\mathcal{N}_n}} \sum_{l=0}^{N_c-1} e^{-il\mathbf{k}\cdot\mathbf{R}}\hat{T}^l\,|\bar{n}\rangle\,, \tag{6.7}$$

where $\mathcal{N}_n$ is a normalization factor associated to $\mathcal{C}_n$. These are just sums of the states in a cycle with a phase prefactor. We can check that these are eigenvectors of the translation operator by applying $\hat{T}$ to them:

$$\hat{T}\,|\bar{n}(\mathbf{k})\rangle = \frac{1}{\sqrt{\mathcal{N}_n}} \sum_{l=0}^{M/2-1} e^{-il\mathbf{k}\cdot\mathbf{R}} \hat{T}^{l+1}\,|\bar{n}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{R}}}{\sqrt{\mathcal{N}_n}} \sum_{l=0}^{M/2-1} e^{-i(l+1)\mathbf{k}\cdot\mathbf{R}} \hat{T}^{l+1}\,|\bar{n}\rangle = e^{i\mathbf{k}\cdot\mathbf{R}}\,|\bar{n}(\mathbf{k})\rangle\,,$$

where we used the periodicity of the lattice to change the summation index $l+1 \to l$. Particular care must be given to the normalization factor appearing in equation 6.7. The sum contains $M/2$ terms but not all cycles have the same periodicity than that of the supercell (for example, the fully antiferromagnetic state always translates to itself). The periodicity N_n is defined such that $\hat{T}^{N_n}\,|\bar{n}\rangle = |\bar{n}\rangle$. If $N_n < N_c$, then certain states will appear several times in 6.7. Moreover, not all cycles of the basis will contribute to an eigenstate $|\psi\rangle$ for a given value of $\mathbf{k}$. The only ones that contribute are those that verify the commensurability condition: $e^{iN_n\mathbf{k}\cdot\mathbf{R}} = 1$, i.e $N_n\mathbf{k}\cdot\mathbf{R}$ is an integer multiple of 2π. The states that don't satisfy this condition should be removed from the new basis. The normalization factor can thus be written as:

$$\mathcal{N}_n = \frac{N_c^2}{N_n}, \tag{6.8}$$

to ensure that $\langle\bar{n}(\mathbf{k})|\bar{n}(\mathbf{k})\rangle = 1$. The next step is to construct the Hamiltonian matrix in this basis. The matrix elements are given by $\langle\bar{m}(\mathbf{k})|\hat{\mathcal{H}}|\bar{n}(\mathbf{k})\rangle$. To implement this numerically, let's first consider the action of the Hamiltonian on one of the basis states:

$$\hat{\mathcal{H}}\,|\bar{n}(\mathbf{k})\rangle = \frac{1}{\sqrt{\mathcal{N}_n}} \sum_{l=0}^{N_c-1} e^{-il\mathbf{k}\cdot\mathbf{R}} \hat{\mathcal{H}}\hat{T}^{l}\,|\bar{n}\rangle = \frac{1}{\sqrt{\mathcal{N}_n}} \sum_{l=0}^{N_c-1} e^{-il\mathbf{k}\cdot\mathbf{R}} \hat{T}^{l}\hat{\mathcal{H}}\,|\bar{n}\rangle\,, \tag{6.9}$$

where we exploited translational symmetry in going to the last equality. Next, we reintroduce the decomposition of $\hat{\mathcal{H}}$ into a sum of operators $\hat{\mathcal{H}}_j$ that map single Fock states to other single Fock states or 0. This gives:

$$\hat{\mathcal{H}}\,|\bar{n}(\mathbf{k})\rangle = \frac{1}{\sqrt{\mathcal{N}_n}} \sum_j \sum_{l=0}^{M/2-1} e^{-il\mathbf{k}\cdot\mathbf{R}} \hat{T}^{l}\alpha_j\,|m_j\rangle\,. \tag{6.10}$$

The notation used is quite general: the $|m_j\rangle$ may to be a representatives and they may not even belong to a valid cycle for a given value of $\mathbf{k}$. If this is the case, we can discard the contribution from this state since it is not in the basis. If it is a valid state, then we can always write it as some translation of its representative: $|m_j\rangle = \hat{T}^{d_j}\,|\bar{m}_j\rangle$, where d_j is the number of shifts by $\mathbf{R}$ from $|\bar{m}_j\rangle$ needed to reach $|\bar{m}_j\rangle$. We now have:

$$\hat{\mathcal{H}}\,|\bar{n}(\mathbf{k})\rangle = \frac{1}{\sqrt{N_n}} \sum_j \sum_{l=0}^{M/2-1} e^{-il\mathbf{k}\cdot\mathbf{R}} \hat{T}^{l+d_j}\alpha_j\,|\bar{m}_j\rangle = \sum_j \frac{\alpha_j e^{id_j\mathbf{k}\cdot\mathbf{R}}}{\sqrt{\mathcal{N}_n}} \sum_{l=0}^{M/2} e^{-i(l+d_j)\mathbf{k}\cdot\mathbf{R}} T^{l+d_j}\,|\bar{m}_j\rangle\,. \tag{6.11}$$

Again, we can use the periodicity of the lattice to change the summation index $l+d_j \to l$ in the last term. We can recognize this as the state $|\bar{m}_j(\mathbf{k})\rangle$ up to a numerical factor of $\sqrt{\mathcal{N}_m}$. This yields the final result that:

$$\hat{\mathcal{H}}\,|\bar{n}(\mathbf{k})\rangle = \sum_j \alpha_j e^{id_j\mathbf{k}\cdot\mathbf{R}} \sqrt{\frac{\mathcal{N}_m}{\mathcal{N}_n}}\,|\bar{m}_j(\mathbf{k})\rangle \boxed{\Rightarrow\ \langle\bar{m}_j(\mathbf{k})|\hat{\mathcal{H}}_j|\bar{n}(\mathbf{k})\rangle = \langle m_j|\hat{\mathcal{H}}_j|\bar{n}\rangle\, e^{id_j\mathbf{k}\cdot\mathbf{R}} \sqrt{\frac{N_n}{N_m}}.} \tag{6.12}$$

For a diagonal operator, the matrix element will simply be $\langle\bar{n}|\hat{\mathcal{H}}|\bar{n}\rangle$ since $d_j = 0$.

7 The Lanczos Algorithm

We've seen how to construct the matrix representation of a correlated electron Hamiltonian on a lattice, as well as how to use symmetries to reduce the dimension of the basis. We're now ready to discuss how to diagonalize the Hamiltonian and find its eigenvalues and eigenstates. There are powerful numerical algorithms for full matrix diagonalization that produce the full spectrum, however these scale like $\mathcal{O}(d^3)$ where d is the dimension of the matrix, making this completely intractable for even moderately sized systems. Instead, we can use two facts. First, correlated phenomena are only present at very low temperatures. Hence, we're only interested in the ground state and a few excited states of the Hamiltonian. Second, we saw that the Hamiltonian can be very sparse. As it turns out, there exists a numerical scheme that finds the ground state of sparse hermitian matrices: the Lanczos algorithm.

7.1 Power method

The goal here is to solve the time independent Schrödinger equation for the ground state:

$$\hat{\mathcal{H}} \left|\psi_0\right\rangle = E_0 \left|\psi_0\right\rangle , \tag{7.1}$$

where E_0 is the ground state energy and $|\psi_0\rangle$ is the ground state eigenvector. The power method [6] is used to determine the dominant eigenvalue of a Hermitian matrix $\hat{\mathcal{H}}$. The dominant eigenvalue has the greatest modulus of all the eigenvalues. By introducing a spectral shift, we can make the ground state E_0 have the maximal eigenvalue. The spectral shift is given by:

$$\hat{\mathcal{H}}' = \hat{\mathcal{H}} - \lambda_s. \tag{7.2}$$

This transformation has the effect of adding a constant offset λ_s to the eigenvalues but leaves the spectrum unchanged. If λ_s is large enough, then the ground state will become the dominant eigenvalue. In the power method, we start with a random initial vector $|\phi_0\rangle$, which can be expanded in the eigenbasis of the Hamiltonian:

$$\left|\phi\right\rangle = \sum_n c_n \left|\psi_n\right\rangle .$$

Then, we repeatedly apply the Hamiltonian $\hat{\mathcal{H}}'$ to this state. After k iterations, we have:

$$\left|\tilde{\phi}_k\right\rangle = \hat{\mathcal{H}}'^k \left|\phi_0\right\rangle = \sum_n c_n E_n'^k \left|\psi_n\right\rangle = E_0'^k \left(c_0 \left|\psi_0\right\rangle + \sum_n c_n \left(\frac{E_n'}{E_0'}\right)^k \left|\psi_n\right\rangle \right). \tag{7.3}$$

Since $|E_0'|/|E_n'| < 1$, the expression gains an increasingly large component along the ground state eigenvector $|\psi_0\rangle$. After normalizing equation 7.3, we get the following expression:

$$\left|\phi_k\right\rangle = \frac{c_0 \left|\psi_0\right\rangle + \sum_n c_n \left(\frac{E_n'}{E_0'}\right)^k \left|\psi_n\right\rangle}{\sqrt{|c_0|^2 + \sum_n |c_n|^2 \left(\frac{E_n'}{E_0'}\right)^{2k}}} \overset{k\to\infty}{\to} e^{i\theta} \left|\psi_0\right\rangle . \tag{7.4}$$

The power method returns the ground state eigenvector up to a phase from which we can extract the ground state energy by computing the expectation value: $\langle\phi_k|\hat{\mathcal{H}}|\phi_k\rangle \approx E_0$. The power method as we've presented it relies on two assumptions: 1) that $|\phi_0\rangle$ is not orthogonal to $|\psi_0\rangle$ and 2) that the ground state is non-degenerate. If it is, the power method will project us in the degenerate subspace.

7.2 Lanczos algorithm

The Lanczos algorithm [7] is a more sophisticated variant of the power method that uses all of the information it provides. This section closely follows the explanations from [8]. In the Lanczos algorithm, brings the Hamiltonian to tri-diagonal form by constructing its *Krylov space* [9]. The Krylov space of the Hamiltonian is given by:

$$\mathcal{K} = \{|\phi_0\rangle, \hat{\mathcal{H}}|\phi_0\rangle, \hat{\mathcal{H}}^2|\phi_0\rangle, \ldots\}. \tag{7.5}$$

In the Lanczos method, one again starts with a random normalized vector $|\phi_0\rangle$. At each Lanczos iteration, we generate the next vector in the orthogonalized Krylov basis, which we call the Lanczos basis, using the Gram-Schmidt procedure [10]. Supposing we have generated. Assuming we have generated $k+1$ orthonormal Lanczos vectors, the next one is obtained using:

$$\begin{aligned} |\tilde{\phi}_{k+1}\rangle &= \hat{\mathcal{H}}|\phi_k\rangle - \alpha_k|\phi_k\rangle - \beta_k|\phi_{n-1}\rangle, \quad \alpha_k = \langle\phi_k|\hat{\mathcal{H}}|\phi_k\rangle, \quad \beta_n = \langle\phi_{k-1}|\hat{\mathcal{H}}|\phi_k\rangle \\ |\phi_{k+1}\rangle &= \frac{|\tilde{\phi}_{k+1}\rangle}{||\,|\tilde{\phi}_{k+1}\rangle\,||}. \end{aligned} \tag{7.6}$$

We can explicitly verify that this constructs the Lanczos basis by induction. Letting $|\phi_{-1}\rangle = \mathbf{0}$, we see that: $|\tilde{\phi}_1\rangle = \hat{\mathcal{H}}|\phi_0\rangle - \alpha_0|\phi_0\rangle$ is orthogonal to $|\phi_0\rangle$ since $\langle\phi_0|\tilde{\phi}_1\rangle = \langle\phi_0|\hat{\mathcal{H}}|\phi_0\rangle - \langle\phi_0|\hat{\mathcal{H}}|\phi_0\rangle = 0$. At the next iteration, we get:

$$|\tilde{\phi}_2\rangle = \hat{\mathcal{H}}|\phi_1\rangle - \alpha_1|\phi_1\rangle - \beta_1|\phi_0\rangle.$$

We can explicitly compute the overlap of this new vector with the previous ones: $\langle\phi_1|\tilde{\phi}_2\rangle = \langle\phi_1|\hat{\mathcal{H}}|\phi_1\rangle - \langle\phi_1|\hat{\mathcal{H}}|\phi_1\rangle\langle\phi_1|\phi_1\rangle - \langle\phi_0|\hat{\mathcal{H}}|\phi_1\rangle\langle\phi_0|\phi_1\rangle = 0$ and $\langle\phi_0|\tilde{\phi}_2\rangle = \langle\phi_0|\hat{\mathcal{H}}|\phi_1\rangle - \langle\phi_1|\hat{\mathcal{H}}|\phi_1\rangle\langle\phi_0|\phi_1\rangle - \langle\phi_0|\hat{\mathcal{H}}|\phi_1\rangle\langle\phi_0|\phi_0\rangle = 0$. Then, supposing that the $k+1$ previous vectors $\{|\phi_0\rangle, |\phi_1\rangle, \ldots|\phi_k\rangle\}$ are orthonormal, we can complete the proof by first taking the overlap of equation 7.6 with the two previous vectors:

$$\begin{aligned} \langle\phi_k|\tilde{\phi}_{k+1}\rangle &= \langle\phi_k|\hat{\mathcal{H}}|\phi_k\rangle - \alpha_k - \beta_k\langle\phi_k|\phi_{k-1}\rangle = \alpha_k - \alpha_k = 0 \\ \langle\phi_{k-1}|\tilde{\phi}_{k+1}\rangle &= \langle\phi_{k-1}|\hat{\mathcal{H}}|\phi_k\rangle - \beta_k = \beta_k - \beta_k = 0. \end{aligned} \tag{7.7}$$

Then we look at the overlap with all vectors $|\phi_j\rangle$, $j \leq k-2$. This gives:

$$\langle\phi_j|\tilde{\phi}_{k+1}\rangle = \langle\phi_j|\hat{\mathcal{H}}|\phi_k\rangle - \alpha_k\langle\phi_j|\phi_k\rangle - \beta_k\langle\phi_j|\phi_{k-1}\rangle = \langle\phi_j|\hat{\mathcal{H}}|\phi_k\rangle. \tag{7.8}$$

The matrix element of the Hamiltonian between two Lanczos vectors such that $j \leq k-2$ can be evaluated using the fact that $\hat{\mathcal{H}}$ is Hermitian and that $\hat{\mathcal{H}}|\phi_j\rangle = |\phi_{j+1}\rangle + \alpha_j|\phi_j\rangle + \beta_j|\phi_j\rangle$. We can write this as:

$$\langle\phi_j|\hat{\mathcal{H}}|\phi_k\rangle = \langle\phi_k|\hat{\mathcal{H}}|\phi_j\rangle^* = \langle\phi_k|\left(|\phi_{j+1}\rangle + \alpha_j|\phi_j\rangle + \beta_j|\phi_j\rangle\right)^* = 0. \tag{7.9}$$

This shows that each Lanczos vector generated is orthogonal to all previous ones. It also tells us that in the Lanczos basis, the Hamiltonian takes a tri-diagonal form:

$$\hat{\mathcal{H}} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & 0 & \ldots \\ \beta_0 & \alpha_1 & \beta_1 & 0 & \ldots \\ 0 & \beta_1 & \alpha_2 & \beta_2 & \ldots \\ 0 & 0 & \beta_2 & \alpha_3 & \ldots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix} \tag{7.10}$$

The size of the Hamiltonian in the Lanczos basis is usually taken to be a few tens or hundreds of rows. Each time we find new matrix elements using the Lanczos vectors, we diagonalize the corresponding tri-diagonal matrix which gives us an estimate for the energy. Then, we check the difference in magnitude with the previous energy to see if it has converged to within some tolerance. Diagonalizing a small tri-diagonal matrix is extremely fast.

References

[1] John Hubbard. Electron correlations in narrow energy bands. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences*, 276(1365):238–257, 1963.

[2] Richard T Scalettar. An introduction to the hubbard hamiltonian. *quantum materials: experiments and theory*, 6, 2016.

[3] Assa Auerbach. *Interacting electrons and quantum magnetism*. Springer Science & Business Media, 2012.

[4] Daniel P Arovas, Erez Berg, Steven A Kivelson, and Srinivas Raghu. The hubbard model. *Annual review of condensed matter physics*, 13:239–274, 2022.

[5] Efthimios Kaxiras and John D Joannopoulos. *Quantum theory of materials*. Cambridge university press, 2019.

[6] Herman Müntz et al. Solution directe de l'équation séculaire et de quelques problemes analogues transcendants. *CR Acad. Sci. Paris*, 156:43–46, 1913.

[7] Cornelius Lanczos. An iteration method for the solution of the eigenvalue problem of linear differential and integral operators. 1950.

[8] E. Arrigoni Wolfgang von der Linden. Extract from the lecture notes "Numerical Many Body Physics". `https://itp.tugraz.at/~evertz/QD/Ref/CP_mbook.pdf`, 2010.

[9] Aleksey Nikolaevich Krylov. On the numerical solution of the equation by which in technical questions frequencies of small oscillations of material systems are determined. *Izvestija AN SSSR (News of Academy of Sciences of the USSR), Otdel. mat. i estest. nauk*, 7(4):491–539, 1931.

[10] Ward Cheney and David Kincaid. Linear algebra: Theory and applications. *The Australian Mathematical Society*, 110:544–550, 2009.

A Hubbard dimer

In this section, we explicitly calculate the Hamiltonian matrix elements for the Hubbard dimer with periodic boundary conditions:

$$\hat{\mathcal{H}} = -t\left(\hat{c}^\dagger_{1\uparrow}\hat{c}_{2\uparrow} + \hat{c}^\dagger_{2\uparrow}\hat{c}_{1\uparrow} + \hat{c}^\dagger_{1\downarrow}\hat{c}_{2\downarrow} + \hat{c}^\dagger_{2\downarrow}\hat{c}_{1\downarrow}\right) + U\left(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{1\uparrow}\hat{n}_{1\downarrow}\right). \tag{A.1}$$

The size of the full basis is $4^2 = 16$. We list the basis states sorted in 2. Now, we can begin explicitly calculating the matrix elements.

$$\begin{aligned}
&\hat{\mathcal{H}}\left|\downarrow,0\right\rangle = -t\hat{c}^\dagger_{2\downarrow}\hat{c}_{1\downarrow}\hat{c}^\dagger_{1\uparrow} = -t\left|0,\downarrow\right\rangle, \quad \hat{\mathcal{H}}\left|0,\downarrow\right\rangle = -t\left|\downarrow,0\right\rangle \\
&\hat{\mathcal{H}}\left|\uparrow,0\right\rangle = -t\left|\uparrow,0\right\rangle, \quad \hat{\mathcal{H}}\left|0,\uparrow\right\rangle = -t\left|\uparrow,0\right\rangle \\
&\hat{\mathcal{H}}\left|\downarrow,\uparrow\right\rangle = -t\left|\downarrow\uparrow,0\right\rangle - t\left|0,\downarrow\uparrow\right\rangle, \quad \hat{\mathcal{H}}\left|\uparrow,\downarrow\right\rangle = -t\left|0,\downarrow\uparrow\right\rangle - t\left|\downarrow\uparrow,0\right\rangle \\
&\hat{\mathcal{H}}\left|\downarrow\uparrow,0\right\rangle = -t\left|\downarrow,\uparrow\right\rangle - t\left|\uparrow,\downarrow\right\rangle + U\left|\downarrow\uparrow,0\right\rangle, \quad \hat{\mathcal{H}}\left|0,\downarrow\uparrow\right\rangle = -t\left|\downarrow,\uparrow\right\rangle - t\left|\uparrow,\downarrow\right\rangle + U\left|0,\downarrow\uparrow\right\rangle \\
&\hat{\mathcal{H}}\left|\downarrow\uparrow,\downarrow\right\rangle = -t\left|\downarrow,\downarrow\uparrow\right\rangle + U\left|\downarrow\uparrow,\downarrow\right\rangle, \quad \hat{\mathcal{H}}\left|\downarrow,\downarrow\uparrow\right\rangle = -t\left|\downarrow\uparrow,\downarrow\right\rangle + U\left|\downarrow,\downarrow,\uparrow\right\rangle \\
&\hat{\mathcal{H}}\left|\uparrow\downarrow,\uparrow\right\rangle = -t\left|\uparrow,\downarrow\uparrow\right\rangle + U\left|\uparrow\downarrow,\uparrow\right\rangle, \quad \hat{\mathcal{H}}\left|\uparrow,\downarrow\uparrow\right\rangle = -t\left|\downarrow\uparrow,\uparrow\right\rangle + U\left|\uparrow,\downarrow\uparrow\right\rangle \\
&\hat{\mathcal{H}}\left|\downarrow\uparrow,\downarrow\uparrow\right\rangle = 2U\left|\downarrow\uparrow,\downarrow\uparrow\right\rangle.
\end{aligned} \tag{A.2}$$

state	particle number	S^z
$\|0,0\rangle$	0	0
$\|\downarrow,0\rangle$, $\|0,\downarrow\rangle$	1	-1/2
$\|\uparrow,0\rangle$, $\|0,\uparrow\rangle$	1	1/2
$\|\downarrow,\downarrow\rangle$	2	-1
$\|\downarrow,\uparrow\rangle$, $\|\uparrow,\downarrow\rangle$, $\|\downarrow\uparrow,0\rangle$, $\|0,\downarrow\uparrow\rangle$	2	0
$\|\uparrow,\uparrow\rangle$	2	1
$\|\downarrow\uparrow,\downarrow\rangle$, $\|\downarrow,\downarrow\uparrow\rangle$	3	-1/2
$\|\downarrow\uparrow,\uparrow\rangle$, $\|\uparrow,\downarrow\uparrow\rangle$	3	1/2
$\|\downarrow\uparrow,\downarrow\uparrow\rangle$	4	0

Table 2: Full basis of the Hubbard dimer ordered from increasing particle number and then increasing total S^z.

When using symmetries, the integer representation of a particular state does not correspond to its position in the basis. Hence, we construct a hash table where the keys are the basis states and the values are their position in the basis.

B The translation operator

B.1 Definition

In this section, we introduce the translation operator $\hat{T}(\mathbf{R})$. It is defined by its action on an eigenvector of the position operator:

$$\hat{T}(\mathbf{R})\left|\mathbf{r}\right\rangle = \left|\mathbf{r}+\mathbf{R}\right\rangle. \tag{B.1}$$

From this definition alone, we can infer its properties. For example, $\hat{T}(\mathbf{R}')\hat{T}(\mathbf{R}) = \hat{T}(\mathbf{R}+\mathbf{R}')$, which means that $\hat{T}^{-1}(\mathbf{R}) = \hat{T}(-\mathbf{R})$. We also see that $\hat{T}(\mathbf{R})$ is unitary since it preserves the norm of kets. This means that $\hat{T}^{\dagger}(\mathbf{R}) = \hat{T}(-\mathbf{R})$. Let's find the matrix elements of the translation operator in the momentum basis $\mathbf{p} = \hbar\mathbf{k}$:

$$\begin{aligned}
\langle \mathbf{k}'|\hat{T}(\mathbf{R})|\mathbf{k}\rangle &= \int \mathrm{d}^3\mathbf{r}'\mathrm{d}^3\mathbf{r}\, \langle \mathbf{k}'|\mathbf{r}'\rangle\ \langle \mathbf{r}'|\hat{T}(\mathbf{R})|\mathbf{r}\rangle\, \langle \mathbf{r}|\mathbf{k}\rangle \\
&= \frac{1}{\mathcal{N}} \int \mathrm{d}^3\mathbf{r}\mathrm{d}^3\mathbf{r}' e^{i\mathbf{k}'\cdot\mathbf{r}'} e^{-i\mathbf{k}\cdot\mathbf{r}} \delta(\mathbf{r}+\mathbf{R}-\mathbf{r}') \\
&= \frac{1}{\mathcal{N}} \int \mathrm{d}^3\mathbf{r} e^{-i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')} e^{i\mathbf{k}\cdot\mathbf{R}} \\
&= e^{i\mathbf{k}\cdot\mathbf{R}}\delta(\mathbf{k}-\mathbf{k}'). \qquad \text{(B.2)}
\end{aligned}$$

So we conclude that the translation operator is diagonal in the momentum basis and has eigenvalues $e^{i\mathbf{k}\cdot\mathbf{R}}$.

B.2 Four site Heisenberg chain

We consider the basis states of a four site Heisenberg chain at 0 spin and their integer representation:

$$\{|\downarrow\downarrow\uparrow\uparrow\rangle = |3\rangle, |\downarrow\uparrow\downarrow\uparrow\rangle = |5\rangle, |\downarrow\uparrow\uparrow\downarrow\rangle = |6\rangle, |\uparrow\downarrow\downarrow\uparrow\rangle = |9\rangle, |\uparrow\downarrow\uparrow\downarrow\rangle = |10\rangle, |\uparrow\uparrow\downarrow\downarrow\rangle = |12\rangle\}$$

If the states are labelled in such a way that shifting spins one entry to the right in the ket representation corresponds to a translation by $\mathbf{a}_1$, we see that we can construct two cycles of states:

$$\mathcal{C}_3 = \{|3\rangle, |9\rangle, |12\rangle, |6\rangle\}, \quad \mathcal{C}_5 = \{|5\rangle, |10\rangle\}. \qquad \text{(B.3)}$$

The periodicities are $N_3 = 4$ and $N_5 = 2$. By ordering the basis like in equation B.3, we can represent the translation operator as a matrix:

$$\hat{T} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \qquad \text{(B.4)}$$

It takes the form of a permutation matrix. We can even compute its spectrum, noting that it decouples into one 4×4 block and one 2×2 block. For the lower 2×2 block, we have: $\lambda^2 = 1 \Rightarrow \lambda = \pm 1$. And for the upper 4×4 block, we have $\lambda^4 = 1 \Rightarrow \lambda = \pm 1, \pm i$. The reciprocal supercell vector is $\mathbf{B}_1 = \mathbf{b}_1/N_c$, so there are 4 allowed values of $\mathbf{k} = k\mathbf{B}_1$. The phase will be $\mathbf{k}\cdot\mathbf{a}_1 = 2\pi k/4 = k\pi/2$

k	phase	eigenvalue
0	e^{0}	1
1	$e^{i\pi/2}$	i
2	$e^{i\pi}$	-1
3	$e^{i3\pi/2}$	$-i$

Table 3: Allowed values of k and the corresponding eigenvalue $e^{i\mathbf{k}\cdot\mathbf{a}_1}$ of $\hat{T}$ for the 4 site Heisenberg chain.

The allowed k and the corresponding eigenvalues of $\hat{T}$ are listed in table 3. For all the values of k, the eigenvector corresponding to $\mathcal{C}_3$ is given by:

$$|\bar{3}(k)\rangle = \frac{1}{2}\left(|3\rangle + e^{-i\pi k/2}\,|9\rangle + e^{-i\pi k}\,|12\rangle + e^{-3i\pi k/2}\,|6\rangle\right). \tag{B.5}$$

For the cycle $\mathcal{C}_5$, the only allowed values of k are such that $k\pi = 2\pi$ which means that $k = 0$ or 2 and in these cases, the eigenvectors are given by:

$$|\bar{5}(k)\rangle = \frac{1}{2\sqrt{2}}\left(2\,|5\rangle + 2e^{-i\pi k/2}\,|10\rangle\right). \tag{B.6}$$

Let's now build the matrix representation of $\hat{\mathcal{H}}$ in this basis. We start by computing the matrix elements for the individual Fock states, using that fact that the distinct pairs of first neighbors are $(3,0),(1,0),(2,1),(3,2)$.

$$\langle\bar{3}(k)|\hat{\mathcal{H}}|\bar{3}(k)\rangle = 0, \quad \langle\bar{5}(k)|\hat{\mathcal{H}}|\bar{3}(k)\rangle = \frac{1}{\sqrt{2}}(1 + e^{ik\pi/2}), \quad \langle\bar{5}(k)|\hat{\mathcal{H}}|\bar{5}(k)\rangle = 1/2. \tag{B.7}$$

Using this, we can write the matrix representation for the Hamiltonian. It will take a block diagonal form where each block corresponds to fixed k sector:

$$\hat{\mathcal{H}} = \begin{pmatrix} 0 & \frac{2}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ \frac{2}{\sqrt{2}} & 1/2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1+i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1-i}{\sqrt{2}} & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{B.8}$$