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Implementing superconducting corrections to the ground state Hamiltonian in `MeanFi`

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Abstract

Understanding the ground-state properties of many-body systems is a computational challenge in condensed-matter physics. `MeanFi` is a Python package that performs self-consistent Hartree-Fock calculations on non-superconducting tight-binding models and aims to find the ground state solution of a Hamiltonian with density-density interactions. This thesis presents how this package is generalized to also perform these calculations for superconducting tight-binding models. First, a complete derivation of the mean-field expansion is given by applying Wick's contractions and the mean-field approximation. This expansion is then transformed into the Bogoliubov-de Gennes basis to explicitly include superconducting terms in the Hamiltonian. Second, the self-consistency criterion is adapted by constraining the solution space by enforcing symmetries on the solution by using `Qsymm`. Third, finite-temperature calculations are added to the algorithm and the total charge of the system replaces the electron filling-factor that was used in `MeanFi`, introducing a minimization problem to the algorithm. Last, the updated algorithm is applied to a 1D-Hubbard model with attractive interactions and the resulting superconducting gap as a function of temperature matches theoretical predictions from BCS-theory.

1 Introduction

Superconductivity is a state of matter observed in some materials where electrical resistance vanishes and magnetic fields are expelled.[1] As the electrical resistance vanishes, superconductors can conduct electricity with very little heat dissipation.[2] Practical applications of superconductors include systems that require strong magnetic fields; MRI scanners are an example of such a system.[3] Superconducting materials have material-dependent critical parameters that determine their suitability for different applications. The critical temperature, the temperature under which a material can be superconducting, is one example of such a parameter. Two more parameters are the critical current and critical field of a superconductor. These are the maximum current and maximum magnetic field that a superconductor can withstand before losing its superconducting properties. Understanding these parameters supports both scientific innovation and practical development.

While material properties can be measured experimentally, theoretical understanding is essential for interpreting results and making predictions. It helps guide which variables to measure and what outcomes to expect. If observations deviate from expectations, theory aids in identifying experimental errors or uncovering novel effects.

Developing a theoretical understanding of the properties of a physical system can be done through its ground state. The ground state encodes many of the system's physical properties, and various observables can be derived directly from it. The ground state of a system is the lowest energy solution to the Hamiltonian of that system. The Hamiltonian captures all relevant interactions within a material, both for individual particles and for interactions between multiple particles. In superconducting systems, for example, the Hamiltonian describes how electrons can interact attractively to form Cooper pairs, which leads to the superconducting properties of a material.[4,5]

Ground states can sometimes be found analytically when systems have few degrees of freedom.[6] In materials however, the Hamiltonian will include a lot of interactions because of the many atoms these systems contain. The number of degrees of freedom grows exponentially with the number of atoms in a system, making it impossible to find an analytical solution. If a system has only a few particles it could be possible to find a solution through direct numerical approximation, but the system size will be limited by what is computationally feasible.[7]

Generally, for many-body systems, approximation have to be made to simplify the interaction in the Hamiltonian to avoid computational issues. Mean-field theory is one example of an approximation used for finding solutions to many-body problems.[8] It replaces interactions on individual particles with an average field from all other particles, reducing the many-body problem to an effective single-particle one. Solutions for a Hamiltonian approximated using a mean-field method are good approximations for the ground state of the original many-body Hamiltonian when there are no big fluctuations from the ground state in the system.[9]

`MeanFi` is a Python package that performs mean-field calculations on tight-binding models for non-superconducting systems.[10] We extend the package to also handle superconducting systems. To achieve this we derive the mean-field approximation of the density-density many-body Hamiltonian with superconducting terms and transform it to the Bogoliubov-de Gennes basis which allows us to diagonalize the Hamiltonian and find a ground state solution for it. Additionally, we add finite-temperature effects to the algorithm and interface `MeanFi` with `Qsymm` to impose symmetry constraints and optimize performance.[11]

2 Second Quantization

Second quantization is a formalism used to describe quantum many-body systems. A many-body system contains many particles in various states, which can be cumbersome to describe using standard bra-ket notation. If the basis of possible states is $\{|0\rangle, |1\rangle, |2\rangle, \dots\}$, then the complete state of the system is some combination of all particles with all of their respective states. A state $|i\rangle$ can encode both the state of the particle and the location of a particle in a system. Second quantization treats particles as indistinguishable and describes the full system by specifying the occupation number of each basis state:

$$|n_1, n_2, n_3, \dots\rangle. \tag{1}$$

Here n_i refers to the number of particles in state $|i\rangle$. A state like equation 1 is called a Fock state and all Fock states form a complete basis of the many-body Hilbert space. Any generic quantum many-body state can be expressed as a linear combination of Fock states.

In the second quantization representation there are operators that act on a system which add or remove a particle. These operators are known as the raising or creation operator $\hat{a}^\dagger$ and lowering or annihilation operator $\hat{a}$ respectively. On a single-particle state, the operators act as follows:

$$\begin{aligned} \hat{a}^\dagger|0\rangle &= |1\rangle, \\ \hat{a}|1\rangle &= |0\rangle, \\ \hat{a}|0\rangle &= 0, \end{aligned} \tag{2}$$

where $|0\rangle$ is the vacuum state. The last formula in equation 2 follows from it being impossible to lower the ground state further. Applying these operators to a Fock state will either add a particle or remove a particle in a certain state:

$$\begin{aligned} \hat{a}_i^\dagger|n_1, n_2, \dots, n_i, \dots\rangle &= |n_1, n_2, \dots, n_i + 1, \dots\rangle, \\ \hat{a}_i|n_1, n_2, \dots, n_i + 1, \dots\rangle &= |n_1, n_2, \dots, n_i, \dots\rangle, \end{aligned} \tag{3}$$

with $\hat{a}_i^\dagger$ the creation operator acting on state $|i\rangle$ and $\hat{a}_i$ the respective annihilation operator.

The operators have certain commutation and anti-commutation identities depending on the type of operator. Specifically, bosonic and fermionic operators commute and anti-commute respectively. For bosons, the commutation relations are as follows:

$$\begin{aligned} [\hat{a}_k, \hat{a}_q^\dagger] &= \hat{a}_k\hat{a}_q^\dagger - \hat{a}_q^\dagger\hat{a}_k = \delta_{kq}\hat{\mathbb{I}}, \\ [\hat{a}_k, \hat{a}_q] &= \hat{a}_k\hat{a}_q - \hat{a}_q\hat{a}_k = \hat{0}, \\ [\hat{a}_k^\dagger, \hat{a}_q^\dagger] &= \hat{a}_k^\dagger\hat{a}_q^\dagger - \hat{a}_q^\dagger\hat{a}_k^\dagger = \hat{0}. \end{aligned} \tag{4}$$

From these identities, we can also see that swapping the order of operators is symmetric. $\hat{a}_k\hat{a}_q = \hat{a}_q\hat{a}_k$. In general, it is possible to write any operator acting on a many-body state as a sum of products of creation and annihilation operators:

$$\hat{O} = \sum_{ijkl\dots} C_{ijkl\dots}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l\dots. \tag{5}$$

The position and momentum operators for a quantum harmonic oscillator are an example of this:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^\dagger - \hat{a}). \tag{6}$$

Fermionic operators must anti-commute due to the Pauli Exclusion principle and are antisymmetric when exchanged, so we know that $\hat{c}_k^\dagger\hat{c}_k^\dagger = 0$ and that $\hat{c}_k\hat{c}_q = -\hat{c}_q\hat{c}_k$.[12] For fermionic operators, we have these similar anti-commutation relations:

$$\begin{aligned} \{\hat{c}_k, \hat{c}_q^\dagger\} &= \hat{c}_k\hat{c}_q^\dagger + \hat{c}_q^\dagger\hat{c}_k = \delta_{kq}\hat{\mathbb{I}}, \\ \{\hat{c}_k, \hat{c}_q\} &= \hat{c}_k\hat{c}_q + \hat{c}_q\hat{c}_k = \hat{0}, \\ \{\hat{c}_k^\dagger, \hat{c}_q^\dagger\} &= \hat{c}_k^\dagger\hat{c}_q^\dagger + \hat{c}_q^\dagger\hat{c}_k^\dagger = \hat{0}. \end{aligned} \tag{7}$$

For this thesis, a relevant example of a fermionic operator would be the Hamiltonian of a tight-binding system:

$$\hat{H} = \sum_{ij} h_{ij} \hat{c}_i^\dagger \hat{c}_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l, \tag{8}$$

where h_{ij} corresponds to the hopping between states $|i\rangle$ and $|j\rangle$ and v_{ijkl} corresponds to the interaction between multiple particles in states $|i\rangle$ and $|j\rangle$. In the context of the tight-binding Hamiltonian a product like $\hat{c}_i^\dagger \hat{c}_j$, means that we destroy a particle in state $|j\rangle$ and create one in state $|i\rangle$, denoting a hopping. For this thesis it is important to realize that the interacting term of the Hamiltonian also encodes the ability to create Cooper pairs, essential for superconductivity.[5] Specifically, any terms like $\hat{c}_i^\dagger \hat{c}_j^\dagger$ or $\hat{c}_i \hat{c}_j$ create or annihilate a pair of electrons respectively.

3 Wick's Contractions

The number of terms in the Hamiltonian in equation 8 grows exponentially with the number of possible states of the system. Every added particle increases the number of possible states and therefore also the complexity of the Hamiltonian. To be able to find a ground state solution for the tight-binding Hamiltonian we have to lower the order of the $\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l$ term. A tool that can help reduce the complexity of these terms is Wick's theorem.[13] Wick's theorem is a method to reduce arbitrary products of annihilation and creation operators to a sum of products of pairs of these operators.

To achieve this, Wick's theorem makes use of normal ordering of operators. Creation and annihilation operators are said to be normal ordered when all creation operators are left of all annihilation operators. The product in equation 8 is normal-ordered, but if the operators are shuffled like $\hat{c}_i^\dagger \hat{c}_j \hat{c}_k^\dagger \hat{c}_l$ you would normal-order it as follows:

$$: \hat{c}_i^\dagger \hat{c}_j \hat{c}_k^\dagger \hat{c}_l := -\hat{c}_i^\dagger \hat{c}_k^\dagger \hat{c}_j \hat{c}_l. \tag{9}$$

The normal ordered product's sign is flipped because the order of two operators had to be swapped. This happens specifically because the operators here are fermionic, bosonic products would not have their sign change.

Another mathematical concept used in Wick's theorem, contractions, are defined as follows for any two operators $\hat{A}$ and $\hat{B}$:

$$\overline{\hat{A}\hat{B}} = \hat{A}\hat{B} - : \hat{A}\hat{B} :, \tag{10}$$

where $: \hat{A}\hat{B} :$ is the normal-ordered product of the operators. In cases where $\hat{A}$ and $\hat{B}$ are equal to the creation or annihilation operators and by using the commutation relations from equation 7, we can find some relations for contractions. Normal ordering the operators in these special cases results in the contraction being equal to the commutation or anti-commutation relations shown in equation 11.

$$\begin{aligned}
\overline{\hat{c}_i \hat{c}_j^\dagger} &= \hat{c}_i \hat{c}_j^\dagger - : \hat{c}_i \hat{c}_j^\dagger := \{\hat{c}_i, \hat{c}_j^\dagger\} = && \delta_{ij}\hat{\mathbb{I}}, \\
\overline{\hat{c}_i^\dagger \hat{c}_j^\dagger} &= \hat{c}_i^\dagger \hat{c}_j^\dagger - : \hat{c}_i^\dagger \hat{c}_j^\dagger := \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = && 0, \\
\overline{\hat{c}_i \hat{c}_j} &= \hat{c}_i \hat{c}_j - : \hat{c}_i \hat{c}_j := \{\hat{c}_i, \hat{c}_j\} = && 0, \\
\overline{\hat{c}_i^\dagger \hat{c}_j} &= \hat{c}_i^\dagger \hat{c}_j - : \hat{c}_i^\dagger \hat{c}_j := && 0.
\end{aligned} \tag{11}$$

The last three relations can also be obtained through realizing that the contraction is already normal ordered. Furthermore, from equation 11, we note that contractions are c-numbers: The δ_{ij} is a scalar that commutes with all operators and does not act on the state.

Wick's theorem states that a string of operators can be written as the normal-ordered product of the string plus the normal ordered product of all possible contractions. A string of operators like $\hat{A}\hat{B}\hat{C}\hat{D}\hat{E}\hat{F}\ldots$ can be expressed as in equation 12.

$$\begin{aligned}
\hat{A}\hat{B}\hat{C}\hat{D}\hat{E}\hat{F}\cdots = &: \hat{A}\hat{B}\hat{C}\hat{D}\hat{E}\hat{F}\cdots : \\
&+ \sum_{\text{singles}} : \overline{\hat{A}\hat{B}}\hat{C}\hat{D}\hat{E}\hat{F}\cdots : \\
&+ \sum_{\text{doubles}} : \overline{\hat{A}\overline{\hat{B}\hat{C}}\hat{D}}\hat{E}\hat{F}\cdots : \\
&+ \ldots .
\end{aligned} \tag{12}$$

Applying Wick's theorem to the product in the tight-binding Hamiltonian in equation 8, the complex term is reduced to a sum of at most pairs of the operators in equation 13.

$$\begin{aligned}
\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l = &: \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l : \\
&+ : \overline{\hat{c}_i^\dagger \hat{c}_j^\dagger} \hat{c}_k \hat{c}_l : - : \overline{\hat{c}_i^\dagger \hat{c}_k} \hat{c}_j^\dagger \hat{c}_l : - : \overline{\hat{c}_i^\dagger \hat{c}_l} \hat{c}_k \hat{c}_j^\dagger : + : \overline{\hat{c}_j^\dagger \hat{c}_k} \hat{c}_i^\dagger \hat{c}_l : - : \overline{\hat{c}_j^\dagger \hat{c}_l} \hat{c}_i^\dagger \hat{c}_k : + : \overline{\hat{c}_k \hat{c}_l} \hat{c}_i^\dagger \hat{c}_j^\dagger : \\
&+ : \overline{\hat{c}_i^\dagger \hat{c}_j^\dagger}\, \overline{\hat{c}_k \hat{c}_l} : - : \overline{\hat{c}_i^\dagger \hat{c}_k}\, \overline{\hat{c}_j^\dagger \hat{c}_l} : - : \overline{\hat{c}_i^\dagger \hat{c}_l}\, \overline{\hat{c}_k \hat{c}_j^\dagger} : .
\end{aligned} \tag{13}$$

Flipping the signs of the different terms is a consequence of the anti-commutators in equations 7; Swapping the order of any two fermionic operators flips the sign.

A useful thing to realize about contractions is that they are commutators themselves. If we have two operators $\hat{A}$ and $\hat{B}$, which we know from equation 5 can be written as a sum of creation and annihilation operators, then the difference between $\hat{A}\hat{B}$ and $:\hat{A}\hat{B}:$ is just shuffling the creation and annihilation operators:

$$\begin{aligned}
\hat{A}\hat{B} = (\hat{A}^\dagger + \hat{A})(\hat{B}^\dagger \hat{B}) &= \hat{A}^\dagger \hat{B}^\dagger + \hat{A}^\dagger \hat{B} + \hat{A}\hat{B}^\dagger + \hat{A}\hat{B}, \\
: \hat{A}\hat{B} : &= \hat{A}^\dagger \hat{B}^\dagger + \hat{A}^\dagger \hat{B} - \hat{B}^\dagger \hat{A} + \hat{A}\hat{B}, \\
\hat{A}\hat{B} - : \hat{A}\hat{B} : &= \hat{A}\hat{B}^\dagger + \hat{B}^\dagger \hat{A} = \{\hat{A}, \hat{B}^\dagger\}.
\end{aligned} \tag{14}$$

In equation 14 we assume that the operators that make up $\hat{A}$ and $\hat{B}$ are fermionic; If they are bosonic the sign in the difference would be flipped, and we find a commutator instead. We will evaluate terms like $\langle gs|\hat{A}\hat{B}|gs\rangle$, a ground state expectation value of a string of operators, to find the mean-field approximation for the Hamiltonian. Inserting $\hat{A}\hat{B} = \overline{\hat{A}\hat{B}} + :\hat{A}\hat{B}:$ and realizing that a normal ordered product acting on the ground state $|gs\rangle$ is 0 allows us to find equation 15.

$$\langle \hat{A}\hat{B} \rangle = \langle gs|\hat{A}\hat{B}|gs\rangle = \langle gs|\overline{\hat{A}\hat{B}} + :\hat{A}\hat{B}:|gs\rangle = \langle gs|\overline{\hat{A}\hat{B}}|gs\rangle + \langle gs|:\hat{A}\hat{B}:|gs\rangle = \langle gs|\overline{\hat{A}\hat{B}}|gs\rangle = \langle \overline{\hat{A}\hat{B}} \rangle. \tag{15}$$

And because $\overline{\hat{A}\hat{B}}$ is a c-number, $\overline{\hat{A}\hat{B}} = \langle \overline{\hat{A}\hat{B}} \rangle = \langle \hat{A}\hat{B} \rangle$.

4 Derivation of the mean-field Hamiltonian

The tight-binding Hamiltonian in equation 8 captures the essential physics of electrons in a lattice, making it useful for effective models of materials. For this project we only consider density-density interactions in the system, so rather than $\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_l$ describing the interactions, we will set $i = k$ and $j = l$. The full tight-binding Hamiltonian consists of a non-interacting and an interacting term so for clarity we write the full Hamiltonian as follows:

$$\begin{aligned}
\hat{H} &= \sum_{ij} h_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ij} v_{ij} c_i^\dagger c_j^\dagger c_i c_j, \\
&= \hat{H}_0 + \hat{V},
\end{aligned} \tag{16}$$

where $\hat{H}_0$ and $\hat{V}$ correspond to the on-site and interacting terms respectively. Finding a ground state solution to this Hamiltonian means solving the Schrödinger equation:

$$\hat{H}|\Psi\rangle = E|\Psi\rangle, \tag{17}$$

where the ground state solution is the solution $|\Psi\rangle$ with the lowest energy E. We demonstrate how to find the mean-field approximation for the interacting term $\hat{V}_{\mathrm{MF}}$ by applying Wick's theorem and show how to rewrite the resulting term in the Bogoliubov-de Gennes basis to explicitly include superconducting pairing terms.[14] The resulting matrix representation of $\hat{H}_0 + \hat{V}_{\mathrm{MF}}$ is diagonalizable, and it is thus possible to find a ground state solution for $\hat{H}$.

The first step into finding $\hat{V}_{\mathrm{MF}}$ is to define what the mean-field approximation of an operator is. The mean-field approximation assumes that any fluctuations from the average field are small compared to that average, so the mean-field approximation is defined as follows:

$$\hat{A} = \langle \hat{A} \rangle + (\hat{A} - \langle \hat{A} \rangle), \tag{18}$$

where we assume that $\hat{A} - \langle \hat{A} \rangle \approx 0$. We also compute the mean-field approximation for a product of operators $\hat{A}\hat{B}$:

$$\begin{aligned}
\hat{A}\hat{B} &= (\langle \hat{A} \rangle + (\hat{A} - \langle \hat{A} \rangle))(\langle \hat{B} \rangle + (\hat{B} - \langle \hat{B} \rangle)), \\
&= \langle \hat{A} \rangle \langle \hat{B} \rangle + \langle \hat{A} \rangle (\hat{B} - \langle \hat{B} \rangle) + (\hat{A} - \langle \hat{A} \rangle)\langle \hat{B} \rangle + (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle), \\
&= \langle \hat{A} \rangle \langle \hat{B} \rangle + \langle \hat{A} \rangle \hat{B} - \langle \hat{A} \rangle \langle \hat{B} \rangle + \hat{A}\langle \hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle + (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle), \\
&\approx \langle \hat{A} \rangle \hat{B} + \hat{A}\langle \hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle.
\end{aligned} \tag{19}$$

From the mean-field approximation in equation 18 we find the mean-field approximation for the Hamiltonian $\hat{V}_{\text{MF}}$:

$$\hat{V} \approx \hat{V}_{\text{MF}} = \langle \hat{V} \rangle = \frac{1}{2} \sum_{ij} \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j \rangle. \tag{20}$$

The term $\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j \rangle$ can not be computed directly, so we apply Wick's theorem to find the single-particle operator sum from equation 13 but with $i = k$ and $j = l$:

$$\begin{aligned} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j = &: \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j : \\ &+ : \overline{\hat{c}_i^\dagger \hat{c}_j^\dagger} \hat{c}_i \hat{c}_j : - : \overline{\hat{c}_i^\dagger \hat{c}_i} \hat{c}_j^\dagger \hat{c}_j : - : \overline{\hat{c}_i^\dagger \hat{c}_j} \hat{c}_i \hat{c}_j^\dagger : + : \overline{\hat{c}_j^\dagger \hat{c}_i} \hat{c}_i^\dagger \hat{c}_j : - : \overline{\hat{c}_j^\dagger \hat{c}_j} \hat{c}_i^\dagger \hat{c}_i : + : \overline{\hat{c}_i \hat{c}_j} \hat{c}_i^\dagger \hat{c}_j^\dagger : \\ &+ : \overline{\hat{c}_i^\dagger \hat{c}_j^\dagger}\, \overline{\hat{c}_i \hat{c}_j} : - : \overline{\hat{c}_i^\dagger \hat{c}_i}\, \overline{\hat{c}_j^\dagger \hat{c}_j} : - : \overline{\hat{c}_i^\dagger \hat{c}_j}\, \overline{\hat{c}_i \hat{c}_j^\dagger} : . \end{aligned} \tag{21}$$

Combining the mean-field approximation in equation 19 with the expectation value of the contractions in equation 15, we establish two formulas to change contractions into products of expectation values and single-particle operators:

$$\begin{aligned} \overline{\hat{c}_i^\dagger \hat{c}_i}\, \overline{\hat{c}_j^\dagger \hat{c}_j} &\approx \langle \overline{\hat{c}_i^\dagger \hat{c}_i} \rangle \overline{\hat{c}_j^\dagger \hat{c}_j} + \overline{\hat{c}_i^\dagger \hat{c}_i} \langle \overline{\hat{c}_j^\dagger \hat{c}_j} \rangle - \langle \overline{\hat{c}_i^\dagger \hat{c}_i} \rangle \langle \overline{\hat{c}_j^\dagger \hat{c}_j} \rangle = \langle \hat{c}_i^\dagger \hat{c}_i \rangle \langle \hat{c}_j^\dagger \hat{c}_j \rangle, \\ \overline{\hat{c}_i^\dagger \hat{c}_i} : \hat{c}_j^\dagger \hat{c}_j : &\approx \langle \overline{\hat{c}_i^\dagger \hat{c}_i} \rangle : \hat{c}_j^\dagger \hat{c}_j : + \overline{\hat{c}_i^\dagger \hat{c}_i} \langle : \hat{c}_j^\dagger \hat{c}_j : \rangle - \langle \overline{\hat{c}_i^\dagger \hat{c}_i} \rangle \langle : \hat{c}_j^\dagger \hat{c}_j : \rangle = \langle \hat{c}_i^\dagger \hat{c}_i \rangle : \hat{c}_j^\dagger \hat{c}_j : . \end{aligned} \tag{22}$$

With these formulas applied and all operators normal-ordered and signs appropriately flipped, we find the full mean-field expansion:

$$\begin{aligned} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j = &: \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j : \\ &+ \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle \hat{c}_i \hat{c}_j - \langle \hat{c}_i^\dagger \hat{c}_i \rangle \hat{c}_j^\dagger \hat{c}_j + \langle \hat{c}_i^\dagger \hat{c}_j \rangle \hat{c}_j^\dagger \hat{c}_i + \langle \hat{c}_j^\dagger \hat{c}_i \rangle \hat{c}_i^\dagger \hat{c}_j - \langle \hat{c}_j^\dagger \hat{c}_j \rangle \hat{c}_i^\dagger \hat{c}_i + \langle \hat{c}_i \hat{c}_j \rangle \hat{c}_i^\dagger \hat{c}_j^\dagger \\ &+ \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle \langle \hat{c}_i \hat{c}_j \rangle - \langle \hat{c}_i^\dagger \hat{c}_i \rangle \langle \hat{c}_j^\dagger \hat{c}_j \rangle + \langle \hat{c}_i^\dagger \hat{c}_j \rangle \langle \hat{c}_j^\dagger \hat{c}_i \rangle. \end{aligned} \tag{23}$$

This expansion still contains a term $: \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j :$, but it is possible to subtract this term from both sides of the expansion to end up with pairs of operators on the right side, and a quadruple contraction on the left.

$$\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j - : \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j := \overline{\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j} \approx \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j \rangle. \tag{24}$$

The next step is to substitute this expansion into $\hat{V}_{\text{MF}}$ in equation 20:

$$\begin{aligned} \hat{V}_{\text{MF}} = \frac{1}{2} \sum_{ij} v_{ij} (&\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle \hat{c}_i \hat{c}_j - \langle \hat{c}_i^\dagger \hat{c}_i \rangle \hat{c}_j^\dagger \hat{c}_j + \langle \hat{c}_i^\dagger \hat{c}_j \rangle \hat{c}_j^\dagger \hat{c}_i + \langle \hat{c}_j^\dagger \hat{c}_i \rangle \hat{c}_i^\dagger \hat{c}_j - \langle \hat{c}_j^\dagger \hat{c}_j \rangle \hat{c}_i^\dagger \hat{c}_i + \langle \hat{c}_i \hat{c}_j \rangle \hat{c}_i^\dagger \hat{c}_j^\dagger) \\ &+ \frac{1}{2} \sum_{ij} v_{ij} (\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle \langle \hat{c}_i \hat{c}_j \rangle - \langle \hat{c}_i^\dagger \hat{c}_i \rangle \langle \hat{c}_j^\dagger \hat{c}_j \rangle + \langle \hat{c}_i^\dagger \hat{c}_j \rangle \langle \hat{c}_j^\dagger \hat{c}_i \rangle). \end{aligned} \tag{25}$$

In `MeanFi` the superconducting pairing terms containing $\hat{c}_i \hat{c}_j$ and $\hat{c}_i^\dagger \hat{c}_j^\dagger$ were neglected, but we retain these terms in our equations. From now on we do neglect the second sum of $\hat{V}_{\text{MF}}$ because this is a constant of motion. The exact value of this term can be calculated by evaluating $\langle 0 | \hat{V}_{\text{MF}} | 0 \rangle$ because all the terms with normal-ordered operators will go to zero and only the second sum will remain. This means that the full interacting mean-field Hamiltonian we consider is as follows:

$$\hat{V}_{\text{MF}} = \frac{1}{2} \sum_{ij} v_{ij} (\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle \hat{c}_i \hat{c}_j - \langle \hat{c}_i^\dagger \hat{c}_i \rangle \hat{c}_j^\dagger \hat{c}_j + \langle \hat{c}_i^\dagger \hat{c}_j \rangle \hat{c}_j^\dagger \hat{c}_i + \langle \hat{c}_j^\dagger \hat{c}_i \rangle \hat{c}_i^\dagger \hat{c}_j - \langle \hat{c}_j^\dagger \hat{c}_j \rangle \hat{c}_i^\dagger \hat{c}_i + \langle \hat{c}_i \hat{c}_j \rangle \hat{c}_i^\dagger \hat{c}_j^\dagger). \tag{26}$$

While the original single-particle operator basis remains valid, the presence of superconducting pairing terms in the Hamiltonian makes it less convenient for practical calculations. The Bogoliubov-de Gennes basis offers a more natural description of our system by combining particle and hole operators into single operators, preserving the bilinear structure of the original basis and simplifying the diagonalization of the Hamiltonian.[14] In this basis we define new operators $\hat{\Psi} = \begin{pmatrix} \vec{c} \\ \vec{c}^\dagger \end{pmatrix}$ and a matrix H_{BdG} such that the full form of the interacting mean-field Hamiltonian is

$$\hat{V}_{\text{MF}} = \frac{1}{2} \hat{\Psi}^\dagger H_{\text{BdG}} \hat{\Psi}. \tag{27}$$

In $\hat{\Psi}$ the $\overrightarrow{c}$ term corresponds with a vector of annihilation operators and creation operators for $\overrightarrow{c^\dagger}$. We think of this as the first half of $\hat{\Psi}$ being composed out of annihilation operators of electrons. The second half is made up of annihilation operators for an extra set of holes, that way doubling the degrees of freedom of the system. The matrix H_{BdG} has the following structure:

$$H_{\text{BdG}} = \begin{pmatrix} H & \Delta \\ \Delta^\dagger & -H \end{pmatrix}, \tag{28}$$

where through equation 27 we see that H will work on the $\hat{c}^\dagger\hat{c}$ terms and Δ on the $\hat{c}^\dagger\hat{c}^\dagger$ terms in $\hat{\Psi}$. All that remains is to rewrite $\hat{V}_{\text{MF}}$ in this new basis.

First we reframe the basis so that an operator $\hat{\Psi}_i = \begin{pmatrix} \hat{c}_i \\ \hat{c}_i^\dagger \end{pmatrix}$ corresponds to a vector where only the $|i\rangle$ state operators are non-zero:

$$\hat{\Psi} = \sum_i \hat{\Psi}_i. \tag{29}$$

We also say that $H_{ij} = \begin{pmatrix} \alpha_{ij} & \beta_{ij} \\ \gamma_{ij} & \eta_{ij} \end{pmatrix}$ where α_{ij} is the ij-th entry of the submatrix H of the main H_{BdG} matrix such that the sum of all H_{ij} is H_{BdG}. This allows us to write the full Hamiltonian as:

$$\hat{V}_{\text{MF}} = \frac{1}{2}\sum_{ij} \Psi_i^\dagger H_{ij} \Psi_j = \frac{1}{2}\sum_{ij} \begin{pmatrix} \hat{c}_i^\dagger & \hat{c}_i \end{pmatrix} \begin{pmatrix} \alpha_{ij} & \beta_{ij} \\ \gamma_{ij} & \eta_{ij} \end{pmatrix} \begin{pmatrix} \hat{c}_j \\ \hat{c}_j^\dagger \end{pmatrix}. \tag{30}$$

We compute the product inside the sum and find a familiar shape for the Hamiltonian:

$$\frac{1}{2}\sum_{ij} \Psi_i^\dagger H_{ij} \Psi_j = \frac{1}{2}\sum_{ij} \alpha_{ij}\hat{c}_i^\dagger\hat{c}_j + \beta_{ij}\hat{c}_i^\dagger\hat{c}_j^\dagger + \gamma_{ij}\hat{c}_i\hat{c}_j + \eta_{ij}\hat{c}_i\hat{c}_j^\dagger, \tag{31}$$

in which we recognize the pairs of operators we found in equation 26. The only terms from that equation that are not yet in equation 31 are the $\hat{c}_i^\dagger\hat{c}_i$ and $\hat{c}_j^\dagger\hat{c}_j$ terms. It is thankfully possible to group these together with other terms by isolating $\langle\hat{c}_i^\dagger\hat{c}_j\rangle\hat{c}_j^\dagger\hat{c}_i$ and $\langle\hat{c}_i^\dagger\hat{c}_i\rangle\hat{c}_j^\dagger\hat{c}_j$ in the sum and introducing an extra index:

$$\begin{aligned} \frac{1}{2}\sum_{ij} v_{ij}\langle\hat{c}_i^\dagger\hat{c}_j\rangle\hat{c}_j^\dagger\hat{c}_i - v_{ij}\langle\hat{c}_i^\dagger\hat{c}_i\rangle\hat{c}_j^\dagger\hat{c}_j &= \frac{1}{2}\left(\sum_{ij} v_{ij}\langle\hat{c}_i^\dagger\hat{c}_j\rangle\hat{c}_j^\dagger\hat{c}_i - \sum_{ijk} v_{ij}\langle\hat{c}_i^\dagger\hat{c}_i\rangle\hat{c}_j^\dagger\hat{c}_k\delta_{jk}\right), \\ &= \frac{1}{2}\left(\sum_{ij} v_{ij}\langle\hat{c}_i^\dagger\hat{c}_j\rangle\hat{c}_j^\dagger\hat{c}_i - \sum_{ijk} v_{kj}\langle\hat{c}_k^\dagger\hat{c}_k\rangle\hat{c}_j^\dagger\hat{c}_i\delta_{ij}\right), \\ &= \frac{1}{2}\left(\sum_{ij} v_{ij}\langle\hat{c}_i^\dagger\hat{c}_j\rangle\hat{c}_j^\dagger\hat{c}_i - \sum_{ij}\delta_{ij}\left(\sum_k v_{kj}\langle\hat{c}_k^\dagger\hat{c}_k\rangle\right)\hat{c}_j^\dagger\hat{c}_i\right), \\ &= \frac{1}{2}\left(\sum_{ij}\left(v_{ij}\langle\hat{c}_i^\dagger\hat{c}_j\rangle - \delta_{ij}\sum_k v_{kj}\langle\hat{c}_k^\dagger\hat{c}_k\rangle\right)\hat{c}_j^\dagger\hat{c}_i\right). \end{aligned} \tag{32}$$

We perform the exact same steps for the $\langle\hat{c}_j^\dagger\hat{c}_i\rangle\hat{c}_i^\dagger\hat{c}_j$ and $\langle\hat{c}_j^\dagger\hat{c}_j\rangle\hat{c}_i^\dagger\hat{c}_i$ terms and find a similar expression:

$$\frac{1}{2}\sum_{ij} v_{ij}\langle\hat{c}_j^\dagger\hat{c}_i\rangle\hat{c}_i^\dagger\hat{c}_j - v_{ij}\langle\hat{c}_j^\dagger\hat{c}_j\rangle\hat{c}_i^\dagger\hat{c}_i == \frac{1}{2}\left(\sum_{ij}\left(v_{ij}\langle\hat{c}_j^\dagger\hat{c}_i\rangle - \delta_{ij}\sum_k v_{ik}\langle\hat{c}_k^\dagger\hat{c}_k\rangle\right)\hat{c}_i^\dagger\hat{c}_j\right). \tag{33}$$

Substituting these two expressions into the mean-field approximation we find a V_{MF} ready to be transformed to the BdG basis:

$$\begin{aligned} \hat{V}_{\text{MF}} = \frac{1}{2}\sum_{ij} & \left(v_{ij}\langle\hat{c}_j^\dagger\hat{c}_i\rangle - \delta_{ij}\sum_k v_{ik}\langle\hat{c}_k^\dagger\hat{c}_k\rangle\right)\hat{c}_i^\dagger\hat{c}_j + v_{ij}\langle\hat{c}_i\hat{c}_j\rangle\hat{c}_i^\dagger\hat{c}_j^\dagger \\ & + v_{ij}\langle\hat{c}_i^\dagger\hat{c}_j^\dagger\rangle\hat{c}_i\hat{c}_j + \left(v_{ij}\langle\hat{c}_i^\dagger\hat{c}_j\rangle - \delta_{ij}\sum_k v_{kj}\langle\hat{c}_k^\dagger\hat{c}_k\rangle\right)\hat{c}_j^\dagger\hat{c}_i. \end{aligned} \tag{34}$$

To express H_{ij} in terms of our Hamiltonian we must determine $\alpha_{ij}, \beta_{ij}, \gamma_{ij}, \eta_{ij}$. We now read these off directly from equation 34:

$$\begin{aligned}
\alpha_{ij} &= \left(v_{ij} \langle \hat{c}_j^\dagger \hat{c}_i \rangle - \delta_{ij} \sum_k v_{ik} \langle \hat{c}_k^\dagger \hat{c}_k \rangle \right), \\
\beta_{ij} &= v_{ij} \langle \hat{c}_i \hat{c}_j \rangle, \\
\gamma_{ij} &= v_{ij} \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle, \\
\eta_{ij} &= - \left(v_{ij} \langle \hat{c}_i^\dagger \hat{c}_j \rangle - \delta_{ij} \sum_k v_{kj} \langle \hat{c}_k^\dagger \hat{c}_k \rangle \right),
\end{aligned} \tag{35}$$

where η_{ij}'s sign is flipped because the operator product in equation 31 was not normal ordered yet. We have now found the Hamiltonian in BdG representation with

$$H_{ij} = \begin{pmatrix} v_{ij} \langle \hat{c}_j^\dagger \hat{c}_i \rangle - \delta_{ij} \sum_k v_{ik} \langle \hat{c}_k^\dagger \hat{c}_k \rangle & v_{ij} \langle \hat{c}_i \hat{c}_j \rangle \\ v_{ij} \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle & - \left(v_{ij} \langle \hat{c}_i^\dagger \hat{c}_j \rangle - \delta_{ij} \sum_k v_{kj} \langle \hat{c}_k^\dagger \hat{c}_k \rangle \right) \end{pmatrix}, \tag{36}$$

where we recognize that the symmetries from equation 28 are maintained.

As a final simplification, we introduce the density operator $\hat{\rho}$, which is used to determine expectation values of observables of the physical system. The density operator essentially encodes which states are occupied in any given state of the system:

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i^\dagger |, \tag{37}$$

where p_i corresponds to the occupation probability of a many-body state $|\psi_i\rangle$. We use the same convention with indices as with H_{ij}, where the i and j correspond to the appropriate indices in the four sections of the BdG representation. Using this, we find the density matrix ρ_{ij} by taking the outer product between $\Psi_i^\dagger$ and Ψ_j:

$$\rho_{ij} = \hat{\Psi}_i^\dagger \otimes \hat{\Psi}_j = \begin{pmatrix} \langle \hat{c}_j^\dagger \hat{c}_i \rangle & \langle \hat{c}_i \hat{c}_j \rangle \\ \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle & -\langle \hat{c}_i^\dagger \hat{c}_j \rangle \end{pmatrix}. \tag{38}$$

With this density matrix we express H_{ij} in terms of $v_{ij}\rho_{ij}$:

$$H_{ij} = v_{ij} \begin{pmatrix} \langle \hat{c}_j^\dagger \hat{c}_i \rangle & \langle \hat{c}_i \hat{c}_j \rangle \\ \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle & -\langle \hat{c}_i^\dagger \hat{c}_j \rangle \end{pmatrix} - \begin{pmatrix} \delta_{ij} \sum_k v_{ik} \langle \hat{c}_k^\dagger \hat{c}_k \rangle & 0 \\ 0 & -\delta_{ij} \sum_k v_{kj} \langle \hat{c}_k^\dagger \hat{c}_k \rangle \end{pmatrix} \tag{39}$$

and substituting ρ_{ij} into this we get:

$$H_{ij} = v_{ij}\rho_{ij} - \delta_{ij} \sum_k \begin{pmatrix} v_{ik} & 0 \\ 0 & -v_{kj} \end{pmatrix} \mathrm{diag}(\rho_{kk}), \tag{40}$$

where $\mathrm{diag}(\rho_{kk})$ is a matrix with the values of ρ_{kk} on the diagonal and zero off-diagonal. Now finally we use the fact that in density-density interactions $v_{ik} = -v_{ki}$ to write

$$H_{ij} = v_{ij}\rho_{ij} - \delta_{ij} \sum_k v_{ik} \mathrm{diag}(\rho_{kk}). \tag{41}$$

Through these steps we have reduced the interacting term of tight-binding Hamiltonian to a matrix in the BdG basis:

$$\hat{V}_{\mathrm{MF}}(\rho) = \frac{1}{2} \sum_{ij} \hat{\Psi}_i^\dagger H_{ij} \hat{\Psi}_j, \tag{42}$$

but to solve the eigenvalue problem in equation 17 we require the full Hamiltonian $\hat{H}$. It is easy to see that $\hat{H}_0$ can be expressed in the BdG basis:

$$\begin{aligned}
\hat{H}_0 &= \sum_{ij} h_{ij} \hat{c}_i^\dagger \hat{c}_j, \\
&= \sum_{ij} \hat{\Psi}_i^\dagger H_{0,ij} \hat{\Psi}_j = \sum_{ij} \alpha_{0,ij} \hat{c}_i^\dagger \hat{c}_j + \beta_{0,ij} \hat{c}_i^\dagger \hat{c}_j^\dagger + \gamma_{0,ij} \hat{c}_i \hat{c}_j + \eta_{0,ij} \hat{c}_i \hat{c}_j^\dagger,
\end{aligned} \tag{43}$$

where we define $H_{0,ij}$ the same way we define H_{ij}. Clearly, $\beta_{0,ij}$ and $\gamma_{0,ij}$ are zero and $\alpha_{0,ij} = h_{ij}$, but for $\eta_{0,ij}$ we remember that from equation 28 we have that this should be the reversed form of $\alpha_{0,ij}$, so $\eta_{0,ij} = -h_{ij}$:

$$H_{0,ij} = \begin{pmatrix} h_{ij} & 0 \\ 0 & -h_{ij} \end{pmatrix}. \tag{44}$$

Finding the full $\hat{H}$ is as simple as adding $\hat{H}_0$ and $\hat{V}_{\text{MF}}$ together:

$$\begin{aligned} \hat{H} &= \hat{H}_0 + \hat{V}_{\text{MF}}, \\ &= \sum_{ij} \hat{\Psi}_i^\dagger H_{0,ij} \hat{\Psi}_j + \frac{1}{2} \sum_{ij} \hat{\Psi}_i^\dagger H_{ij} \hat{\Psi}_j, \\ &= \frac{1}{2} \sum_{ij} \hat{\Psi}_i^\dagger H_{0,ij} + H_{ij} \hat{\Psi}_j, \\ &= \frac{1}{2} \hat{\Psi}^\dagger H_{\text{BdG}} \hat{\Psi}, \end{aligned} \tag{45}$$

where H_{BdG} has a structure like in equation 28, but now also includes $\hat{H}_0$. This completes the derivation of the mean-field Hamiltonian in the Bogoliubov–de Gennes basis. By expanding the interacting term through Wick's theorem, we have successfully reduced the complexity of the original many-body problem to an effective single-particle description. The resulting Hamiltonian is diagonalizable and is used to compute the ground state solution to the Schrödinger equation 17.

5 The Hartree-Fock Algorithm

Solving the Schrödinger equation 17 should be as simple as diagonalizing the Hamiltonian in equation 45, but it is not. Although it is possible to diagonalize the Hamiltonian, it is not immediately obvious what the expectation values $\langle \hat{c}_j^\dagger \hat{c}_i \rangle$ etc. used to construct the Hamiltonian are. The expectation values in ρ_{ij} depend on the occupied states in the ground state of the system according to equation 37, but which states are occupied in the ground state depend on the Hamiltonian. We have a new problem: we have $\rho \to H_{\text{BdG}}$ and $H_{\text{BdG}} \to \rho$.

To solve this problem, we have to solve for both the mean-field interaction and the density matrix at the same time. We only consider the interaction term $\hat{V}_{\text{MF}}$ because $\hat{H}_0$ does not depend on ρ. The Hartree-Fock method is an application of mean-field theory, typically used to find solutions for many-electron systems like materials.[15] We solve for both the ground state density matrix and mean-field interaction $\hat{V}_{\text{MF}}$ self-consistently: we calculate the interacting mean-field Hamiltonian $\hat{V}_{\text{MF}}$ based on an initial density matrix ρ_{init} and find a new ground state density matrix by diagonalizing $\hat{V}_{\text{MF}}(\rho_{\text{init}})$. One iteration follows three steps,

$$\rho_{\text{init}} \to \hat{V}_{\text{MF}}(\rho_{\text{init}}) \to \rho_{\text{new}}(\hat{V}_{\text{MF}}), \tag{46}$$

starting with some initial guess for the mean-field Hamiltonian of the system $\hat{V}_{\text{MF, init}}$:

1. Based on an initial guess for the interacting mean-field Hamiltonian, calculate the total Hamiltonian from equation 45 and equation 41.
2. Compute the ground state density matrix as per equation 37:
   (a) Diagonalize the Hamiltonian to obtain eigenvalues and eigenstates.
   (b) Determine the occupation probability for the eigenvectors.
   (c) Calculate the density matrix using the eigenvectors and the occupation probability.
3. Calculate a new mean-field Hamiltonian with the ground state density matrix using equation 41.
4. Repeat steps until some self-consistent criterion has been met.

To determine when the solution is self-consistent, we require some function $f : \rho \to f(\rho)$ which minimally parametrizes ρ. The self-consistency criterion is a fixed-point problem which we treat as a root-finding problem.

$$\begin{aligned} f(\rho_{\text{new}}) &= f(\rho_{\text{init}}), \\ f(\rho_{\text{new}}) - f(\rho_{\text{init}}) &= 0, \end{aligned} \tag{47}$$

where ρ_{new} and ρ_{init} refer to the starting point and result of one iteration of the algorithm. In `MeanFi`, f was chosen to be a vectorization of the density matrix using the free parameters of ρ to reach self-consistency.

We could select the same f, but we pick a different function because we impose additional symmetries on the density matrix which constrain the solution space. In the BdG basis we explicitly assume we have electron-hole symmetry present and in specific systems it is possible to define more symmetries in for example the crystal structure of a material. In general, it is possible to find a basis of matrices for a Hamiltonian that is constrained by certain symmetries.[11] This basis will span all possible Hamiltonians that have those symmetries, and we know that the basis will have at most N matrices, where N is the total number of individual values of the Hamiltonian. The more constraints there are, the smaller the basis will be and therefore the more efficient the algorithm will be.

We choose f to be a projection coefficient of the density matrix onto a basis constrained by those symmetries. The final density matrix is constructed from a matrix basis $B = \{B_1, B_2, \dots\}$ and a coefficient vector $\overrightarrow{c} = [c_1, c_2, \dots]^T$, where the values correspond with the scalar projection of the appropriate basis. We generate the basis B using `Qsymm` and have added an interface to `Qsymm` in the `MeanFi` code.

$$\hat{H} = \sum_i c_i B_i. \tag{48}$$

Because the basis needs to be found only once for a given symmetry, this approach is equally efficient at the worst, and faster in most cases.

6 Fermi level

The final aspect of the algorithm that needs to be adapted, is the way that the occupation probability of equation 37 is determined. We consider closed systems, where the total charge is fixed. In `MeanFi`, all calculations are done at zero-temperature, where every possible state has a well-defined charge associated with it: the total number of electrons filling that state. For the probability distribution of `MeanFi`, the electron filling-factor was chosen to determine the occupied states. For example, if the system is at half-filling, then the eigenstates are counted until the half are filled from the lowest energy and up. More specifically, the Fermi energy is chosen such that half of the eigenstates have a lower energy.

However, in superconducting systems, the electron filling-factor can not be used in the same way; Every state is occupied by either an electron or a hole, so the total filling is constant. We still fix the total charge of the system, because this is still useful in superconductors: holes and electrons have opposite charge, so the total charge of a superconducting system can be expressed like

$$\begin{aligned} Q_{\text{tot}} &= Q_{\text{electrons}} + Q_{\text{holes}}, \\ &= -\nu q + (N - \nu) q, \end{aligned} \tag{49}$$

where ν is the electron filling-factor and N is the number of total possible states in the system.

The total charge is not a good quantum number in superconductors though, it is not possible to directly place the Fermi energy and count states until enough are filled. Instead, we fix the total charge via

$$\begin{aligned} \langle \hat{Q} \rangle(\mu) &= \text{tr}(\rho(\mu)\hat{Q}), \\ &= \sum_i f_{\text{FD},i}(\mu) \langle \psi_i | \hat{Q} | \psi_i \rangle, \end{aligned} \tag{50}$$

where $\hat{Q}$ is the charge operator for the system and $f_{\text{FD},i}(\mu)$ is value of the Fermi-Dirac distribution at the energy of state $|\psi_i$.[16,17] The value of $f_{\text{FD},i}(\mu)$ will depend on the Fermi level, or chemical potential, μ. In non-superconducting systems, $\hat{Q}$ is simply an identity matrix because all particles have the same charge, but for a superconducting system it is defined differently. In the BdG basis we assume we have electrons and holes, so the charge operator reflects that and looks something like in equation 51, but scaled to the same dimension as the BdG basis.

$$\hat{Q} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{51}$$

Fixing the charge this way yields an additional minimization problem, because $\langle \hat{Q} \rangle(\mu)$ depends on $f_{\text{FD},i}(\mu)$, and we can't directly set μ to fix the distribution. If we choose the system to have total charge Q_0, we have to find the root for

$$\langle \hat{Q} \rangle(\mu) - Q_0 = 0. \tag{52}$$

When the optimal μ is found, the occupation distribution that results in the chosen total charge of the system can be defined, and then the density matrix can be constructed. Another parameter that shapes the Fermi-Dirac distribution is the temperature and in principle, the temperature of the system can be picked arbitrarily. For superconducting systems finite temperature adds no computational cost because the minimization has to happen regardless. Therefore, this root finding implementation allows us to generalize `MeanFi` to finite temperatures.

7 Example

To show that our changed algorithm results in a superconducting solution for the mean-field Hamiltonian, we consider a simple interacting electronic system. We choose a 1D chain of sites that allow nearest-neighbour tunnelling with strength t and an on-site interaction between two electrons if they are on the same site of strength U. This model is known as the 1D Hubbard model and is useful to describe the transition between conducting and insulating systems.[18] In our system we hope to see a transition to a superconducting system. The total Hamiltonian for this system is $\hat{H} = \hat{H}_0 + \hat{V}$, with H_0 the non-interacting part and V the interacting part of the Hamiltonian:

$$\begin{aligned} \hat{H}_0 &= -t \sum_{\sigma} \sum_{i} \left(\hat{c}^{\dagger}_{i,B,\sigma} \hat{c}_{i,A,\sigma} + \hat{c}^{\dagger}_{i,A,\sigma} \hat{c}_{i+1,B,\sigma} + \mathbf{h.c.} \right), \\ \hat{V} &= U \sum_{i} \left(\hat{n}_{i,A,\uparrow} \hat{n}_{i,A,\downarrow} + \hat{n}_{i,B,\uparrow} \hat{n}_{i,B,\downarrow} \right), \end{aligned} \tag{53}$$

where **h.c.** is the hermitian conjugate, σ denotes spin ($\uparrow$ or $\downarrow$), A and B are sublattices that correspond to the different sites in one unit cell and $\hat{n}_{i,A,\sigma} = \hat{c}^{\dagger}_{i,A,\sigma} \hat{c}_{i,A,\sigma}$, which is the number operator for sublattice A and spin σ.

We run the algorithm at half-filling, which corresponds to target charge $Q_0 = 0$. Additionally, we set $U < 0$ (-2 in the figures), to promote a superconducting transition. The resulting mean-field Hamiltonian in figure 1 has non-zero values for the electron-hole coupling terms and is Hermitian as expected based on the BdG matrix from equation 28.

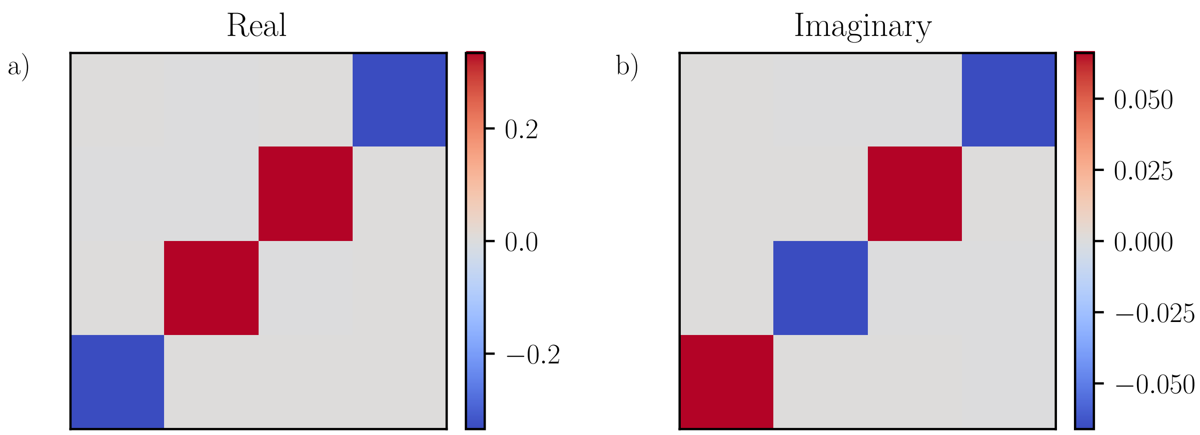

Figure 1: a) Shows the real part of the mean-field Hamiltonian; b) Shows the imaginary part of the mean-field Hamiltonian.

Furthermore, when we diagonalize this Hamiltonian and look at the eigenstates, we can show the bands, which clearly show a gap as can be seen in figure 2 a). We also see that particle-hole symmetry is present, because the bands are symmetric around the Fermi level $E - E_F = 0$.

Finally, to test the finite temperature algorithm we implemented, we compare our superconducting gap at different temperatures with an analytical solution for the gap. For the system we have chosen, there exists a known gap-temperature formula based on BCS-theory.[19]:

$$\Delta(T) = \Delta(0) \tanh\left(1.74\sqrt{\frac{T_c}{T} - 1}\right). \tag{54}$$

We use equation 54 and fit this formula to our results by determining the critical temperature T_c and the gap at $T = 0$, $\Delta(0)$. Then we plot this formula alongside the calculated gap for our system at different temperatures in figure 2, showing that our gap-temperature dependence closely matches the theoretical dependence.

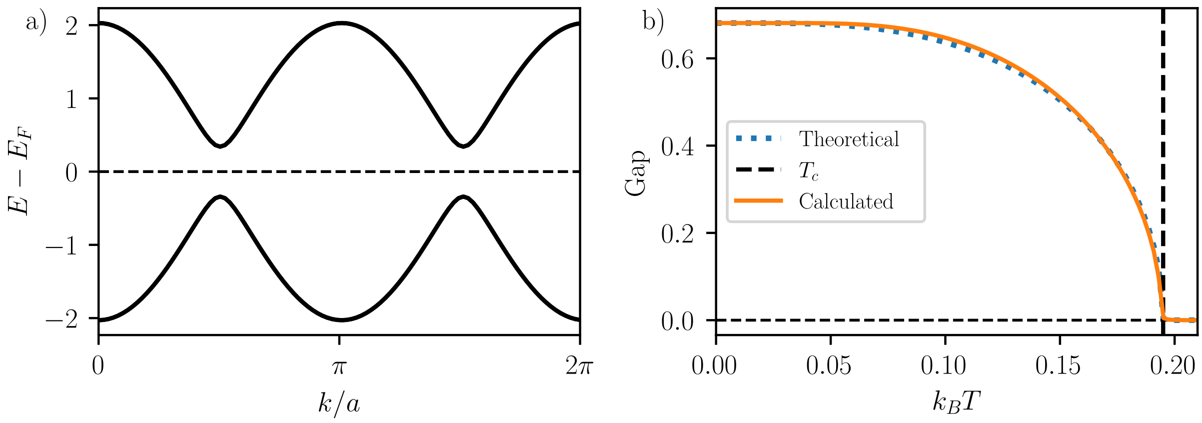

Figure 2: a) Shows the bands of the system at $T = 0$; b) Shows the size of the superconducting gap at different temperatures.

8 Summary

In this thesis, we showed how we derived the tight-binding mean-field Hamiltonian including the superconducting terms previously left out in `MeanFi`. We did this by expanding the tight-binding density-density Hamiltonian using Wick's theorem and mean-field approximation and transformed the resulting expansion into the BdG basis to include the superconducting pairing terms explicitly.

We additionally adapted the self-consistent Hartree-Fock algorithm from `MeanFi` to use a new self-consistency criterion. This new criterion was based on a projection of the density matrix onto a matrix basis constrained by symmetries using `Qsymm`. This was done both for efficiency reasons and to ensure that the electron-hole symmetry is preserved.

In the algorithm itself, we introduced an additional minimization problem to determine the occupation probability of the eigenstates of the Hamiltonian, because total charge is not a good quantum number in superconducting systems. Instead, we calculated the Fermi level μ such that $\langle\hat{Q}\rangle(\mu) - Q_0 = 0$, where Q_0 is the charge of the system. This extra minimization option also enabled us to implement finite temperature as a parameter in the system, rather than performing all calculations at zero-temperature like in `MeanFi`.

Finally, to show that our algorithm returns a mean-field Hamiltonian with superconducting terms, we applied it to a 1D Hubbard model with attractive interactions and calculated the superconducting gap from the bands of the mean-field solution for different temperatures of the system. The gap-temperature dependence closely matched the theoretical dependence predicted by BCS-theory.

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