Topological Superconductors

Lecture notes for the second semester of the course on Topological Insulators at Eotvos University

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Introduction

In the first semester, we used single-particle quantum mechanics to learn that topological insulators host protected edge states. In the Su-Schrieffer-Heeger model, these are bound states whose energy is pinned at 0. In 2-dimensional topological insulators (e.g., the Qi-Wu-Zhang model or the Bernevig-Hughes-Zhang model), edge states form bands which allow for perfect (reflectionless, zero four-terminal resistance) conduction. Single-particle quantum mechanics was good enough for these models: even though the many-body ground state contains many electrons, it can be obtained simply by filling all negative energy eigenstates by one electron each. This was because these models did not contain interaction, and conserved particle number.

This semester, we study topological superconductors. Here the electrons are in contact with a reservoir of Cooper pairs, which we will treat in the mean-field approximation. Cooper pair formation and Cooper pair breaking will be included in the Hamiltonian as pairs of electrons disappearing from the system, or added to the system, coherently. Particle number is no longer conserved, and a straightforward description of the system by a single-particle Hamiltonian is not possible.

There is a way to associate a single-particle Hamiltonian to a superconductor, known as the Bogoliubov-de Gennes trick. Because it is not entirely trivial to interpret its results, we dedicate the first few lessons to this formalism.

Chapter 1

The Bogoliubov-de Gennes Hamiltonian for Superconductors

There is a way to associate a single-particle Hamiltonian to a superconductor, known as the Bogoliubov-de Gennes trick. Because it is not entirely trivial to interpret its results, we dedicate the first few lessons to this formalism.

1.1 Superconductor in the mean-field approximation

A superconductor is a material with an excitation gap Δ due to some process that forced electrons at and near the Fermi surface into Cooper pairs. The Cooper pairs have condensed, and form the superconducting order parameter.

Supercurrent.

Single-particle excitation gap.

In the mean-field approximation, we write down a Hamiltonian for the dynamics of the electrons only, and treat the condensate of Cooper pairs as a fixed order parameter. Mostly, we will not care about actually obtaining superconductivity by some self-consistent calculation. Rather, we will put it in our model as a parameter, coming possibly from a large piece of superconductor which is touching our system, via the so-called proximity effect. We will consider lattice models, where these electrons live in a crystal (lattice with a basis), having a unit cell coordinate and some internal state, including sublattice and spin. We will also consider models of coupled quantum dots. Electrons can hop, possibly changing their internal state in the process. Importantly, spin may or may not be conserved due to possible spin-orbit coupling. The electrons also appear or disappear from the system pairwise, as Cooper pairs are broken or formed.

1.1.1 Simplest example: quantum dot with superconductivity

The simplest toy model for a superconductor describes a quantum dot with a single energy level, which can be occupied by an electron with its spin up or down. The grand canonical Hamiltonian reads,

$$\hat{H} = B(\hat{c}_\uparrow^\dagger \hat{c}_\uparrow - \hat{c}_\downarrow^\dagger \hat{c}_\downarrow) - \mu(\hat{c}_\uparrow^\dagger \hat{c}_\uparrow + \hat{c}_\downarrow^\dagger \hat{c}_\downarrow) + \Delta \hat{c}_\uparrow^\dagger \hat{c}_\downarrow^\dagger + \Delta^* \hat{c}_\downarrow \hat{c}_\uparrow. \tag{1.1}$$

The first term is a magnetic field $B \in \mathbb{R}$ tuning the energy difference between the two spin states, the second a chemical potential $\mu \in \mathbb{R}$. The third and fourth terms describe Cooper-pair breaking – with the electrons that constituted the pair appear on the dot –, and Cooper-pair creation – two electrons both exit the dot and form a Cooper pair. These processes have coherent amplitudes $\Delta \in \mathbb{C}$ and Δ^*.

For such a small system, we can actually calculate its eigenstates in the Fock space. The matrix of the Hamiltonian reads,

$$\hat{H} = \begin{pmatrix} |0\rangle & |\uparrow\downarrow\rangle & |\uparrow\rangle & |\downarrow\rangle \end{pmatrix} \begin{pmatrix} 0 & \Delta^* & & \\ \Delta & -2\mu & & \\ & & -\mu + B & \\ & & & -\mu - B \end{pmatrix} \begin{pmatrix} \langle 0| \\ \langle\uparrow\downarrow| \\ \langle\uparrow| \\ \langle\downarrow| \end{pmatrix} \tag{1.2}$$

$$\tag{1.3}$$

Superconductivity conservers fermion parity. Notice how this 4 by 4 matrix is composed of 2 blocks of 2 by 2 matrices. Even though the upper block connects sectors of the Hilbert space with different particle number, Cooper pair formation and breaking both conserve the parity of the particle number, so there are no off-diagonal blocks. The upper-left block acts in the subspace with even particle number, the lower-rght block in the subspace with odd particle number.

Since matrices of the form $d_0\sigma_0 + d_x\sigma_x + d_y\sigma_y + d_z\sigma_z$ will occur often later on, we remind the reader of their spectrum here:

$$\begin{pmatrix} d_0 + d_z & d_x - id_y \\ d_x + id_y & d_0 - d_z \end{pmatrix} \begin{pmatrix} d_x - id_y \\ \pm E - d_z \end{pmatrix} = E_\pm \begin{pmatrix} d_x - id_y \\ \pm E - d_z \end{pmatrix}; \tag{1.4}$$

$$E_\pm = d_0 \pm \sqrt{d_x^2 + d_y^2 + d_z^2}. \tag{1.5}$$

We obtain the energy levels,

$$E_{e\pm} = -\mu \pm \sqrt{|\Delta|^2 + \mu^2}; \qquad |e\pm\rangle \propto \Delta^* |0\rangle + (E_{e\pm} - \mu) |\uparrow\downarrow\rangle \tag{1.6}$$

$$E_{o\pm} = -\mu \pm B; \qquad |o_+\rangle = |\uparrow\rangle; \qquad |o_-\rangle = |\downarrow\rangle. \tag{1.7}$$

The odd energy eigenstates the same as the odd basis states, and independent of all system parameters. The even eigenstates are superpositions of the two even basis states, with amplitudes that depend on the parameters. In the shorthand

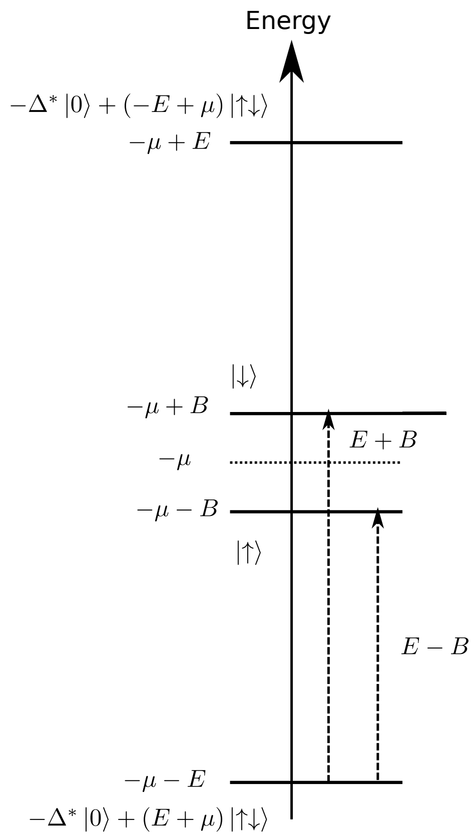

Figure 1.1: Energy levels of the simplest superconducting system: a quantum dot with a single energy level, which can be doubly unoccupied, with two electrons with opposite spin, Eq. (1.1). We assume $0 < |\Delta| < B < \mu$.

used above, $E = \sqrt{\mu^2 + |\Delta|^2}$. In the limit where $0 < |\Delta| \ll \mu$, we have $E \approx \mu + |\Delta|^2/(2\mu)$, and

$$E_{e+} \approx \frac{|\Delta|^2}{2\mu}; \qquad |e+\rangle \approx |0\rangle + \frac{\Delta}{2\mu}|\uparrow\downarrow\rangle \tag{1.8}$$

$$E_{e-} \approx -2\mu - \frac{|\Delta|^2}{2\mu}; \qquad |e-\rangle \approx -\frac{\Delta^*}{2\mu}|0\rangle + |\uparrow\downarrow\rangle\,. \tag{1.9}$$

The energy levels cross as the magnetic field is tuned across a critical value, $B_{\text{crit}} = \sqrt{\Delta^2 + \mu^2}$. The nature of the ground state changes abruptly at this critical field:

$$-\sqrt{|\Delta|^2 + \mu^2} < B < \sqrt{|\Delta|^2 + \mu^2} \quad : \quad |GS\rangle = |e-\rangle\,; \tag{1.10}$$

$$\sqrt{|\Delta|^2 + \mu^2} < B \quad : \quad |GS\rangle = |o-\rangle\,. \tag{1.11}$$

The crossing does not become an avoided crossing, because there is no term in the Hamiltonian that changes the parity of the particle number: the parity is a conserved quantity. It is represented by

$$\hat{P} = (-1)^{\hat{c}_\uparrow^\dagger \hat{c}_\uparrow + \hat{c}_\downarrow^\dagger \hat{c}_\downarrow}. \tag{1.12}$$

We can also interpret this spectrum using the concept of quasiparticles. For this purpose, we define the operators $\hat{d}_1$ and $\hat{d}_2$ as exciting from the ground state to the first and to the second excited state. In the regime $0 < |\Delta| < B < \mu$, this amounts to the requirements,

$$\hat{d}_1^\dagger |e-\rangle = |\uparrow\rangle\,; \qquad \hat{d}_1^\dagger |\downarrow\rangle = |e+\rangle\,; \tag{1.13}$$

$$\hat{d}_2^\dagger |e-\rangle = |\downarrow\rangle\,; \qquad \hat{d}_2^\dagger |\uparrow\rangle = -|e+\rangle\,; \tag{1.14}$$

$$\hat{d}_1^2 = \hat{d}_2^2 = 0. \tag{1.15}$$

We now just state that this system of equations can always be solved, we will find a systematic way of solving them in the next Section.

The spectrum of $\hat{H}$, shown in Fig. 1.1, is symmetric around $E = -\mu$. This symmetry has nothing to do with superconductivity, it is a generic feature of free Hamiltonians (i.e., where $\hat{H}$ is a quadratic function of the operators $\hat{c}_m$ and $\hat{c}_m^\dagger$), which can be explained simply. All energy levels can be obtained from the bottom up, starting with $|GS\rangle$, and adding particles by operating with excitation operators $\hat{d}^\dagger$, as indicated by the slashed lines. Alternatively, one can go top-down: with the state where all $\hat{d}$ fermions are present, and subtract the $\hat{d}$'s. The symmetry point can be shifted by onsite potentials, but is always there. We will now describe a systematic way to obtain the operators $\hat{d}$

1.1.2 Superconducting wire

The next step towards topological superconductors is to study a superconducting quantum wire, a system which has a bulk and two ends. The mean-field

Hamiltonian of a superconducting wire with N sites, and with periodic boundary conditions (no ends, i.e., a ring) reads

$$\hat{H}_s = \sum_{m=1}^{N} \Big(\sum_{\sigma=\uparrow,\downarrow} \Big[-v\hat{c}^\dagger_{m,\sigma}\hat{c}_{m+1,\sigma} - \frac{\mu}{2}\hat{c}^\dagger_{m,\sigma}\hat{c}_{m,\sigma} \Big] + \Delta\hat{c}^\dagger_{m,\uparrow}\hat{c}^\dagger_{m,\downarrow} \Big) + h.c. \tag{1.16}$$

We assume $N+1=1$.

1.1.3 Spinless superconducting wire - Kitaev wire

The simplest model of a topological superconductor is not the superconducting wire introduced above, but a superconducting wire where only one spin species is present. In this model we will therefore suppress the spin label, and call this a spinless superconducting wire. This simplest Hamiltonian reads,

$$\hat{H}_p = \sum_{m=1}^{N} \Big(- v\hat{c}^\dagger_m\hat{c}_{m+1} - \frac{\mu}{2}\hat{c}^\dagger_m\hat{c}_m + \Delta\hat{c}^\dagger_m\hat{c}^\dagger_{m+1} \Big) + h.c. \tag{1.17}$$

Here too we have Cooper pair breaking with amplitude $\Delta \in \mathbb{C}$ – and the Hermitian conjugate process of Cooper pair production – in the Hamiltonian, but now these involve electrons on neighboring sites, with the same spin. One way this could happen if there is some mechanism for flipping the spin during the formation of the actual Cooper pairs.

1.1.4 General formalism

A generic grand canonical Hamiltonian for a mean-field superconductor reads,

$$\hat{H} = \sum_{m,l=1}^{N} \hat{c}^\dagger_m h_{ml}\hat{c}_l + \frac{1}{2}\sum_{m<l=1}^{N} \hat{c}^\dagger_m\Delta_{ml}\hat{c}^\dagger_l - \frac{1}{2}\sum_{m<l=1}^{N} \hat{c}_m\Delta^*_{ml}\hat{c}_l. \tag{1.18}$$

Here, we don't distinguish between internal and external degrees of freedom, and so the sums over m, l denote both unit cell and spin or sublattice or other degrees of freedom. The operator $\hat{c}_m$ annihilates an electron from site m. The first term describes the onsite potentials, the hopping, and the the chemical potential. The last two terms are the effects of superconductivity in the mean-field approximation, via the pair potential Δ_{ml}, a set of complex parameters, corresponding to the wave function of the Cooper pair condensate. Note the $-$ in front of the last term, which appears because we reorder the operators $\hat{c}_m$ and $\hat{c}_l$.

1.2 Fock space

Superconducting Hamiltonians do not conserve the particle number. Therefore, the dynamics they describe take place in the Fock space.

1.2.1 Computational basis notation

A set of 2^N basis states that spans the Fock space can be defined using the operators $\hat{c}_m$. We start with the state $|\varnothing\rangle$ of the system with no particles present,

$$\hat{c}_m |\varnothing\rangle = 0 \quad \text{for } m = 1, \ldots, N. \tag{1.19}$$

We then specify for each site m whether it is occupied or not. In the case of $N = 3$ sites, the set of basis states reads

$$\begin{aligned} &|000\rangle = |\varnothing\rangle ; &&|100\rangle = \hat{c}_1^\dagger |\varnothing\rangle ; &&|010\rangle = \hat{c}_2^\dagger |\varnothing\rangle ; &&|110\rangle = \hat{c}_2^\dagger \hat{c}_1^\dagger |\varnothing\rangle ; \\ &|001\rangle = \hat{c}_3^\dagger |\varnothing\rangle ; &&|101\rangle = \hat{c}_3^\dagger \hat{c}_1^\dagger |\varnothing\rangle ; &&|011\rangle = \hat{c}_3^\dagger \hat{c}_2^\dagger |\varnothing\rangle ; &&|111\rangle = \hat{c}_3^\dagger \hat{c}_2^\dagger \hat{c}_1^\dagger |\varnothing\rangle . \end{aligned}$$

Note that the order of the operators is important, e.g.,

$$|010\rangle = -\hat{c}_1 |110\rangle = \hat{c}_3 |001\rangle . \tag{1.20}$$

1.2.2 Matrices for the operators

Describe the construction of the matrix of fermion operators $\hat{c}_m$.

Build the matrix of the Hamiltonian $\hat{H}_K$.

1.3 The ground state and normal modes

In the mean-field approximation, a superconductor such as the Kitaev wire is described by a free Hamiltonian, i.e., quadratic in the electron creation and annihilation operators. Note that although the number of fermions is not conserved, the parity is. Since this is a free Hamiltonian (quadratic), it can be diagonalized by introducing new fermionic operators, in the sense that

$$\hat{H} = \sum_{n=1}^{N} E_n \hat{d}_n^\dagger \hat{d}_n + \text{const}, \tag{1.21}$$

where "const." is a number (not an operator), and the $\hat{d}_n$'s are linear combinations of the original fermionic operators, with fermionic anticommutation relations,

$$\{\hat{d}_n, \hat{d}_l\} = 0; \qquad \{\hat{d}_n, \hat{d}_l^\dagger\} = \delta_{nl}. \tag{1.22}$$

Because of the superconductivity, the operator $\hat{d}_n$ has to be a linear combination of both electron annihilation and creation operators,

$$\hat{d}_n = \sum_m u_{nm} \hat{c}_m + v_{nm} \hat{c}_m^\dagger ; \qquad \hat{d}_n^\dagger = \sum_m u_{nm}^* \hat{c}_m^\dagger + v_{nm}^* \hat{c}_m . \tag{1.23}$$

Thus, in a sense the new operators $\hat{d}_n$ and $\hat{d}_n^\dagger$ are described on the same footing. We will use this freedom to ensure that all of the $\hat{d}$ operators describe positive energy excitations:

$$E_n \geq 0 \quad \text{for } n = 1, \dots, N. \tag{1.24}$$

This can be achieved by redefining the negative energy fermions $\hat{d}_n$ as $\hat{d}_n \leftrightarrow \hat{d}_n^\dagger$.

> What requirements do the commutation relations of the $\hat{d}_n$ impose on the coefficients u_{nm} and v_{nm}?

Once we have found the operators $\hat{d}_n$, we can construct the ground state $|GS\rangle$ of the Hamiltonian. This is the vacuum of the operators $\hat{d}_n$, i.e.,

$$\forall n = 1, \dots, N : \quad \hat{d}_n |GS\rangle = 0. \tag{1.25}$$

The ground state is a complicated state when expressed in the basis of the original fermions $\hat{c}_m$. It is in general a superposition of states with different particle numbers, since the Hamiltonian does not conserve particle number. However, since the Hamiltonian conserves the parity of the particle number, the ground state is a superposition of states with only odd, or only even number of particles ($\hat{c}_m$ fermions).

One way to construct the ground state $|GS\rangle$ is to turn the logic of the previous paragraph around. Starting from any "seed" state, we can proceed to take away all the components of it that contain excitations $\hat{d}$: then we are left with $|GS\rangle$, if the seed state had a $|GS\rangle$ component. A frequent choice for the seed state is $|00\dots0\rangle$, the vacuum of the $\hat{c}_m$ fermions, which gives

$$\hat{d}_N \hat{d}_{N-1} \dots \hat{d}_1 |\varnothing\rangle \propto |GS\rangle \text{ or } 0. \tag{1.26}$$

If the initial state had no component of the ground state (because, e.g., the ground state is odd), we can continue this procedure with other seed states. [1]

1.3.1 Using the eigenmodes, we can construct the whole spectrum

If we have the ground state $|GS\rangle$ and the eigenmodes $\hat{d}_n$ of the Hamiltonian, we can construct all 2^N of its eigenstates. We simply specify which of the $\hat{d}_m$ fermions are present in the system, e.g.,

$$|000\dots0\rangle_d = |GS\rangle; \qquad |100\dots0\rangle_d = \hat{d}_1^\dagger |GS\rangle \tag{1.28}$$

$$|010\dots0\rangle_d = \hat{d}_2^\dagger |GS\rangle; \qquad |110\dots0\rangle_d = \hat{d}_2^\dagger \hat{d}_1^\dagger |GS\rangle. \tag{1.29}$$

[1] Alternatively, the projector to the ground state can be obtained if we remove all single-particle excitations from the mixture of all possible states,

$$|GS\rangle\langle GS| = \hat{d}_N \hat{d}_{N-1} \dots \hat{d}_1 \left(\sum_{n_1=0}^{1} \dots \sum_{n_N=0}^{1} \hat{c}_N^{\dagger n_N} \dots \hat{c}_1^{\dagger n_1} |0\rangle\langle 0| \hat{c}_1^{n_1} \dots \hat{c}_N^{n_N} \right) \hat{d}_1^\dagger \hat{d}_2^\dagger \dots \hat{d}_N^\dagger. \tag{1.27}$$

1.4 Normal modes from Bogoliubov–de Gennes Hamiltonian

To construct eigenstates of the superconductor we need to obtain the coefficients $u_{n,j}, v_{n,j}$ of Eq. (1.23). An efficient way to obtain the coefficients is the Bogoliubov–de Gennes formalism.

We begin by symmetrizing each term in the Hamiltonian. We use the fermionic anticommutation relations, whereby,

$$\hat{c}_m\hat{c}_j = \frac{1}{2}\hat{c}_m\hat{c}_j - \frac{1}{2}\hat{c}_j\hat{c}_m; \qquad \hat{c}_m^\dagger\hat{c}_j = \frac{1}{2}\hat{c}_m^\dagger\hat{c}_j - \frac{1}{2}\hat{c}_j\hat{c}_m^\dagger + \frac{1}{2}\delta_{mj}.; \tag{1.30a}$$

$$\hat{c}_m^\dagger\hat{c}_j^\dagger = \frac{1}{2}\hat{c}_m^\dagger\hat{c}_j^\dagger - \frac{1}{2}\hat{c}_j^\dagger\hat{c}_m^\dagger; \qquad \hat{c}_m\hat{c}_j^\dagger = \frac{1}{2}\hat{c}_m\hat{c}_j^\dagger - \frac{1}{2}\hat{c}_j^\dagger\hat{c}_m + \frac{1}{2}\delta_{mj}. \tag{1.30b}$$

We substitute these into the Hamiltonian, to obtain its symmetrized form,

$$\hat{H} = \frac{1}{2}\sum_{j,m=1}^{N}\Big(h_{mj}\left(\hat{c}_m^\dagger\hat{c}_j - \hat{c}_j\hat{c}_m^\dagger\right) + \Delta_{mj}\hat{c}_m^\dagger\hat{c}_j^\dagger + \Delta_{mj}^*\hat{c}_j\hat{c}_m\Big) + \frac{1}{2}\sum_{m=1}^{N}h_{mm}. \tag{1.31}$$

The complex numbers h_{mj} and Δ_{mj}, read out from the Hamiltonian, are grouped into matrices. Hermiticity of the Hamiltonian ensures that the matrix h is Hermitian, while the symmetrization, Eq. (1.30), ensures that the matrix Δ is antisymmetric, i.e.,

$$h_{jm} = h_{mj}^*; \qquad \Delta_{jm} = -\Delta_{mj}. \tag{1.32}$$

As an example, for the Kitaev wire, Eq. (**??**), on $N = 4$ sites, the matrices h and Δ read,

$$h = \begin{pmatrix} u_1 & t_1 & 0 & 0 \\ t_1 & u_2 & t_2 & 0 \\ 0 & t_2 & u_3 & t_3 \\ 0 & 0 & t_3 & u_4 \end{pmatrix}; \qquad \Delta = \begin{pmatrix} 0 & -\Delta_1 & 0 & 0 \\ \Delta_1 & 0 & -\Delta_2 & 0 \\ 0 & \Delta_2 & 0 & -\Delta_3 \\ 0 & 0 & \Delta_3 & 0 \end{pmatrix}; \tag{1.33}$$

Using a practical shorthand,

$$\hat{\mathbf{c}}^\dagger = (\hat{c}_1^\dagger, \hat{c}_2^\dagger, \ldots, \hat{c}_N^\dagger), \tag{1.34}$$

the Hamiltonian can be written in a compact form as

$$\hat{H} = \frac{1}{2}\begin{pmatrix}\hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}}\end{pmatrix}\mathcal{H}\begin{pmatrix}\hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger\end{pmatrix} + \frac{1}{2}\mathrm{Tr}h; \qquad \mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}. \tag{1.35}$$

The matrix $\mathcal{H}$ is known as the Bogoliubov-de Gennes (BdG) Hamiltonian. It is Hermitian because h is Hermitian and Δ is skew symmetric.

1.4.1 Particle-Hole Symmetry

The BdG Hamiltonian has particle-hole symmetry (PHS), because of the symmetrization procedure involved in its construction. This is a symmetry which, like chiral symmetry, connects $\mathcal{H}$ with $-\mathcal{H}$, and, like time-reversal symmetry, is represented by an antiunitary operator, $\hat{\mathcal{P}} = \sigma_x K$. Here by σ_x we mean the $2N \times 2N$ matrix,

$$\sigma_x = \begin{pmatrix} 0 & \mathbb{I}_{N\times N} \\ \mathbb{I}_{N\times N} & 0 \end{pmatrix}, \tag{1.36}$$

and K is the operator of complex conjugation in real space (and some fixed internal basis), i.e., for any matrix A,

$$KAK = A^*, \tag{1.37}$$

where A^* is the matrix obtained from the matrix A by elementwise complex conjugation. The requirement of particle-hole symmetry reads,

$$\sigma_x \mathcal{H}^\star \sigma_x = -\mathcal{H}. \tag{1.38}$$

1.4.2 Diagonalization

Due to the particle-hole symmetry of $\mathcal{H}$, we can diagonalize it using only the positive energy eigenstates,

$$\mathcal{H}\begin{pmatrix} u_n^* \\ v_n^* \end{pmatrix} = E_n \begin{pmatrix} u_n^* \\ v_n^* \end{pmatrix}, \quad \text{with } E_n \geq 0 \text{ for } n = 1, \dots, N; \tag{1.39}$$

$$\mathcal{H}\begin{pmatrix} v_n \\ u_n \end{pmatrix} = -E_n \begin{pmatrix} v_n \\ u_n \end{pmatrix}, \quad \text{for } n = 1, \dots, N, \tag{1.40}$$

where the nth eigenvector of $\mathcal{H}$ was written as $(u_n, v_n)^\dagger$, with u_n and v_n both N-component vectors. Remember that $\mathcal{H}$ was a Hermitian matrix, and thus its eigenvectors form an orthonormal basis.

We can use the components u_{nm} and v_{nm} to define new operators as per Eq. (1.23),

$$\hat{d}_n = \sum_m u_{nm}\hat{c}_m + v_{nm}\hat{c}_m^\dagger; \qquad \hat{d}_n^\dagger = \sum_m u_{nm}^*\hat{c}_m^\dagger + v_{nm}^*\hat{c}_m. \tag{1.41}$$

Orthonormality of the eigenvectors translates to the required anticommutation relations.

We can check that the fermions introduced above really are the eigenmodes of the Hamiltonian. We can write $\mathcal{H}$ as

$$\mathcal{H} = \sum_n E_n \begin{pmatrix} u_n^* \\ v_n^* \end{pmatrix} \begin{pmatrix} u_n & v_n \end{pmatrix} - \sum_n E_n \begin{pmatrix} v_n \\ u_n \end{pmatrix} \begin{pmatrix} v_n^* & u_n^* \end{pmatrix}. \tag{1.42}$$

Comparing this with Eq. (1.35), we find that it corresponds to

$$\hat{H} = \frac{1}{2}\sum_{n=1}^{N} E_n(\hat{d}_n^\dagger \hat{d}_n - \hat{d}_n \hat{d}_n^\dagger) + \frac{1}{2}\sum_{n=1}^{N} E_n = \sum_{n=1}^{N} E_n \hat{d}_n^\dagger \hat{d}_n, \tag{1.43}$$

the form that we were looking for.

1.5 Summary: single-particle Bogoliubov-de Gennes Hamiltonian

General superconducting Hamiltonian in mean-field approximation:

$$\hat{H} = \sum_{m,l=1}^{N} \hat{c}_m^\dagger h_{ml} \hat{c}_l + \frac{1}{2}\sum_{m,l=1}^{N} \hat{c}_m^\dagger \Delta_{ml} \hat{c}_l^\dagger - \frac{1}{2}\sum_{m,l=1}^{N} \hat{c}_m \Delta_{ml}^* \hat{c}_l. \tag{1.44}$$

Diagonalized by fermionic operators (Bogoliubov transformation)

$$\hat{H} = \sum_{n=1}^{N} \hat{d}_n^\dagger \hat{d}_n + \text{const.}; \qquad \hat{d}_n = \sum_{m=1}^{N} u_{nm}\hat{c}_m + v_{nm}\hat{c}_m^\dagger. \tag{1.45}$$

To find the matrices of coefficients u and v, associate a single-particle BdG Hamiltonian $\mathcal{H}$ to the system:

$$\hat{H} = \frac{1}{2}\begin{pmatrix}\hat{\mathbf{c}}^\dagger & \hat{\mathbf{c}}\end{pmatrix}\mathcal{H}\begin{pmatrix}\hat{\mathbf{c}} \\ \hat{\mathbf{c}}^\dagger\end{pmatrix} + \frac{1}{2}\text{Tr}h; \qquad \mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}, \tag{1.46}$$

with matrices h complex Hermitian, Δ complex skew symmetric.

Eigenvectors of BdG Hamiltonian $\mathcal{H}$ collected into matrices:

$$\mathcal{H} = \begin{pmatrix} u^* & v \\ v^* & u \end{pmatrix}\begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}\begin{pmatrix} u^T & v^T \\ v^\dagger & u^\dagger \end{pmatrix}. \tag{1.47}$$

Here E is a diagonal matrix of nonnegative eigenvalues. Unitarity of the matrix of eigenvectors ensures fermionic commutation relations of the $\hat{d}$'s.

We can construct all of the Fock spectrum using the data from the BdG trick.

$$|GS\rangle = \hat{d}_N \ldots \hat{d}_2 \hat{d}_1 |\Psi\rangle, \tag{1.48}$$

where $|\Psi\rangle$ is any Fock state.

$$|n_N, \ldots, n_2, n_1\rangle = (\hat{d}_N^\dagger)^{n_N} \ldots (\hat{d}_2^\dagger)^{n_2} (\hat{d}_1^\dagger)^{n_1} |GS\rangle, \tag{1.49}$$

with all of the n_j either 1 or 0. The corresponding Fock state energy values are,

$$E_{(n_1,\ldots,n_N)} = E_{GS} + (E_1)^{n_1} + \ldots + (E_N)^{n_N}. \tag{1.50}$$