

Quantum Non-Linear Transformations and Third Quantization

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Abstract

In quantum many body physics, namely in the second quantization formalism, the Schrödinger equation for non-interacting Hamiltonians that are quadratic in operators can be simply solved using linear transformations of operators. However, for interacting systems (quartic in operators), one resorts to doing linear transformations of many-particle states, which is far more challenging. On the other hand, when expressed in the representation of Majorana fermions, the door opens to non-linear canonical transformations as an alternative way to engage with these interacting problems. By introducing a gauge degree of freedom with a decoupled auxiliary orbital to the Hamiltonian of the particle-hole symmetric Hubbard model in the single site case and in the insulating phase, non-linear transformations on the Majorana operators take this interacting system (due to Coulomb repulsion) to an effectively non-interacting form. The language of third quantization is used to provide a lens into these interacting problems, by defining an orthonormal basis of operators and the transition Hamiltonian, investigating how the basis operators connect to one another under the action of the Hamiltonian. Transition Hamiltonians with only zero entries inside blocks connecting the linear Majoranas to higher order products determines if the Hamiltonian is non-interacting in a chosen basis. This transition Hamiltonian also offers a way to view the change in dynamics of the system after a set of non-linear canonical transformations have acted on the basis of operators, and is constructed for simple Hubbard and Heisenberg model systems.

Keywords: second quantization, non-linear canonical transformations, Majorana fermions, third quantization

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Declaration of Authorship

I declare that all material in this project is my own work, except where there is clear acknowledgement and appropriate reference to the work of others.

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Acronyms

LCG Local Canonical Group. 11, 12

NLCTs Non-Linear Canonical Transformations. 1, 2, 15, 16, 28

P-H symmetry particle-hole symmetry. iv, v, 9, 15, 17–20, 22, 23, 25, 28, 29

QCMT quantum condensed matter theory. 1, 2, 6, 8, 12, 28

1 Introduction

The field of quantum condensed matter theory (QCMT) aims to find useful ways to describe the physics of many-body systems. P.W. Anderson describes the necessity for quantum condensed matter physicists best: ‘More is different’ [1]. Emergent properties arise from systems as they scale up in size in ways that cannot be predicted by merely looking at the sum of their parts. The degrees of freedom of problems involving fermions in QCMT are encoded in creation and annihilation operators with which the Hamiltonian may be defined by. In this formalism, problems wherein fermions may interact with one another are known as interacting problems, and are quartic in the fermionic operators, while systems where the fermions behave independently are known as non-interacting problems. These simpler systems are quadratic in the fermionic operators, and are solved with the aid of linear transformations of the fermionic operators. However, solving the Schrödinger equation for the interacting model requires performing linear transformations on the multiparticle states of the system, a far more complicated endeavour that requires either more computational power or analytical ingenuity.

However, a Hamiltonian written in the Majorana representation introduces the possibility of performing Non-Linear Canonical Transformations (NLCTs). These transformations, performed on the Majorana operators, are able to swap products of any odd number of operators with single, linear Majoranas. These non-linear transformations are, in effect, able to change the very structure and interpretation of a Hamiltonian with their ability to alter which terms contribute to the interaction. This feature of NLCTs is highlighted when introducing gauge freedoms to our Hamiltonian in the form of a decoupled auxiliary site, which may swap one of its Majoranas with higher order operator products in the interacting system of interest. Thus, performing a series of NLCTs may be able to render interacting models effectively non-interacting.

The dynamics of interacting systems can be further explored with a different formalism known as third quantisation. While second quantization is built in the language of operator

space, third quantization is built in the language of operator commutator space. In this formalism, an operator inner product and thus an orthonormal basis of operators is defined. The transition Hamiltonian matrix is constructed using these tools and the operator inner product. This sheds light into the dynamics and structure of a Hamiltonian, and is also a way to determine whether a Hamiltonian is in a non-interacting form after a series of transformations. This thesis seeks to use the language of third quantization to explore the nature of interacting Hamiltonians, and the scope of what becomes possible with the advent of NLCTs.

2 Background

2.1 Second Quantization

Second quantization is a formalism in QCMT that describes states in terms of occupation numbers and number operators, as opposed to attempting to describe the entire system by a wavefunction like one may see in single-particle systems. The latter method, also known as first quantization, is inefficient for describing systems with many particles due to the increasing complexity of the wavefunction as it attempts to encode more and more particles. Instead, second quantization simply asks how many particles are in what state of each orbital of a system. This formalism works thanks to the notion of indistinguishability in quantum mechanics. The assumption states that, for N-particle systems, any two particles described by the same quantum numbers i.e. spin, charge, mass, etc. are indistinguishable from one another [2].

To build the formalism of second quantization, we take an ordered, complete single particle basis $|j\rangle$. The number operator \hat{n}_j defines how many particles occupy a given state $|j\rangle$ defined by a set of quantum numbers. The number operator acts on a set of basis states defined by the quantum number n_j (known as the occupation number). The eigenvalue equation for the number operator for an N-particle system is thus,

$$\hat{n}_j |n_1, \dots, n_j, \dots\rangle = n_j |n_1, \dots, n_j, \dots\rangle \quad (1)$$

where $\sum_j n_j = N$. Solely focusing on fermionic systems, in which particles have a half-odd integer spin, n_j is restricted to taking a value of either 0 or 1 for fermions due to the Pauli exclusion principle. A value of 0 corresponds to an empty state, while an occupied state will have the occupation number equal 1. The state given in (1) is known as a Fock state, as they live in what is known as the Fock space, denoted by \mathcal{F} . The Fock space can be thought of as the sum of the Hilbert spaces corresponding to zero particle states, single particle states, double particle states, and so on. Mathematically, this is expressed as $\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \dots$, where $\mathcal{F}_N = \text{span}\{|n_1, n_2, \dots\rangle \mid \sum_j n_j = N\}$.

Several number operators may act on an eigenstate, but their ordering is of paramount importance for fermions. To understand why, we introduce the fermionic creation operator (\hat{c}_j^\dagger) and its adjoint, the annihilation operator (\hat{c}_j). The creation and annihilation operators are related to the number operator by,

$$\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j \quad (2)$$

Individually, they act on the basis states by,

$$\hat{c}_j |0\rangle_j = 0, \quad \hat{c}_j |1\rangle_j = |0\rangle_j, \quad \hat{c}_j^\dagger |0\rangle_j = |1\rangle_j, \quad \hat{c}_j^\dagger |1\rangle_j = 0 \quad (3)$$

The creation and annihilation operators obey the following anticommutation relations,

$$\{\hat{c}_j, \hat{c}_k\} = 0, \quad \{\hat{c}_j^\dagger, \hat{c}_k^\dagger\} = 0, \quad \{\hat{c}_j^\dagger, \hat{c}_k\} = \delta_{jk} \quad (4)$$

The basis states of the number operator is defined by the creation operators acting on a vacuum state $|vac\rangle$. The order in which the operators act on the vacuum state is important, and for our convention we take the creation operators of higher j to act on the vacuum state first. By the anticommutation relations in (4), swapping around two creation operators incurs a minus sign. For example,

$$\begin{aligned} |101\rangle &= \hat{c}_3^\dagger \hat{c}_1^\dagger |vac\rangle \\ &= -\hat{c}_1^\dagger \hat{c}_3^\dagger |vac\rangle \end{aligned} \quad (5)$$

Hence it is imperative to be meticulous with the order in which the operators act on a pre-existing state in order to build another state.

Problems involving particles which do not communicate with one another are known as non-interacting problems. These Hamiltonians are quadratic with respect to the fermionic operators. They may be solved by writing the Hamiltonian in the form $\hat{H} = \vec{\hat{C}}^\dagger \mathbb{T} \vec{\hat{C}}$, where $\vec{\hat{C}}$ and $\vec{\hat{C}}^\dagger$ represent vectors with the individual fermionic operators as elements, and \mathbb{T} represents the single-particle Hamiltonian. The diagonalization of \mathbb{T} is the equivalent of solving Schrödinger's equation, and reduces the Hamiltonian to the form $\hat{H} = \sum_k \epsilon_k \hat{n}_k$. This \mathbb{T} matrix is of dimension $N \times N$, and the eigenstates of such a Hamiltonian are simply the products of single particle states.

In contrast, problems involving interactions between particles, such as a Coulomb repulsion between two fermions, are quartic (or even higher order) with respect to the fermionic operators. This Hamiltonian cannot be written as a single particle Hamiltonian, and must be constructed using the multiparticle states of a system, i.e. $[\hat{H}]_{nm} = \langle \phi_n | \hat{H} | \phi_m \rangle$, which must then be diagonalised to solve Schrödinger's equation. This matrix, in contrast, is of dimension $2^N \times 2^N$, and the eigenstates are superpositions of products of single particle states. It is thus evident that interacting problems are very different in their nature from non-interacting problems. The fundamental structure of these interacting models are investigated, especially in the face of the possibility of non-linear transformations which are able to change the structure of these interacting models.

2.2 Majorana fermions

2.2.1 Ettore Majorana and the Dirac Equation

The Dirac equation is a historic relativistic wave equation for electrons that famously implied the existence of antimatter [3]. The equation, originally derived by Paul Dirac in 1928 but written here in covariant notation used in quantum field theory, and taking the convention of

$\hbar = c = 1$, reads,

$$(i\gamma^\mu \partial_\mu - m)\psi = 0 \quad (6)$$

Where ψ represents the Dirac spinor field that describes fundamental fermions and γ^μ represent the four Dirac matrices that obey the rules of the Clifford algebra,

$$\{\gamma^\mu, \gamma^\nu\} \equiv 2\eta^{\mu\nu} \quad (7)$$

Here, $\eta^{\mu\nu}$ is the metric tensor of flat space [4]. The components $\mu = \{0, 1, 2, 3\}$ are coordinates in spacetime, with 0 representing the time coordinate and 1, 2, 3 the spacial coordinates. To ensure the Dirac equation describes the wavefunction ψ of a spin-1/2 particle of mass m , it is required that γ_0 be Hermitian with the other elements being anti-Hermitian. Finding suitable real and imaginary matrices for the Dirac matrices implies that ψ must be a complex field with an associated, and different, complex conjugate ψ^* that also satisfies the Dirac equation. In the language of quantum field theory, particles generated by a field ϕ would annihilate with particles generated by the complex conjugate field ϕ^* .

Ten years after Paul Dirac first published his famous equation, Ettore Majorana posed the question, would it be possible to obtain a real Dirac spinor field that would thus be its own complex conjugate, generating particles that are their own antiparticle [5]? Majorana indeed found four purely imaginary matrices satisfying the Clifford algebra,

$$\begin{aligned} \tilde{\gamma}^0 &= \sigma_2 \otimes \sigma_1 \\ \tilde{\gamma}^1 &= i\sigma_2 \otimes 1 \\ \tilde{\gamma}^2 &= i\sigma_3 \otimes 1 \\ \tilde{\gamma}^3 &= i\sigma_2 \otimes \sigma_2 \end{aligned} \quad (8)$$

With these matrices, Dirac's equation may be reduced to Majorana's equation, describing a

real Dirac spinor field $\tilde{\psi}$ that generates a spin-1/2 particle that is its own antiparticle.

$$(i\tilde{\gamma}^\mu\partial_\mu - m)\tilde{\psi} = 0 \quad (9)$$

These particles are thus known as the Majorana fermions. There are several examples of particles which are their own antiparticles; most notably the photon which has spin 1, and neutral pions which are spin 2 particles. However, the obstacle which exists for spin-1/2 particles in achieving this symmetry is their charge. Under charge conservation, these particles cannot simply annihilate with another particle of the same charge. Thus, antiparticles of spin-1/2 particles always have opposite charges, making them distinct from their particle counterparts. A chargeless spin-1/2 particle would be a prime candidate for being a Majorana fermion. At the time of writing, fundamental particles with the behaviour of a Majorana fermion have not been detected. There is some discussion about the possibility of right-handed neutrinos being a candidate for exhibiting the behaviour of a Majorana fermion, but there is no experimental evidence supporting this hypothesis [6]. Majorana fermions however do appear as Bogoliubov quasiparticles on the surfaces and vertex cores of topological superconductors, and obey non-Abelian statistics, notably distinct from bose and fermi statistics [7]. Their potential in topological quantum computation is a source of research interest in the QCMT community [8].

2.2.2 Mathematical Construction of Majorana Fermions

Venturing away from the relativistic nature of the theory of the Dirac equation, we seek a representation of the Majorana fermions in QCMT. When constructing the operators for Majorana fermions, denoted by γ_i , it is imperative they follow the correct anticommutation relations as

described by the Clifford algebra, this time in a non-relativistic setting.

$$\begin{aligned}\{\gamma_i, \gamma_j\} &= 2\delta_{ij} \\ \gamma_i^\dagger &= \gamma_i \\ \gamma_i^2 &= 1\end{aligned}\tag{10}$$

The above relationships highlight the key properties of Majorana fermions; they are self-adjoint Hermitian operators that annihilate with themselves and anticommute. Majorana operators are related to the canonical fermionic creation and annihilation operators via the linear transformation,

$$\hat{c}_i = \frac{\gamma_{2i-1} + i\gamma_{2i}}{2}, \quad \hat{c}_i^\dagger = \frac{\gamma_{2i-1} - i\gamma_{2i}}{2}\tag{11}$$

It is evident that for every N fermions present in a system, $2N$ Majoranas are required to describe them. Majorana operators also hold another unique quality; the product of an odd number of Majorana fermions also obey the Clifford algebra, and thus are also considered Majorana fermions. In particular, the set $\{i\gamma_i\gamma_k\}$ behave exactly like Majorana fermions, where they are multiplied by a factor i to ensure the set obeys the Clifford algebra [9]. This property is crucial to achieving the non-linear canonical transformations discussed later.

When constructing the explicit matrix form of a Majorana fermion, the above relationships must all be considered. One way to construct them which ensures they obey the Clifford algebra is the Jordan-Wigner transformation which transforms spin-1/2 systems into fermions (and vice versa) which not only preserves the correct anticommutation relations and operator algebra, but also the dimensionality of the Hilbert space [10]. By utilizing this transform and the connection between fermionic operators and Majoranas, we are able to construct Majoranas as tensor products of the Pauli spin matrices [11],

$$\hat{\gamma}_{2n-1} = \prod_{i=1}^{n-1} \sigma_i^z \sigma_n^x \quad \hat{\gamma}_{2n} = \prod_{i=1}^{n-1} \sigma_i^z \sigma_n^y$$

It is also possible to decompose spin-1/2 operators into Majorana fermions via the Martin transformation [12], which preserves the SU(2) algebra of the spin operators.

$$\begin{aligned}\hat{S}^x &= -\frac{i}{2}\gamma_j\gamma_k \\ \hat{S}^y &= -\frac{i}{2}\gamma_k\gamma_i \\ \hat{S}^z &= -\frac{i}{2}\gamma_i\gamma_j\end{aligned}\tag{12}$$

2.3 Interacting Fermionic and Spin Models

2.3.1 The Hubbard Model

One of the simplest and most famous cases of an interacting model in QCMT is the Hubbard model, which comprises a tight-binding fermionic lattice, with strong on-site Coulomb repulsion (the long-range Coulomb interaction is neglected) [13]. For the general Hubbard model, the Hamiltonian reads as follows,

$$\hat{H} = \epsilon \sum_{\sigma=\uparrow,\downarrow} \sum_i \hat{n}_{i\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - t \sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}\tag{13}$$

The ϵ term corresponds to the single-particle potential energy of each site on the lattice, and a kinetic term t arises from fermions tunnelling to nearest neighbour sites. A Coulomb repulsion term U describe from two opposite-spin fermions occupying the same site. Physically, given this is an interaction between two different fermions, it makes sense why this Coulomb term is quartic in terms of the fermionic operators. Specifically, in this short range case where two opposite spin fermions interact with each other in the same site, it is also called the Hubbard interaction. Without this interacting term, the Hubbard model would simply describe a tight-binding model which can be easily solved using a set of linear transformations on the fermionic operators. The Hubbard model is useful in investigating the Mott transition between conducting and insulating systems driven by electronic interactions, such as in transition metal oxide materials [14]. This may be seen by focusing on the half-filled case, where

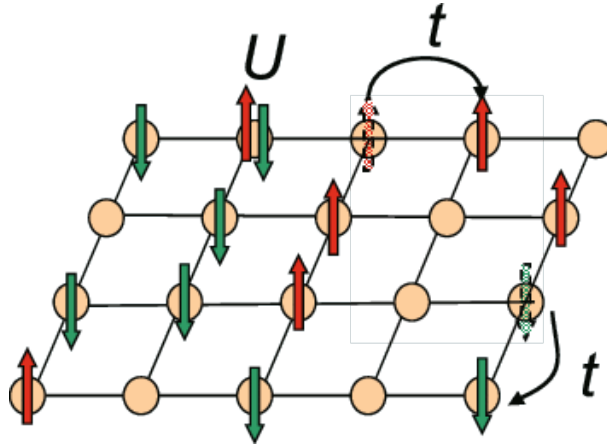


Figure 1: Schematic of the 2D Hubbard model. A Hubbard interaction U is present in sites containing two anti-aligned fermions, with a tunnelling parameter t to account for fermions hopping to neighbouring sites [15].

there is approximately one fermion per site on average which may be either up or down spin. Known as particle-hole symmetry (P-H symmetry), this is the case wherein $\langle \hat{n}_i \rangle = 1$, arising for $\epsilon - \frac{U}{2}$. In the case where $U \ll t$, the kinetic term dominates and fermions more freely tunnel to neighbouring sites, generating phenomena such as particle-hole excitations called excitons and magnetic excitations known as magnons. In this regime, the system is said to be in a metallic phase. In contrast, in the insulating phase, we have $U \gg t$. Any tunnelling into neighbouring atoms generates a large Coulomb interaction U , an extremely unfavourable energy level. The lifetimes of any doubly occupied states are very short as a result.

2.3.2 The Heisenberg Model

Another interacting model of interest is the Heisenberg model, written in terms of spin operators. The system describes a set of N spins which interact with their nearest neighbour via an exchange coupling parameter J [16]. The Heisenberg Hamiltonian simply reads,

$$\hat{H} = J \sum_{\langle i,j \rangle} \vec{\hat{S}}_i \cdot \vec{\hat{S}}_j \quad (14)$$

Considering a 1D chain of N spins, the Hamiltonian may thus be re-expressed as,

$$\hat{H} = J \sum_{i=1}^{N-1} \left[\hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2} (\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+) \right] \quad (15)$$

The \hat{S}_i^z operators represents a magnetic interaction between two neighbouring spins, which may prefer to be anti-aligned (antiferromagnetic) for $J > 0$ or aligned (ferromagnetic) for $J < 0$. The second term with the \hat{S}_i^+ and \hat{S}_i^- operators encode spin flips, in which two neighbouring anti-aligned spins may switch positions in a quantum fluctuation. In the antiferromagnetic phase, the Heisenberg model acts as an effective low energy description of the Hubbard model in the insulating phase where $U \gg t$ [17]. In this regime, the coupling constant J is related to the Hubbard constants by $J = 4t^2/U$.

A more interesting case, the triangular lattice, may also be considered. In its simplest case, with three spins oriented in a triangle, the Hamiltonian becomes,

$$\hat{H} = J \left(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_3 \cdot \vec{S}_1 + \vec{S}_2 \cdot \vec{S}_3 \right) \quad (16)$$

In this case, for $J > 0$, the system experiences magnetic frustration as it becomes impossible to satisfy simultaneously all antiferromagnetic bonds. In other words, with two anti-aligned spins, or a valence bond, the third site will always be aligned with one of them. This produces a large degeneracy in the ground state of the system.

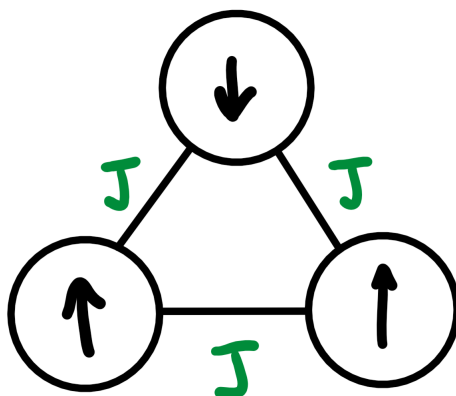


Figure 2: Heisenberg model for three spins oriented in a triangular lattice.

2.4 The Local Canonical Group in the Majorana Representation

Canonical transformations are those which are able to change the Fock structure of a Hilbert space while preserving the fermionic anticommutation relations [18]. In other words, this group of transformations may take us from one set of fermionic operators describing the degrees of freedom of the system $\{\hat{c}_\sigma\}$, to another set $\{\hat{d}_\sigma\}$ which acts on the same Hilbert space. The group of transformations that correctly preserve the fermionic anticommutation relations is referred to as the Local Canonical Group (LCG), given by,

$$SU(2^{n-1}) \otimes SU(2^{n-1}) \otimes U(1) \otimes \mathbb{Z}_2 \quad (17)$$

The transformations performed must remain consistent for all of the elements of the Clifford algebra given below, for N unique fermions,

$$\begin{aligned} \Gamma^{(0)} &: 1 \\ \Gamma^{(1)} &: \gamma_1, \dots, \gamma_{2N} \\ \Gamma^{(2)} &: \gamma_1\gamma_2, \dots, \gamma_1\gamma_{2N}, \dots, \gamma_{2N-1}\gamma_{2N} \\ &\vdots \\ \Gamma^{(2N)} &: \gamma_1 \dots \gamma_{2N} \end{aligned} \quad (18)$$

Where $\Gamma^{(k)}$ represents all the different independent combinations of k Majoranas accessible from a selection of n total Majoranas. In terms of the Majorana fermions, the \mathbb{Z}_2 component of the transformation simply just refers to a sign change of an odd number of the linear set of Majoranas in $\Gamma^{(1)}$. Linear transformations are encapsulated in the $SU(2^{n-1}) \otimes SU(2^{n-1})$ component of the LCG. This transformation, parameterised by an angle χ , generates a new set of Majoranas $\{\alpha_i\}$ given by,

$$\alpha_i = e^{-\frac{\chi}{2}\gamma_j\gamma_k}\gamma_i e^{\frac{\chi}{2}\gamma_j\gamma_k} \quad (19)$$

Evidently, this rotor may be re-expressed as $e^{\frac{\chi}{2}\gamma_j\gamma_k} = \cos(\chi/2) - \gamma_j\gamma_k \sin(\chi/2)$.

2.4.1 Non-Linear Canonical Transformations

The $U(1)$ component of the LCG represent the non-linear transformations that may be performed on the elements of the Clifford algebra. Problems in QCMT, such as strongly correlated electron systems, require analysis beyond the original electron degrees of freedom and Landau's theory [18]. By utilizing these non-linear basis transformations instead of the typical linear basis transformations that are performed to solve problems in QCMT, the original degrees of freedom associated with the system become less relevant. The door is opened to describing these correlated systems in terms of customized quantum coordinates.

Non-linear transformations in terms of fractionalized Majorana fermions are possible because of their aforementioned property wherein the elements of the Clifford algebra in $\Gamma^{(k)}$ for odd k are themselves Majorana fermions and obey the Majorana anticommutation relations when multiplied by an appropriate imaginary factor. Valid transformations on the Majorana basis must still ensure that the Majoranas fulfill the anticommutation relations in (10) and must be consistent for all elements in the Clifford algebra. One such non-linear canonical transformation would be one that mixes the elements in $\Gamma^{(1)}$ and $\Gamma^{(3)}$ in what is called a Hodge rotation [18]. A rotation of this form would generate a new set of Majorana fermions $\{\mu_i\}$ in the following way,

$$\mu_i = e^{-i\frac{\chi}{2}\gamma_j\gamma_k\gamma_l\gamma_m}\gamma_i e^{i\frac{\chi}{2}\gamma_j\gamma_k\gamma_l\gamma_m} \quad (20)$$

We may define from here the Hodge rotation function $R(\chi) = e^{i\frac{\chi}{2}\gamma_j\gamma_k\gamma_l\gamma_m}$. Similarly to the $SU(2^{n-1}) \otimes SU(2^{n-1})$ component of the LCG, the Hodge rotation may be written as $e^{i\frac{\chi}{2}\gamma_j\gamma_k\gamma_l\gamma_m} = \cos(\chi)\gamma_j + i \sin(\chi)\gamma_k\gamma_l\gamma_m$.

2.5 Third Quantization

Pioneered by Tomaž Prosen, third quantization is a formalism which has been used to solve the Linblad master equations associated with quadratic open systems [19]. The theory works

in the language of operator commutator space, with the commutator being built in directly in the construction of the theory.

To understand the formalism of third quantization, recall that any operator \hat{X} may be decomposed in terms of an orthonormal basis $|n\rangle$ of the appropriate Hilbert space,

$$\hat{X} = \sum_{nm} |n\rangle \langle n| \hat{X} |m\rangle \langle m| = \sum_{nm} \langle n| \hat{X} |m\rangle |n\rangle \langle m| \quad (21)$$

Entering the language of third quantisation, the Hilbert-Schmidt inner product, also known as the operator inner product, is defined as,

$$(\hat{A}|\hat{B}) = \frac{\text{tr}(\hat{A}^\dagger \hat{B})}{2^N} \quad (22)$$

Where we divide by 2^N , the dimension of the Hilbert space, to normalise the inner product such that $(\hat{A}|\hat{A}) = \mathbb{1}$ [11]. Using this inner product, we have that $(|n\rangle \langle m| |\hat{X}) = \langle n| \hat{X} |m\rangle$. This allows us to write the operator decomposition in our new, generalised Dirac vector space notation,

$$|\hat{X}) = \sum_{nm} (|n\rangle \langle m| |\hat{X}) |n\rangle \langle m| \quad (23)$$

In third quantization, the degrees of freedom of the system may be represented in an operator basis consisting of the elements of the Clifford algebra described in (18). A vector $\vec{\Gamma}$ may be

constructed, encoding all possible basis operators of the system,

$$\vec{\Gamma} = \begin{bmatrix} \mathbb{1} \\ \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_{2N} \\ \gamma_1\gamma_2 \\ \vdots \\ \gamma_{2N-1}\gamma_{2N} \\ \vdots \\ \gamma_1\gamma_2 \cdots \gamma_{2N-1}\gamma_{2N} \end{bmatrix} \quad (24)$$

Using the operator inner product, it becomes clear why the elements of $\vec{\Gamma}$ form an orthonormal basis, since they fulfill the property that $(\Gamma_i|\Gamma_j) = \delta_{ij}$.

The transition Hamiltonian \mathcal{H} is constructed using the operator inner product and the orthonormal basis operators,

$$\mathcal{H}_{ij} = (\Gamma_i|[\hat{H}, \Gamma_j]) \quad (25)$$

The transition Hamiltonian is an adjacency matrix that provides a deeper insight into the structures and correlations of a corresponding Hamiltonian. It can be thought of as a unique fingerprint, which when transformed into a matrix plot, provides an interesting topology that reflects details about the individual model or Hamiltonian that we are working with. Each element \mathcal{H}_{ij} details how Γ_i and Γ_j connect to one another under the action of the Hamiltonian. The transition Hamiltonian gets its name from the fact that it also encodes all possible transitions between the eigenstates of the Hamiltonian [11].

Furthermore, in the Heisenberg picture the time derivative of an operator that does not

carry explicit time dependence is solely dependent on the commutators [20].

$$\frac{d\hat{A}}{dt} = \frac{\partial \hat{A}}{\partial t} + i[H, \hat{A}] \quad (26)$$

Hence, it is clear from the definition of \mathcal{H} that its elements also provide insight into the decomposition of time derivatives of the basis operators in terms of other basis operators of the system. Such applications of this would be investigating the decomposition of the time derivative of number operators \hat{n} in a given Majorana basis. Hence, \mathcal{H} provides an expanded view of the dynamics of its associated Hamiltonian.

3 Performing Non-Linear Transforms on Interacting Models

3.1 Hubbard Atom in the Particle-Hole Symmetric Case

As a premiere example for exploring the utility of NLCTs in transforming interacting Hamiltonians to a non-interacting form, the single-site case of the Hubbard model described in (13) is investigated, otherwise known simply as the Hubbard atom. We may further direct focus to the Hubbard atom under P-H symmetry, with $\epsilon = -U/2$. In this specific case, the Hamiltonian simplifies to,

$$\hat{H} = -\frac{U}{2} (\hat{c}_\uparrow^\dagger \hat{c}_\uparrow + \hat{c}_\downarrow^\dagger \hat{c}_\downarrow - 2\hat{c}_\uparrow^\dagger \hat{c}_\uparrow \hat{c}_\downarrow^\dagger \hat{c}_\downarrow) \quad (27)$$

Clearly, this Hamiltonian is quartic in terms of the creation and annihilation operators, and is thus an interacting problem requiring the diagonalization of a $2^2 \times 2^2$ matrix to solve. The aim becomes to reduce the complexity of this Hamiltonian by employing NLCTs.

The first step is to introduce an auxiliary orbital to the system as in Figure 3. The auxiliary orbital is a completely decoupled site from the Hubbard atom, and thus cannot affect the observables of the original Hubbard site in any way. The introduction of this auxiliary orbital

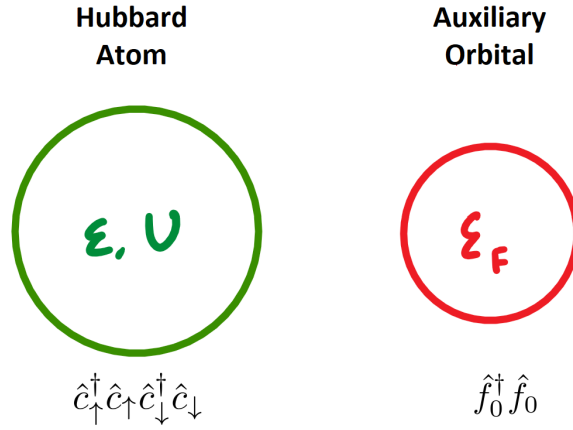


Figure 3: Schematic of the single Hubbard site described by the operators $\hat{c}_{\uparrow}^{\dagger}$, \hat{c}_{\uparrow} , $\hat{c}_{\downarrow}^{\dagger}$, and \hat{c}_{\downarrow} and the decoupled auxiliary orbital described by the operators \hat{f}^{\dagger} and \hat{f} .

introduces an extra set of fermionic operators \hat{f}_0^{\dagger} and \hat{f}_0 that act upon it to the Hamiltonian of the Hubbard model. As this is totally decoupled with our system of interest, it can be treated as a gauge degree of freedom and its energy ϵ_f can be set to be 0 at the end (or indeed, start) of our NLCTs. The Hamiltonian for the overall system including this new auxiliary site is,

$$\hat{H} = -\frac{U}{2} (\hat{c}_{\uparrow}^{\dagger} \hat{c}_{\uparrow} + \hat{c}_{\downarrow}^{\dagger} \hat{c}_{\downarrow} - 2\hat{c}_{\uparrow}^{\dagger} \hat{c}_{\uparrow} \hat{c}_{\downarrow}^{\dagger} \hat{c}_{\downarrow}) + \epsilon_f \hat{f}^{\dagger} \hat{f} \quad (28)$$

A change of representation from the fermionic operators to the Majorana operators is then performed,

$$\begin{aligned} \hat{c}_{\uparrow} &= \frac{\gamma_1 - i\gamma_2}{2}, & \hat{c}_{\downarrow} &= \frac{\gamma_3 - i\gamma_4}{2}, & \hat{f} &= \frac{\gamma_5 - i\gamma_6}{2} \\ \hat{c}_{\uparrow}^{\dagger} &= \frac{\gamma_1 + i\gamma_2}{2}, & \hat{c}_{\downarrow}^{\dagger} &= \frac{\gamma_3 + i\gamma_4}{2}, & \hat{f}^{\dagger} &= \frac{\gamma_5 + i\gamma_6}{2} \end{aligned} \quad (29)$$

The Hamiltonian thus becomes,

$$H = -\frac{U}{4}(1 + \gamma_1\gamma_2\gamma_3\gamma_4) + \frac{\epsilon_f}{2}(1 + i\gamma_5\gamma_6) \quad (30)$$

Employing a Hodge rotation to obtain a new set of Majoranas, $\{\mu_i\}$, where $\mu_i = R^{\dagger} \left(\frac{\pi}{2} \right) \gamma_i R \left(\frac{\pi}{2} \right)$, and $R(\chi) = \exp \left(-\frac{i}{2} \chi \gamma_2 \gamma_3 \gamma_4 \gamma_5 \right)$, the Hamiltonian becomes,

$$H = -\frac{U}{4}(1 + i\mu_1\mu_5) + \frac{\epsilon_f}{2}(1 - \mu_2\mu_3\mu_4\mu_6) \quad (31)$$

By setting $\epsilon_f = 0$, the Hamiltonian becomes effectively quadratic in terms of the Majorana operators. We may then return to the fermionic operator basis by defining a new fermionic operator based on μ_1 and μ_5 ,

$$\hat{d} = \frac{\mu_1 + i\mu_5}{2}, \quad \hat{d}^\dagger = \frac{\mu_1 - i\mu_5}{2} \quad (32)$$

Which reduces the Hamiltonian to a much simpler form, $H = -\frac{U}{2}\hat{d}^\dagger\hat{d}$, with a much more straightforward solution. The Hubbard site is now simply unoccupied, with energy 0, or occupied, with energy $-U/2$. The question may be asked as to what detail is lost in this situation. It may first appear as if we have managed to reduce the degrees of freedom of the system, only describing the Hamiltonian with one pair of fermionic operators instead of two. However, this is not the full picture.

Prior to transformation, by simple analysis it is evident that the eigenstates of the single Hubbard-site under P-H symmetry are simply the ground states $|\uparrow\rangle, |\downarrow\rangle$ with energy $E = -U/2$ and the excited states $|0\rangle, |\uparrow\downarrow\rangle$ with energy $E = 0$. The ground and excited states are hence both doubly degenerate. Introducing the auxiliary orbital doubles the possible eigenstates of the system as the auxiliary may be unoccupied or occupied. Setting $\epsilon_f = 0$, two states with identical quantum numbers only differing between whether the auxiliary orbital is occupied or unoccupied will both have the exact same energy eigenvalue, as seen in Table 1. This increases the degeneracy of the system further, with the energy of the ground state and first excited state now being quadruply degenerate.

To see what happens after transformation, we explicitly write out the transformed Hamiltonian in the fermionic representation, now including the terms associated with the auxiliary site. Defining $\hat{f}_1 = \frac{1}{2}(\mu_2 + i\mu_3)$ and $\hat{f}_2 = \frac{1}{2}(\mu_4 + i\mu_6)$, we get,

$$\hat{H} = -\frac{U}{2}\hat{d}^\dagger\hat{d} + \epsilon_f(2\hat{f}_1^\dagger\hat{f}_1\hat{f}_2^\dagger\hat{f}_2 - \hat{f}_1^\dagger\hat{f}_1 - \hat{f}_2^\dagger\hat{f}_2 + 1) \quad (33)$$

The auxiliary Hilbert space is now of dimension four instead of two, all contributing the same energy once ϵ_f is set to 0. In contrast, the Hilbert space associated with the Hubbard

Pre-Transformation		Post-Transformation	
Eigenstate	Energy	Eigenstate	Energy
$ 0, 0\rangle$	0	$ 0, 00\rangle$	0
$ 0, 1\rangle$		$ 0, 01\rangle$	
$ \uparrow\downarrow, 0\rangle$		$ 0, 10\rangle$	
$ \uparrow\downarrow, 1\rangle$		$ 0, 11\rangle$	
$ \uparrow, 0\rangle$	$-\frac{U}{2}$	$ 1, 00\rangle$	$-\frac{U}{2}$
$ \uparrow, 1\rangle$		$ 1, 01\rangle$	
$ \downarrow, 0\rangle$		$ 1, 10\rangle$	
$ \downarrow, 1\rangle$		$ 1, 11\rangle$	

Table 1: Table explicitly detailing the energy eigenstates and eigenvalues of the Hamiltonian, before and after a non-linear transformation is performed. The comma separates the quantum numbers associated with the Hubbard sites from those associated with the auxiliary orbital. The unoccupied orbitals are denoted by 0, while the occupied sites are denoted by either 1 or an \uparrow/\downarrow , depending on their nature.

atom and the Coulomb interaction were originally 4-dimensional but are now only described by two states (associated with whether the effective d -orbital is occupied or unoccupied). This transformation can thus be seen as the degeneracy shifting from the Hubbard atom over to the auxiliary, which becomes responsible for all of the system's degenerate eigenstates. However, both before and after transformation, there are eight overall eigenstates of the system, seen clearly in Table 1.

3.1.1 Other Configurations of the Hubbard Model

Venturing out of P-H symmetry for the Hubbard site, the picture becomes more complicated. Remaining in the single-site case, the Hamiltonian becomes,

$$\hat{H} = \epsilon(\hat{n}_\uparrow^\dagger + \hat{n}_\downarrow^\dagger) + U\hat{n}_\uparrow\hat{n}_\downarrow + \epsilon_f\hat{f}^\dagger\hat{f} \quad (34)$$

Written in the Majorana representation,

$$\begin{aligned} \hat{H} &= \frac{\epsilon}{2}(2 + i\gamma_1\gamma_2 + i\gamma_3\gamma_4) + \frac{U}{4}(1 + i\gamma_1\gamma_2 + i\gamma_3\gamma_4 - \gamma_1\gamma_2\gamma_3\gamma_4) + \frac{\epsilon_f}{2}(1 + i\gamma_5\gamma_6) \\ &= \epsilon + i\left(\frac{2\epsilon + U}{4}\right)(\gamma_1\gamma_2 + \gamma_3\gamma_4) + \frac{U}{4}(1 - \gamma_1\gamma_2\gamma_3\gamma_4) + \frac{\epsilon_f}{2}(1 + i\gamma_5\gamma_6) \end{aligned} \quad (35)$$

By transforming the set of Majoranas by the same rotor $R(\chi = \pi/2) = \exp\left(-\frac{i\pi}{4}\gamma_2\gamma_3\gamma_4\gamma_5\right)$ in an effort to again reduce the quartic term connected to the Coulomb repulsion into a quadratic one, the Hamiltonian becomes,

$$\hat{H} = \epsilon + i\left(\frac{2\epsilon + U}{4}\right)(i\mu_1\mu_3\mu_4\mu_5 + \mu_3\mu_4) + \frac{U}{4}(1 - i\mu_1\mu_5) + \frac{\epsilon_f}{2}(1 - \mu_2\mu_3\mu_4\mu_6) \quad (36)$$

Evidently, there are terms that are still quartic in terms of the Majorana operators. Further rotations will only shift which term is quartic in the Majoranas away from P-H symmetry. The introduction of more auxiliary orbitals has been explored, encountering the same problem of shifting complexity within the terms related to the Hubbard atom. As of writing, there is no known rotation which will render the Hubbard atom quadratic in the Majoranas.

Similarly, we explore the Hubbard dimer, the 2-site case of the Hubbard model, under P-H symmetry. The Hamiltonian with respect to the fermionic operators is written as,

$$\hat{H} = -\frac{U}{2}(\hat{n}_{1\uparrow}^\dagger + \hat{n}_{1\downarrow}^\dagger + \hat{n}_{2\uparrow}^\dagger + \hat{n}_{2\downarrow}^\dagger) + U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + t(\hat{c}_{1\uparrow}^\dagger\hat{c}_{2\uparrow} + \hat{c}_{2\uparrow}^\dagger\hat{c}_{1\uparrow} + \hat{c}_{1\downarrow}^\dagger\hat{c}_{2\downarrow} + \hat{c}_{2\downarrow}^\dagger\hat{c}_{1\downarrow}) + \epsilon_f\hat{f}^\dagger\hat{f} \quad (37)$$

Again in the Majorana representation,

$$\hat{H} = -\frac{U}{4}(2 + \gamma_1\gamma_2\gamma_3\gamma_4 + \gamma_5\gamma_6\gamma_7\gamma_8) + \frac{it}{2}(\gamma_2\gamma_5 - \gamma_1\gamma_6 + \gamma_4\gamma_7 - \gamma_3\gamma_8) + \frac{\epsilon_f}{2}(1 + \gamma_9\gamma_{10}) \quad (38)$$

Performing two rotations $R_1(\pi/2) = e^{\frac{i\pi}{4}\gamma_2\gamma_3\gamma_4\gamma_9}$ and $R_2(\pi/2) = e^{\frac{i\pi}{4}\gamma_5\gamma_7\gamma_8\gamma_{10}}$ to reduce the

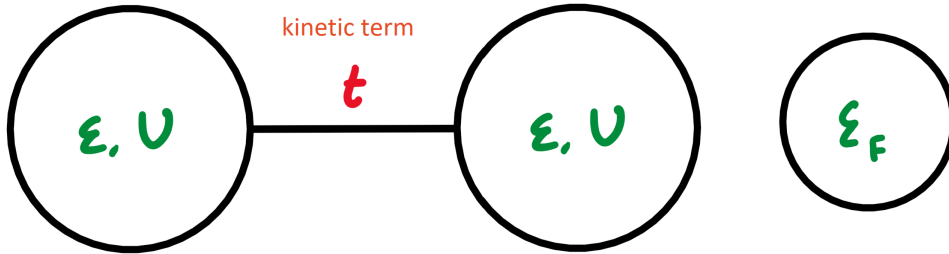


Figure 4: Illustration of the Hubbard dimer with an accompanying auxiliary orbital. A new kinetic term t permits tunnelling between sites.

Coulomb interaction into a quadratic form returns,

$$\begin{aligned} \hat{H} = & -\frac{iU}{4}(2 + \mu_1\mu_9 - \mu_6\mu_{10}) - \frac{\epsilon_f}{2}(1 - i\mu_2\mu_3\mu_4\mu_5\mu_7\mu_8) \\ & + \frac{it}{2}(-\mu_3\mu_4\mu_9\mu_7\mu_8\mu_{10} + \mu_1\mu_6 + \mu_9\mu_2\mu_3\mu_8\mu_{10}\mu_5 - \mu_4\mu_9\mu_2\mu_{10}\mu_5\mu_7) \end{aligned} \quad (39)$$

Similar to the Hubbard atom away from P-H symmetry, the complexity is merely shifted from one term to another as the kinetic term becomes sextic in the Majorana fermions. Again, further non-linear transformations on this Hamiltonian to shift complexity onto the auxiliary orbital also transfers complexity to either the Coulomb or the kinetic terms. It remains a noteworthy result to recognise that the interacting term is no longer the Coulomb repulsion, but the kinetic term that permits site hopping. Thus, the interpretation of this Hamiltonian has effectively changed.

In the insulating phase where $U \gg t$ such that $t \sim 0$, we are still able to render this a non-interacting Hamiltonian using the same methods as in the P-H symmetric single Hubbard case. Even as the number of sites increase, we still only require a single auxiliary orbital for this technique to work. This is easily shown with the example of three Hubbard sites, with the Coulomb interaction in two sites already having been transformed into quadratic terms,

$$\hat{H} = -\frac{iU}{4}(2 + \mu_1\mu_{13} - \mu_6\mu_{14} - i\mu_9\mu_{10}\mu_{11}\mu_{12}) + \frac{\epsilon_f}{2}(1 - i\mu_2\mu_3\mu_4\mu_5\mu_7\mu_8) \quad (40)$$

We may use any one of the Majorana fermions that have been shifted to the auxiliary orbital for the Hodge rotation to turn \hat{H} quadratic. Arbitrarily choosing μ_2 and performing the rotation $R(\chi = \pi/2) = \exp\left(-\frac{i\pi}{4}\mu_{10}\mu_{11}\mu_{12}\mu_2\right)$ to define a new set of $\{\alpha_i\}$ operators,

$$\hat{H} = -\frac{iU}{4}(2 + \alpha_1\alpha_{13} - \alpha_6\alpha_{14} + \alpha_9\alpha_2) - \frac{\epsilon_f}{2}(1 - \alpha_{10}\alpha_{11}\alpha_{12}\alpha_3\alpha_4\alpha_5\alpha_7\alpha_8) \quad (41)$$

Hence, we observe that in the insulator phase, for every site we reduce to quadratic in terms of the Majorana fermions, we obtain three new operators with which we may use to perform Hodge rotations to reduce more sites to quadratic forms. Thus, only one auxiliary orbital is necessary at the start, independent of system size in this limit $U \gg t$.

Performing these Hodge rotations by hand can become tedious with increasing consecutive rotations. A formalism is sought to perform these transformations immediately, with an accompanied diagnosis of whether the transformed Hamiltonian is non-interacting.

4 Third Quantization

4.1 The Transition Hamiltonian Matrix

Consider a simple Hubbard atom away from P-H symmetry, without an additional auxiliary orbital. The system may be described by four Majorana operators,

$$\hat{H} = \frac{\epsilon}{2}(2 + i\gamma_1\gamma_2 + i\gamma_3\gamma_4) + \frac{U}{4}(1 + i\gamma_1\gamma_2 + i\gamma_3\gamma_4 - \gamma_1\gamma_2\gamma_3\gamma_4) \quad (42)$$

A matrix plot of the transition Hamiltonian for this \hat{H} is constructed and plotted in Figure 5. A non-zero entry in the ij^{th} element of the matrix, depicted in the matrix plot by a black square, indicates some connection between Γ_i and Γ_j under the action of the Hamiltonian. The matrix is divided into different blocks, separated by the order of Majoranas that are connecting to one another. Entries in block $A^{(k)}$ indicate how elements in $\Gamma^{(k)}$ connect to Majoranas of the same order. For example, in the $A^{(1)}$ block lies the elements of the transition Hamiltonian where linear Majoranas connect to other linears, and in the $A^{(2)}$ block is where the bilinear Majoranas (product of two Majorana operators) connect to other bilinears.

The entries in the $B^{(kl)}$ blocks represent how combinations of Majoranas connect to other products of Majoranas of different order. For example, the entries in $B^{(13)}$ block detail how linear Majoranas connect to trilinear Majoranas. These off block-diagonal entries are especially of interest, as they are a way of diagnosing whether a Hamiltonian is in an interacting form. Non-interacting Hamiltonians are quadratic with respect to the Majorana operators, hence we do not expect any connections to exist between linear Majoranas to higher order products of Majoranas. In the following results discussed, a non-interacting Hamiltonian will be diagnosed when there exists only zero entries in the $B^{(1k)}$ block, with $2N \geq k > 1$. Equivalently,

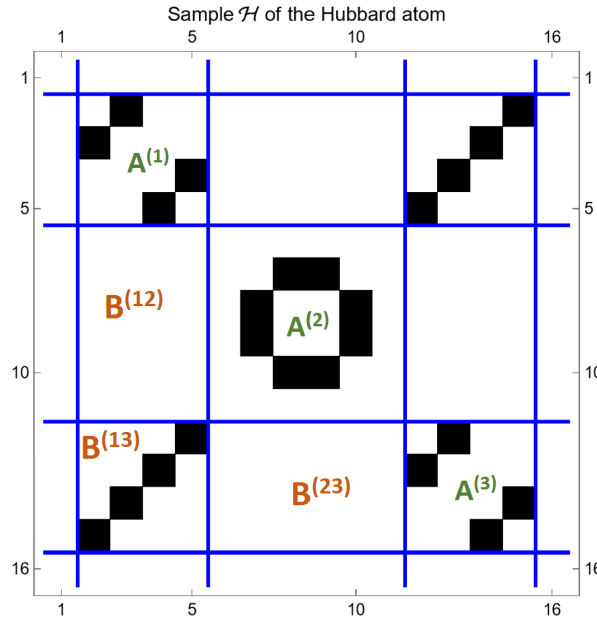


Figure 5: Matrix plot for the transition Hamiltonian of the Hubbard atom without P-H symmetry. Non-zero entries are filled in black. The matrix is segmented into separate blocks. Along the block diagonal, block $A^{(k)}$ represents where the $\Gamma^{(k)}$ elements of the Clifford algebra connect with other elements in $\Gamma^{(k)}$. Off the diagonal, the entries in $B^{(kl)}$ represent where elements in $\Gamma^{(k)}$ connect with elements in $\Gamma^{(l)}$.

the $B^{(k1)}$ blocks may be considered.

Already captured by this \mathcal{H} is charge conservation, with the $B^{(12)}$ block being empty indicating no connections existing between linear and bilinear Majoranas. This observation makes sense; if non-linear canonical transformations can swap out products of odd numbers of Majoranas for linear ones, then a connection present in the $B^{(1k)}$ block for even k would indicate that a transformation is possible that would produce a single fermionic operator in the Hamiltonian that would thus signify a disruption of charge conservation.

The transition Hamiltonian may be symmetric by a more careful construction of $\vec{\Gamma}$, where we multiply different subsets of the Clifford algebra $\Gamma^{(k)}$ by an appropriate imaginary factor. This is not strictly necessary as all non-zero entries appear on the matrix plot the same, represented by a black square, as we are mostly only interested in whether a connection between Γ_i and Γ_j exists at all (not its magnitude). Hence, the matrix plots generated are effectively symmetric. By performing a Hodge rotation and applying it to all elements in $\vec{\Gamma}$ to generate a new set of matrices \vec{M} , we are able to generate a new \mathcal{H} in the basis of operators in \vec{M} .

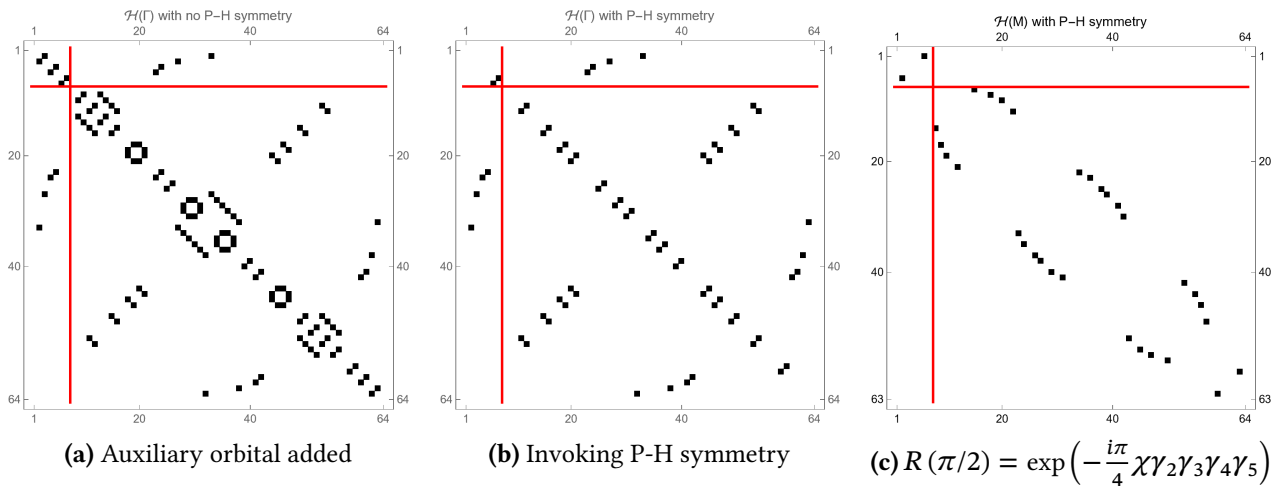


Figure 6: \mathcal{H} for the Hubbard site. An auxiliary orbital added to the system in (a), and P-H symmetry is imposed in (b), A Hodge rotation is then performed on $\vec{\Gamma}$, leaving only zero entries on the off-diagonal blocks. The Hamiltonian is now non-interacting.

4.2 The \mathcal{H} of the P-H symmetric Hubbard Site

Following the same steps that turned this interacting Hamiltonian into an effectively non-interacting form in Section 3.1 and only focusing on eliminating non-zero entries in the $B^{(1k)}$ block, an auxiliary orbital is introduced. The addition of two Majoranas quadruples the size of $\vec{\Gamma}$, and hence the dimensions of \mathcal{H} . By invoking P-H symmetry, some terms along the block diagonal become zero, however there still exists non-zero terms in the off-diagonal blocks.

Performing the same Hodge rotation as before, $R(\chi) = \exp\left(-\frac{i}{2}\chi\gamma_2\gamma_3\gamma_4\gamma_5\right)$, we arrive at a block diagonalised \mathcal{H} . In the basis of operators in \vec{M} , there are no connections between the linear Majorana operators with higher order products of Majoranas. We deduce that this transformation on the Majoranas have reduced the Hamiltonian to a non-interacting form.

4.3 The \mathcal{H} of the Hubbard Site without P-H symmetry

Performing the same Hodge rotation with $\gamma_2\gamma_3\gamma_4\gamma_5$ as before, now removing the condition that $\epsilon = -\frac{U}{2}$, non-zero terms outside of the block diagonal re-appear. An example of three consecutive rotations are performed on the system in Figure 7, transforming from a representation in $\{\gamma_i\}$ to $\{\mu_i\}$, then $\{\alpha_i\}$, and finally $\{\beta_i\}$. However, non-zero terms continue to persist outside of the block-diagonal, indicating that the Hamiltonian in this basis is still interacting. It is

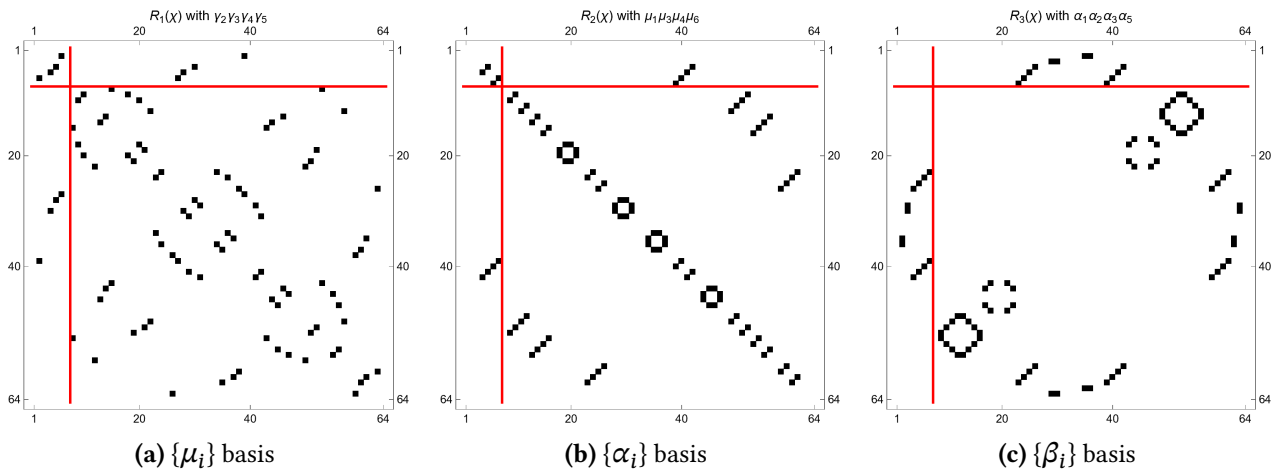


Figure 7: \mathcal{H} for the Hubbard site the transformations $R_1(\pi/2) = e^{\frac{i\pi}{4}\gamma_2\gamma_3\gamma_4\gamma_5}$, $R_2(\pi/2) = e^{\frac{i\pi}{4}\mu_1\mu_3\mu_4\mu_6}$ and $R_3(\pi/2) = e^{\frac{i\pi}{4}\alpha_1\alpha_2\alpha_3\alpha_5}$ are performed.

interesting to watch the vastly different topologies of \mathcal{H} in different operator bases. Notably, represented with the $\{\beta_i\}$ fermions, the achieved \mathcal{H} is empty in its block diagonals. The topology of this graph thus reflects how the Hamiltonian in the basis of the $\{\beta_i\}$ Majoranas, all terms are quartic in the Majorana fermions.

4.4 The \mathcal{H} of the Hubbard Dimer

In Figure 8a we plot \mathcal{H} for the Hubbard dimer with an added auxiliary orbital (see in (38)). It involves twelve individual Majorana operators leading to a \mathcal{H} of dimension 1024×1024 . The structure of \mathcal{H} for the dimer is significantly different to the Hubbard atom with the single site due to the addition of a kinetic term generating new connections. Non-zero entries on the off-block diagonal entries corroborate that this is an interacting system. Performing the same two Hodge rotations as done in Section 3.1.1 drastically changes the structure of \mathcal{H} . The non-zero entries now collect towards the edges of the matrix plot, associated with connections between the linear Majoranas to products of five Majoranas. This is what is expected of the Hamiltonian when written in the basis of the transformed μ_i Majoranas, which is sextic in the Majorana operators as seen in (39).

In the insulating phase, and approximating $t \sim 0$, we observe from Figure 8c the expected block-diagonal structure that indicates that no connections exist between linear and non-linear

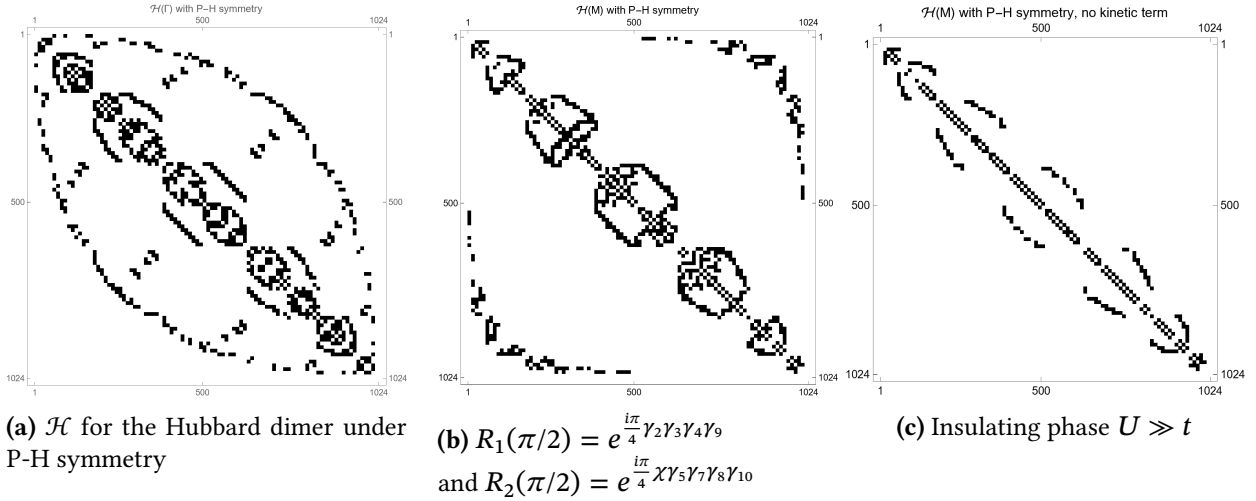


Figure 8: \mathcal{H} for the Hubbard dimer in P-H symmetry.

Majoranas. We have again visually determined the Hamiltonian is written in a basis where it is non-interacting using the transition Hamiltonian.

4.5 The \mathcal{H} for the Heisenberg Model

The Heisenberg spin chain containing two sites may be expressed in two different ways. Directly relating the spins to the Majorana fermions as in (12), the Hamiltonian may be written as,

$$\hat{H} = \frac{-J}{4}(\gamma_2\gamma_3\gamma_5\gamma_6 + \gamma_3\gamma_1\gamma_6\gamma_4 + \gamma_1\gamma_2\gamma_4\gamma_5) \quad (43)$$

The transition Hamiltonian matrix now has a significantly different form than it took for the Hubbard dimer. The non-zero entries indicate connections between the $\Gamma^{(1)}$ and $\Gamma^{(3)}$ sets and $\Gamma^{(2)}$ and $\Gamma^{(4)}$ sets. Unintuitively, the entries in the block diagonal are all zero, including the $A^{(2)}$ block. This is possibly due to an underlying symmetry of the system, presumably $SU(2)$ spin symmetry.

Expressing the Hamiltonian given in (15) in terms of the fermionic creation and annihilation operators,

$$\hat{H} = \frac{J}{2} \left(\frac{1}{2}(\hat{n}_{1\downarrow} - \hat{n}_{1\uparrow})(\hat{n}_{2\downarrow} - \hat{n}_{2\uparrow}) + \hat{c}_{1\uparrow}^\dagger \hat{c}_{1\downarrow} \hat{c}_{2\downarrow}^\dagger \hat{c}_{2\uparrow} + \hat{c}_{1\downarrow}^\dagger \hat{c}_{1\uparrow} \hat{c}_{2\uparrow}^\dagger \hat{c}_{2\downarrow} \right) \quad (44)$$

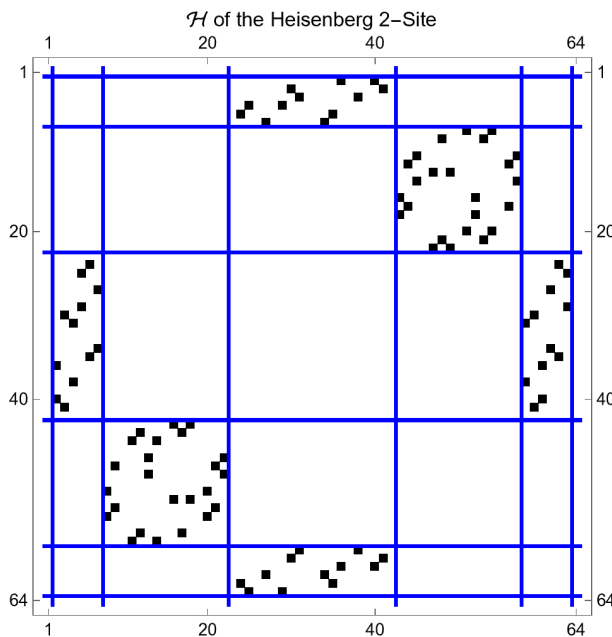


Figure 9: \mathcal{H} for the Heisenberg 2-site model using the Martin transformation. All blocks are clearly defined to highlight its block diagonal structure.

Which then in the Majorana representation becomes,

$$\begin{aligned} \hat{H} = J/16 & (\gamma_1\gamma_3\gamma_7\gamma_5 + \gamma_1\gamma_3\gamma_8\gamma_6 - \gamma_1\gamma_4\gamma_7\gamma_6 + \gamma_1\gamma_4\gamma_8\gamma_5 + \gamma_2\gamma_3\gamma_7\gamma_6 - \gamma_2\gamma_3\gamma_8\gamma_5 \\ & + \gamma_2\gamma_4\gamma_7\gamma_5 + \gamma_2\gamma_4\gamma_8\gamma_6 - \gamma_1\gamma_2\gamma_5\gamma_6 + \gamma_1\gamma_2\gamma_7\gamma_8 + \gamma_3\gamma_4\gamma_5\gamma_6 - \gamma_3\gamma_4\gamma_7\gamma_8) \quad (45) \end{aligned}$$

While this does capture the physics of the problem, the Hilbert space for this site is larger than necessary, as it includes the possibility of having unoccupied or doubly occupied sites, which need not be considered in the Heisenberg model. However, it now has the same dimensions as the Hubbard dimer, allowing us to compare both of their transition Hamiltonians together. A variation of \mathcal{H} is constructed, taking the absolute value of the Hilbert-Schmidt inner product in order to determine the magnitude of connection between Γ_i and Γ_j . This comparison is of interest following the theory in Section 2.3.2, where we discuss how the Heisenberg model is an effective low energy description of the Hubbard model. Evaluating \mathcal{H} for the Hubbard dimer with $U \gg t$ and the Heisenberg model with $J = t^2/U$ we see the topology of both plots are inherently different, with most of the entries in the Heisenberg \mathcal{H} being close to zero, while large terms persist in the Hubbard dimer.

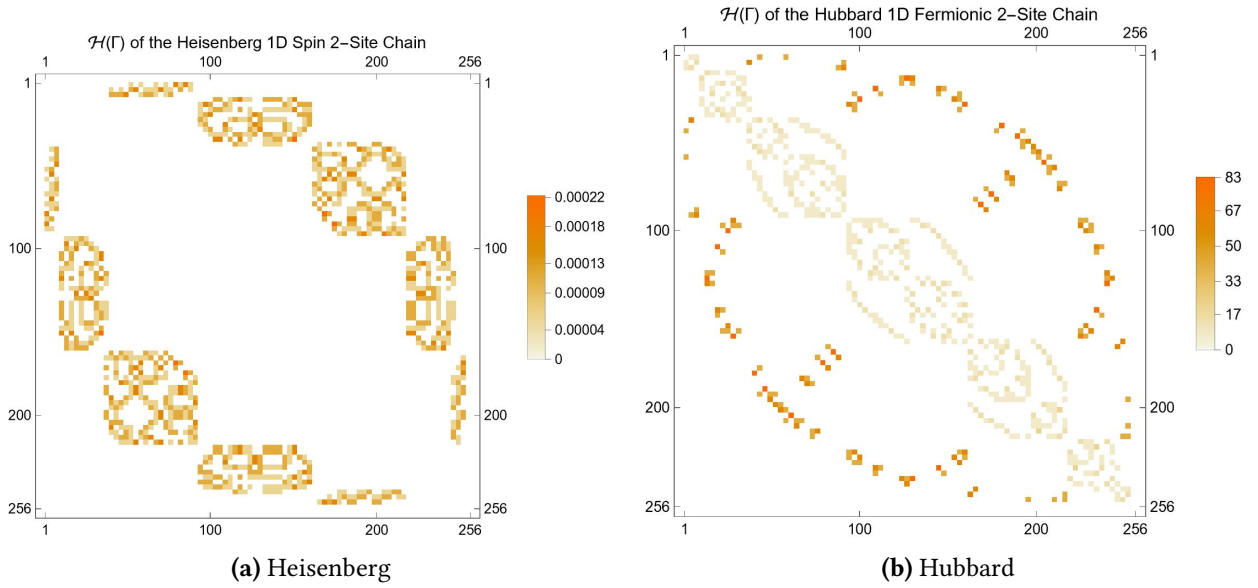


Figure 10: \mathcal{H} for the Hubbard and Heisenberg models for two sites in the limit $U \gg t$ with $U = 1000$, $t = 1$ and $J = 0.001$. Note the different largely different magnitude gradients for both matrix plots.

We may also look at the Hamiltonian of the Heisenberg triangular lattice in terms of the Majorana fermions, obtained again by the Martin transformation, given by,

$$\hat{H} = J/4(\gamma_1\gamma_2\gamma_4\gamma_5 + \gamma_1\gamma_2\gamma_7\gamma_8 + \gamma_2\gamma_3\gamma_5\gamma_6 + \gamma_2\gamma_3\gamma_8\gamma_9 + \gamma_3\gamma_1\gamma_6\gamma_4 + \gamma_3\gamma_1\gamma_9\gamma_7 + \gamma_4\gamma_5\gamma_7\gamma_8 + \gamma_5\gamma_6\gamma_8\gamma_9 + \gamma_6\gamma_4\gamma_9\gamma_7) \quad (46)$$

The matrix plot of \mathcal{H} is plotted in Figure 11. We again observe zero entries along the block

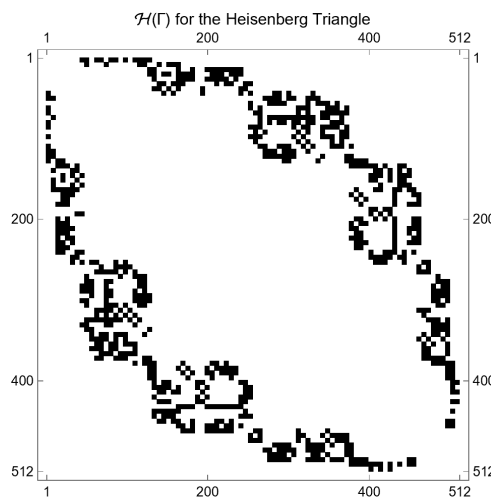


Figure 11: Matrix plot of \mathcal{H} for the Heisenberg model with a triangular lattice.

diagonal of \mathcal{H} . This again is a possible imprint left by the $SU(2)$ symmetry present in the Heisenberg model.

5 Discussion

The nature of interacting problems in QCMT is called into question with the arrival of NLCTs. These transformations are able to shift the very structure and interpretation of Hamiltonians. Utilizing auxiliary orbitals as a gauge freedom, we have rendered the Hubbard atom in P-H symmetry effectively non-interacting, opening the doors to other possible interacting systems which may be reduced to effectively non-interacting forms via these strange NLCTs. This method can be straightforwardly extended to the insulating phase of the Hubbard model in P-H symmetry for any number of sites using only one auxiliary orbital. It is not known as of yet what other systems exist that may be rendered effectively non-interacting in a similar way via these NLCTs. Prime candidates of possible systems that could be transformed into non-interacting models are the transverse Ising field model, and other systems with degeneracies in the eigenstates such as the magnetically frustrated Heisenberg triangular lattice, as we saw how the degeneracy of the system itself seemed to be transferred from the Hubbard atom to being captured by the auxiliary orbital.

However, this ability to perform NLCTs also has interesting consequences for perturbation theory. Since transformations on the Hubbard model may render the Coulomb repulsion term non-interacting at the expense of introducing quartic or even sextic terms to the kinetic term, this changes the nature of the problem when doing perturbation theory or mean-field theory around some reference state. This might prove helpful for dealing with models where the natural reference state can be simplified by NLCTs.

The formalism of third quantization also shows much promise in understanding these interacting systems in a more fundamental light in the face of non-linear transformations. We have shown how the transition Hamiltonian's topology changes with performing non-linear transformations on its basis operators, the Majorana fermions and all possible product combinations. We show that \mathcal{H} is able to visually determine that we have a non-interacting system

after repeating the same transformations that renders the Hubbard model in P-H symmetry and in the insulating phase to a non-interacting form. We discuss how it allows us to see where the connections between the basis operators that construct Hamiltonians themselves lie, and how the matrix describes the deeper dynamics of the system due to it being constructed using the operator commutator between the Hamiltonian and the basis operators that represent the degrees of freedom of the system. We investigate how problems with similar physics, such as the antiferromagnetic Heisenberg model and the Hubbard model in the insulating phase, and see how the topology of their \mathcal{H} matrices are completely different. The structure of \mathcal{H} also signals certain symmetries, such as charge symmetry in the fermionic systems, and possibly SU(2) symmetry in the Heisenberg model where the block diagonal entries are all unintuitively zero.

Further research may be done to study other interacting systems under this framework of third quantization. Hamiltonians with similar features of degeneracy to the insulating P-H symmetric Hubbard model may be investigated to see if these are also possible candidates for reducing to non-interacting forms. Transformations on the level of \mathcal{H} and not just it's elements may also provide a strategy to block diagonalising these matrices, in order to produce a non-interacting model.

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