PROCEEDINGS OF SCIENCE

Topology and symmetry in carbon nanoribbons

Lado Razmadze*

Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn,
53115 Bonn, Germany

E-mail: s6larazm@uni-bonn.de

BCS-Hubbard model is applied to nanoribbons with zigzag and armchair geometries. Dispersion relations and effective Hamiltonian are derived at symmetric lines for ferromagnetic and antiferromagnetic order. Conserved quantities are found for general case of BCS-Hubbard model.

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*Speaker

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1. Introduction

Topology is an interesting mathematical field in and of itself and existing toolkit of topology can be used in condensed matter to extend classification of states of matter.

1.1 Topology in condensed matter

Key concept in topology is *continuity*. Two topological spaces are considered to be equivalent if they can be continuously mapped to each-other. In condensed matter systems we introduce the notion of *topological equivalence* on the space of gapped Hamiltonians. Hamiltonian is gapped if the difference in its ground state and first excited state energies remains finite in the limit where we take the system to be infinitely large.

Consider a space Ω of Hamiltonians. Two Hamiltonians are defined as topologically equivalent if the two can be connected in the Hamiltonian space without closing the energy gap. Physically this corresponds to adiabatically changing the parameters to transform one Hamiltonian into another while every intermediate Hamiltonian remains gapped. In Figure 1 H and H'' are equivalent since there exists a path connecting them while satisfying this requirement. But H' is separated from H and H'' by a wall of gap closing denoted in red, meaning H and H' are topologically inequivalent. Having defined equivalence we have to define a *topologically trivial phase*. For this we choose

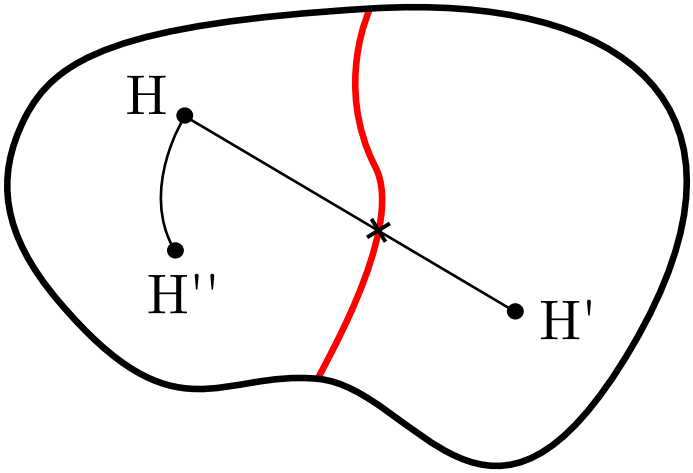


Figure 1: Hamiltonian space with two phases separated by wall of gap closing denoted in red. H and H'' are equivalent while H and H' are not.

atomic insulators which are insulating because electrons are tightly bound to the atomic cores inside the solid. If a system is not topologically equivalent to an atomic insulator then we say that it is topological.

2. Kitaev Chain

Kitaev introduced a 1D toy model [1] in order to argue that Majorana states could be created in solid state systems. His main motivation was development of Majoranas as qubits for quantum computing due to their robustness, which stems from the topological invariant that the system possesses - Parity. The chain is a 1D system with nearest neighbor hopping t, chemical potential μ and nearest neighbor superconductive pairing Δ. These physical properties span our parameter space. Hamiltonian is given as

$$\mathrm{H} = -t\sum_{j=1}^{L-1}(c_j^\dagger c_{j+1} + h.c.) + \Delta\sum_{j=1}^{L-1}(c_j c_{j+1} + h.c.) - \mu\sum_{j=1}^{L} n_j \tag{1}$$

where $n_j = c_j^\dagger c_j$ is the number operator. Note first two sums don't include last lattice site due to *open boundary conditions*. Also note that due to the pairing term $U(1)$ symmetry is broken down to $\mathbb{Z}_2$. In order to investigate this system further we assume each lattice cite to be occupied by two Majorana fermions $c \to \gamma_a, \gamma_b$(see Figure 2a)

$$\gamma_{ja} = c_j + c_j^\dagger \qquad \gamma_{jb} = i(c_j - c_j^\dagger) \tag{2}$$

Ordinary fermion operators c are *nilpotent* meaning $\exists n \in \mathbb{N} \ : \ c^n = 0$. For spin-1/2 particles like we have here, $n = 2$. Majorana fermions γ are superpositions of creation and annihilation operators of ordinary fermions, because of that they are no longer nilpotent, instead $\gamma^2 = 1$. They do, however, still retain the anti-commutation property of ordinary fermions, that is to say $\{\gamma_{i\lambda}, \gamma_{j\lambda'}\} = \delta_{ij}\delta_{\lambda\lambda'}$. parity operator can be constructed by taking products of these operators

$$P = \prod_{j=1}^{L}(-i\gamma_{ja}\gamma_{jb}) \tag{3}$$

Assuming symmetric line conditions($\Delta = t$) results in

$$\mathrm{H} = t\sum_{j=1}^{L-1} i\gamma_{jb}\gamma_{j+1a} - \frac{\mu}{2}\sum_{j=1}^{L}(1 + i\gamma_{ja}\gamma_{jb}) \tag{4}$$

This system admits two limits $\mu \gg t$ and $t \gg \mu$. In first case (Figure 2b) majoranas become bound on the same cites and and there is no more hopping between the neighboring cites. This system has a unique ground state. In the opposite limit we end up with a 2-fold degenerate ground state. Degeneracy is due to parity - $P = \pm 1$. As we can see for two sets of (t, Δ, μ) we get two Hamiltonians with different eigensystems. If we were to smoothly vary these parameters $(0, 0, \mu) \to (t, t, 0)$ there would be gap closing at $(t, t, 2t)$ which, from the definition in section 1.1, means that these two Hamiltonians represent topologically distinct phases.

(a) Each lattice cite is occupied by two Majorana fermions denoted in black and white. Dashed line implies there are nearest neighbor interactions

(b) $\mu \gg \Delta, t$ majorana fermions are bound to each-other on the same cite. There is no more hopping between neighboring cites.

(c) $\mu \ll \Delta, t$ majorana fermions from neighboring cites are bound to each-other there are no hoppings between bound states. There are two unpaired majoranas on the endpoints of the chain.

Figure 2: Diagrammatic representation of various phases in Kitaev chain

3. BCS-Hubbard Model

3.1 Hamiltonian

Consider an N-dimensional general bipartite lattice with nearest neighbor hopping - t and superconductive(SC) pairing - Δ. Hopping and SC are defined only between different sublattices. Here sublattices A and B are color-coded in blue and red to make the equations more amenable to visual parsing. In this chapter i and j will be exclusively referring to cites on sublattice A and B respectively and will be color-coded accordingly as $i \in A$ and $j \in B$. Nearest neighbors are denoted as $\langle i, j \rangle$ and σ is a label for spin. Write Hamiltonian as in [2]

$$\mathrm{H}_{\text{free}} = \sum_{\langle i,j \rangle \sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + \Delta_{ij} c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma} + h.c. \tag{5}$$

Furthermore Hubbard interaction at half filling is defined using the spin degrees of freedom.

$$\mathrm{H}_{\text{hubbard}} = U \sum_{l} \left(n_{l\uparrow} - \frac{1}{2} \right) \left(n_{l\downarrow} - \frac{1}{2} \right) \tag{6}$$

For a homogeneous case $t_{ij} = t$ and $\Delta_{ij} = \Delta$.

3.2 Composite fermions

We go to Majorana basis similar to Kitaev model

$$c_{i\sigma} = \eta_{i\sigma} + i\beta_{i\sigma} \qquad c_{j\sigma} = \beta_{j\sigma} + i\eta_{j\sigma}$$

Resulting in

$$\mathrm{H} = \sum_{\langle i,j \rangle \sigma} 2i(t-\Delta)\eta_{i\sigma}\eta_{j\sigma} - 2i(t+\Delta)\beta_{i\sigma}\beta_{j\sigma} - U \sum_{l} (2i\beta_{l\uparrow}\beta_{l\downarrow})(2i\eta_{l\uparrow}\eta_{l\downarrow}) \tag{7}$$

At Symmetric lines $D_l = 4i\eta_{l\uparrow}\eta_{l\downarrow}$ is conserved for each lattice cite as was shown in [3], [4]. However, $D^1 = \sum_l 4i\beta_{l\uparrow}\beta_{l\downarrow}$ and $D^2 = \sum_l 4i\eta_{l\uparrow}\eta_{l\downarrow}$ are conserved for all values of Δ, t. Which is easy to show by writing $[H, D^a]$ and using commutator-anticommutator identities.

From here we can make another change of basis to composite d-fermions.

$$d_{i1} = \beta_{i\uparrow} - i\beta_{i\downarrow} \qquad d_{j1} = \beta_{j\uparrow} + i\beta_{j\downarrow}$$
$$d_{i2} = \eta_{i\uparrow} + i\eta_{i\downarrow} \qquad d_{j2} = \eta_{j\uparrow} - i\eta_{j\downarrow}$$

For $\Delta = t$ Hamiltonian becomes quadratic for any value of U, hence diagonalizable. Moreover since D_l is conserved and $D_l^2 = 1$ Hilbert space gets split into 2^N sectors where N is the number of lattice cites. In composite fermion basis D_l measures $\hat{y}$-axis spin polarization.

4. Carbon Nanoribbons

Applying BCS-Hubbard model to nanoribbons we derive Bloch matrix for zigzag and armchair geometries and for both ferromagnetic and antiferromagnetic cases. In the rest of the paper D_{am} and D_{bm} are D_l for sublattices A and B respectively. m is the index of lattice cites along the width of the ribbon. Choosing a specific Hilbert space sector is tantamount to setting corresponding D_l's to 1 or -1.

4.1 Zigzag Nanoribbon(ZNR)

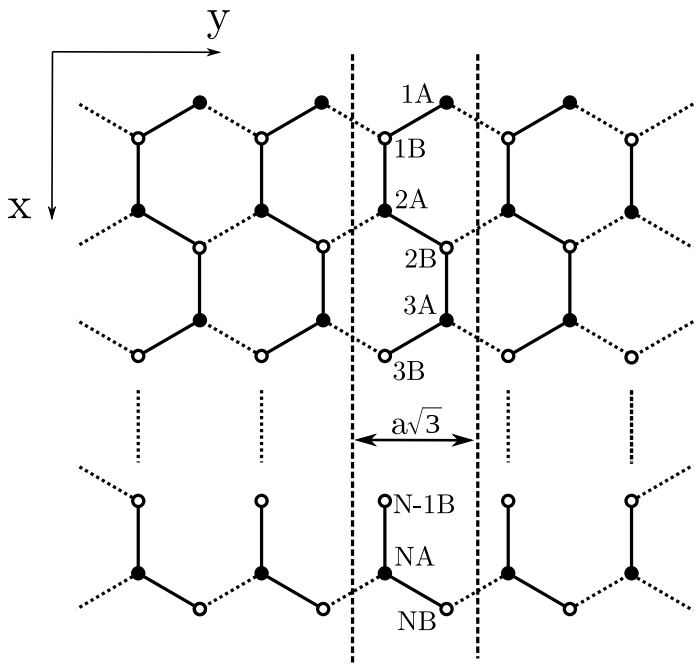


Figure 3: Lattice of an zigzag carbon nanoribbon, with unit cell(dashed) of size $a\sqrt{3}$, width N and length L_y.

4.1.1 Antiferromagnetic(AF) order

In [4] the ground state of this system is shown to belong to the sector of the Hilbert space where $D_{am} = -D_{bm} = -1$. This shall be referred to as *AF order*, since in this sector both sub-lattices are populated by d_2-fermions and on different sub-lattices d_2 has opposite y-polarizations. This can be

verified by examining the transformations between ordinary and composite fermions bases. Now the matrix can be written as

$$\mathrm{H}_k = \begin{pmatrix} -\frac{U}{2} & 0 & 0 & 2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}) \\ 0 & \frac{U}{2} & 2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}) & 0 \\ 0 & -2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}^\dagger) & -\frac{U}{2} & 0 \\ -2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}^\dagger) & 0 & 0 & \frac{U}{2} \end{pmatrix} \tag{8}$$

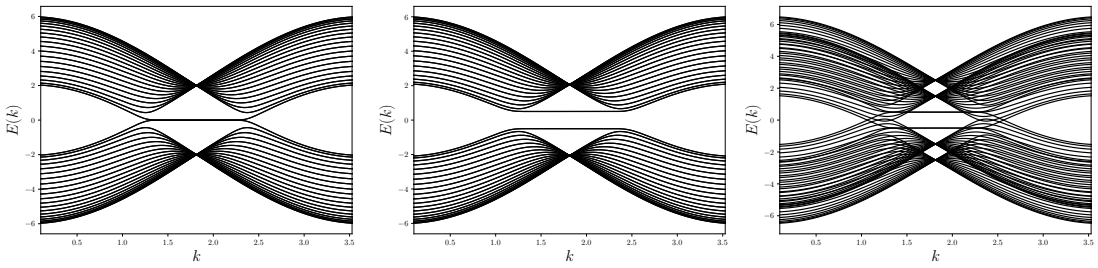
$\mathbb{K} = \sum_m |m\rangle\langle m+1|$ is a unilateral shift operator with ones on the upper diagonal and $g_k = 2\cos(\sqrt{3}ka/2)$. Energy levels are given in Figure 4b. We observe gap opening however the degeneracy is not lifted and every level is still doubly degenerate.

4.1.2 Ferromagnetic(F) order

Ferromagnetic in this context means we are considering the sector of Hilbert space where only one sub-lattice is populated by d_2-fermions. It corresponds to the state in which all d_2 fermions are aligned. It's the same as setting $D_l = 1$ or $D_l = -1$. Now the matrix looks like

$$\mathrm{H}_k = \begin{pmatrix} \mp\frac{U}{2} & 0 & 0 & 2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}) \\ 0 & \pm\frac{U}{2} & 2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}) & 0 \\ 0 & -2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}^\dagger) & \pm\frac{U}{2} & 0 \\ -2i\tilde{t}(g_k\mathbb{1}+\mathbb{K}^\dagger) & 0 & 0 & \mp\frac{U}{2} \end{pmatrix} \tag{9}$$

Since the spectrum is symmetric around zero, ± doesn't change anything, and after solving for the eigenvalues and plotting them w.r.t. momentum (Figure 4c) one can see energy levels splitting.



(a) U=0 **(b)** Antiferromagnetic order **(c)** Ferromagnetic order

Figure 4: Zigzag energy levels for F and AF orders. $E(k)$ and k are measured in units of $\tilde{t}$. Calculation is done for $N = 20$, $U = 1$

4.2 Armchair Nanoribbon(ANR)

Armchair nanoribbon behavior depends on it's width. It can be metallic or have an energy gap.

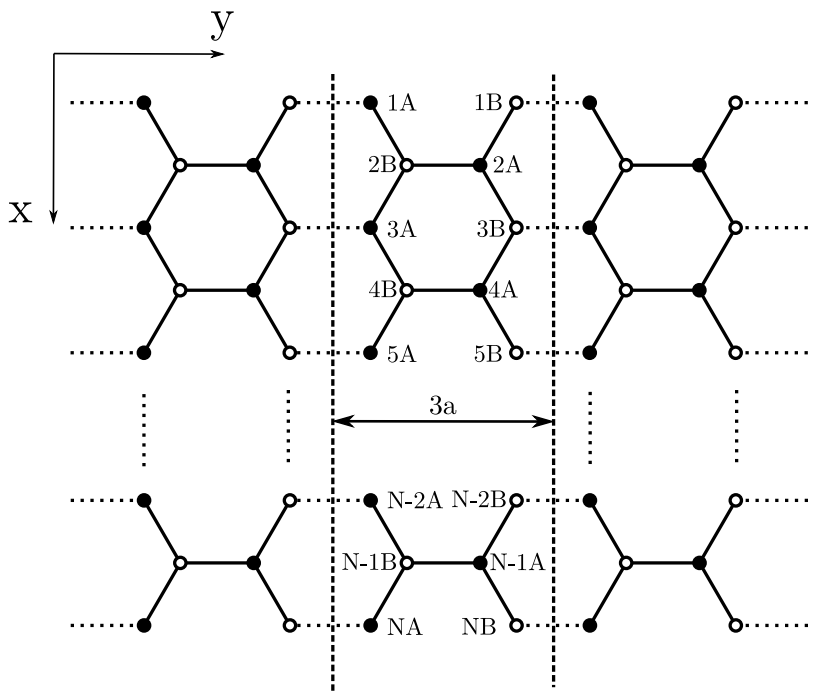


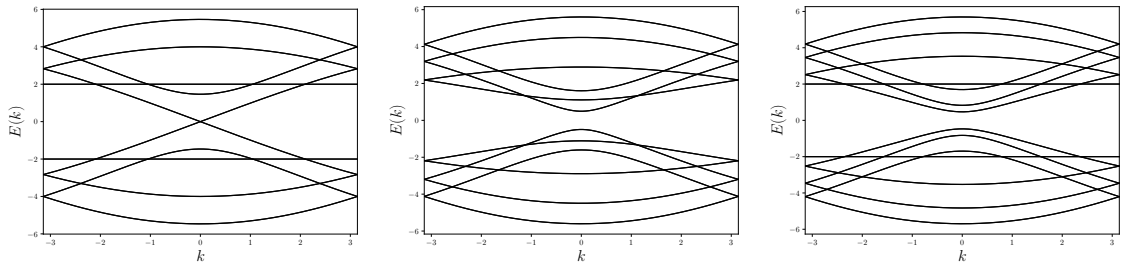
Figure 5: Lattice of an armchair carbon nanoribbon, with unit cell(dashed) of size $3a$, width N and length L_y

4.2.1 Antiferromagnetic(AF) order

As it was for zigzag configuration AF order here means that we are in the Hilbert space sector defined by $D_{am} = -D_{bm} = -1$ and the matrix is rewritten as

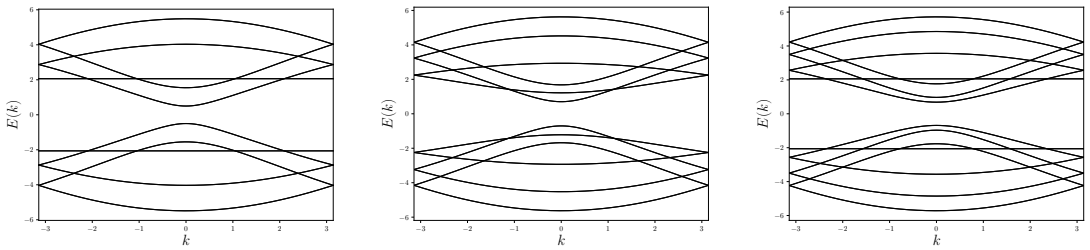
$$\mathrm{H}_k = \begin{pmatrix} -\frac{U}{2} & 0 & 0 & 2i\tilde{t}(\mathbb{1} + e^{-ika_t/2}\mathbb{J}) \\ 0 & \frac{U}{2} & 2i\tilde{t}(\mathbb{1} + e^{ika_t/2}\mathbb{J}) & 0 \\ 0 & -2i\tilde{t}(\mathbb{1} + e^{-ika_t/2}\mathbb{J}) & -\frac{U}{2} & 0 \\ -2i\tilde{t}(\mathbb{1} + e^{ika_t/2}\mathbb{J}) & 0 & 0 & \frac{U}{2} \end{pmatrix} \tag{10}$$

$\mathbb{J} = \sum_m |m\rangle\langle m+1| + |m+1\rangle\langle m|$ is a bilateral shift operator with ones on the upper and lower diagonals. Solving for the eigenvalues for every value of k and plotting the results gives the energy band structure 7a, 7b, 7c. As with zigzag geometry here too we observe gap opening without lifting the degeneracy.



(a) N=5 **(b)** N=6 **(c)** N=7

Figure 6: Energy bands for widths 5,6,7 for the case $U = 0$. Everything is measured in units of $\tilde{t}$.



(a) N=5 (AF) **(b)** N=6 (AF) **(c)** N=7 (AF)

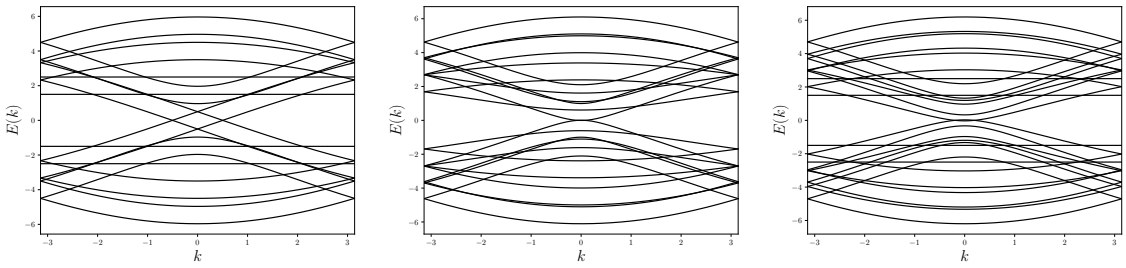
Figure 7: Energy bands for widths 5,6,7 in antiferromagnetic order. Everything is measured in units of $\tilde{t}$. For all calculations $U = 1$

4.2.2 Ferromagnetic(F) order

Ferromagnetic as it was for zigzag nanoribbon means we are considering the sector of Hilbert space where only one sub-lattice is populated by d_2-fermions, resulting in $D_{am} = D_{bm} = \pm 1$. Now the matrix looks like

$$\mathrm{H}_k = \pm \begin{pmatrix} \mp\frac{U}{2} & 0 & 0 & 2i\tilde{t}(\mathbb{1} + e^{-ika_t/2}\mathbb{J}) \\ 0 & \pm\frac{U}{2} & 2i\tilde{t}(\mathbb{1} + e^{ika_t/2}\mathbb{J}) & 0 \\ 0 & -2i\tilde{t}(\mathbb{1} + e^{-ika_t/2}\mathbb{J}) & \pm\frac{U}{2} & 0 \\ -2i\tilde{t}(\mathbb{1} + e^{ika_t/2}\mathbb{J}) & 0 & 0 & \mp\frac{U}{2} \end{pmatrix} \tag{11}$$

Since the spectrum is symmetric ± doesn't change anything. Solving for the eigenvalues and plotting it w.r.t. we can see the same behavior as in zigzag case, degeneracy is lifted (Figure 8a, Figure 8b, Figure 8c). For some widths there exists a critical value of $U = U_c$ where the band gap closes, but if we keep increasing U eventually gap opens again and the band structure becomes that of a trivial insulator. Since band closing is unavoidable initial state must be topologically nontrivial.



(a) N=5 (F) **(b)** N=6 (F) **(c)** N=7 (F)

Figure 8: Energy bands for widths 5,6,7 in ferromagnetic order. Everything is measured in units of $\tilde{t}$. For all calculations $U = 1$

5. Effective Hamiltonian

As we have seen the Hamiltonian can be written as

$$H_{\text{ZNR}} = -\frac{U}{2} D \otimes \sigma_z - 2\tilde{t}\mathbb{1} \otimes \sigma_y \otimes \sigma_x + i\tilde{t} g_k \mathbb{K} \otimes \sigma^+ \otimes \sigma_x - i\tilde{t} g_k \mathbb{K}^\dagger \otimes \sigma^- \otimes \sigma_x \tag{12}$$

or

$$H_{\text{ANR}} = -\frac{U}{2} D \otimes \sigma_z - 2\tilde{t}\,(\mathbb{1} + \mathbb{J}\cos(ka_T/2)) \otimes \sigma_y \otimes \sigma_x - 2\tilde{t}\sin(ka_T/2)\mathbb{J} \otimes \sigma_y \otimes \sigma_y \tag{13}$$

Matrix D depending on Hilbert space sector can take the form $D = \mathbb{1} \otimes \mathbb{1}$ or $D = \mathbb{1} \otimes \sigma_z$. σ_i are Pauli matrices, and $\sigma_\pm = \sigma_x \pm i\sigma_y$. Now we diagonalize the first term in the matrix product. Let $A \in \{\mathbb{J}, \mathbb{K}\}$ Then there exists a unitary transform such that

$$UAU^\dagger = \text{diag}(\lambda_1, \lambda_2, \cdots) \tag{14}$$

where λ's are the eigenvalues and consequently

$$U(\mathbb{1} + A)U^\dagger = \text{diag}(\lambda_1 + 1, \lambda_2 + 1, \cdots) \tag{15}$$

For every λ Equation 12 and Equation 13 become 4d Dirac equations, since direct product of Pauli matrices along with $2x2$ unit matrix spans Clifford algebra. In fact we are free to choose the basis $\{\Gamma_a\}_{a=1\cdots5}$ as long as it satisfies anti-commutation relations

$$\{\Gamma_a, \Gamma_b\} = 2\delta_{ab} \qquad [\Gamma_a, \Gamma_b] = 2i\Gamma_{ab} \tag{16}$$

One possible choice is [5]

$$\{\sigma_x \otimes \mathbb{1},\ \sigma_z \otimes \mathbb{1},\ \sigma_y \otimes \sigma_x,\ \sigma_y \otimes \sigma_y,\ \sigma_y \otimes \sigma_z\} \tag{17}$$

References

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