Merging Weyl-points in the configuration space of symmetry constrained systems

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I. INTRODUCTION

In these notes we investigate how Weyl points of classical systems merge in the configuration space as we tune the control parameters of the sysmmetry constrained system. We assume that the dynamical matrix depends continuously on two periodic parameters α_1 and α_2, moreover we focus on systems whose vibrational spectrum contains two eigenmodes which can be degenerate for specific parameter values. The parameters of the dynamical matrix periodic meaning that the configuration space is a 2D manifold which is topologically equivalent to a 2 torus. The consequence of the topological properties of the configuration space is that the total charge of the Weyl points in the configuration must vanish. Our aim is to show that the only way to go from a configuration of 4 Weyl-points to a configuration of 2 Weyl-points,is that three Weyl-points must merge into a new Weyl-point creating a 2 point configuration. This means that the transition from four Weyl points to two Weyl points is immediate, there are no configuration with three degeneracy points. In what follows we propose a method to generate parameter dependent dynamical matrices whose spectrum contains 4 and 2 Weyl-points.

II. GENERATION OF WEYL-POINT CONFIGURATIONS

In this section we introduce a simple method which can be used to generate parameter dependent dynamical matrices whose spectrum contains Weyl-points in the configuration space. Our aim is to generate systems with 4 and 2 Weyl points.

We assume that our system has two parameters α_1 and α_2 which define a periodic configuration space similar to the Brillouin zone of a 2D periodic lattice. This means that the dynamical matrix is a function of the parameters α_1 and α_2, $D(\alpha_1, \alpha_2)$. Due to the dynamical matrix being real we can decompose it as

$$D(\alpha_1, \alpha_2) = x(\alpha_1, \alpha_2)\sigma_x + z(\alpha_1, \alpha_2)\sigma_z, \tag{1}$$

where x and z are functions of α_1 and α_2 and $\sigma_{x,y}$ are the Pauli x and z matrices. We also impose (somewhat artifically) the following symmetry for the dynamical matrix. The dynamical matrix at (α_1, α_2) is not independent from the dynamical matrix at (α_2, α_1). That is, we require

$$x(\alpha_1, \alpha_2) = -x(\alpha_2, \alpha_1), \tag{2a}$$

$$z(\alpha_1, \alpha_2) = z(\alpha_2, \alpha_1). \tag{2b}$$

This means that the x component must change sign upon the reflection of the angles $\alpha_1 \leftrightarrow \alpha_2$ while the z component does not change sign. At this point it seems to be useful to introduce new coordinates which are either symmetric or antisymmetric under the reflection of the angles. We define $\beta_{1,2}$ as the coordinates in the configration space that replace the old angles with β_1 being symmetric upon the reflection and β_2 being antisymmetric. With these new angles the previous constraint on the dynamical matrix can be written as

$$x(\beta_1, \beta_2) = -x(\beta_1, -\beta_2), \tag{3a}$$

$$z(\beta_1, \beta_2) = z(\beta_1, -\beta_2). \tag{3b}$$

Based on electronic band structures of solids we propose the following functional form for the x and z functions

$$x(\beta_1, \beta_2) = \sum_{i=1,2} \sum_{k=1}^{n} \left(a_{i,k} \sin(k \cdot \beta_i) + b_{i,k} \cos(k \cdot \beta_i) \right), \tag{4a}$$

$$z(\beta_1, \beta_2) = \sum_{i=1,2} \sum_{k=1}^{n} \left(c_{i,k} \sin(k \cdot \beta_i) + d_{i,k} \cos(k \cdot \beta_i) \right). \tag{4b}$$

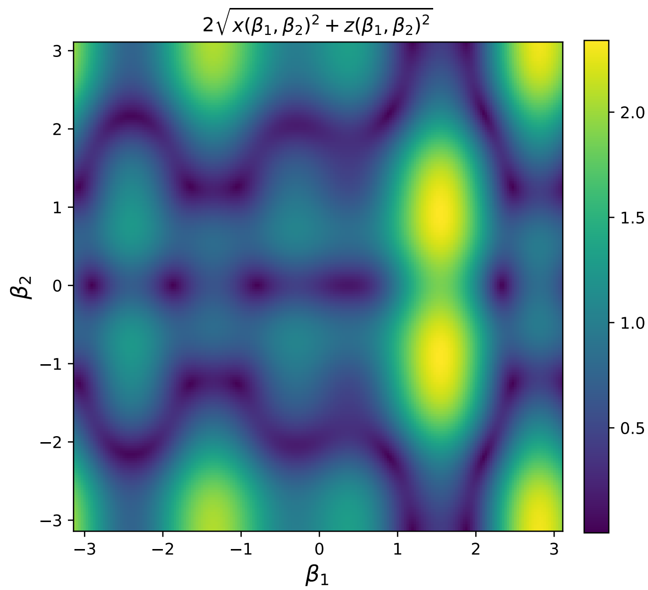

Figure 1. Spectrum of random system with $n = 3$ harmonics. The spectrum contains 18 Weyl-points.

This form is motivated by the fact that the electronic band structures in solids usually involve periodic functions of the lattice vectors k_x and k_y. In the above expressions we include the first n harmonics of the periodic parameters $\beta_{1,2}$. Using the imposed symmetries we can conclude that in the functional form of x only the $a_{2,k}$ can be nonzero. This is due to the fact that β_1 and the function $\cos(\beta_2)$ does not change sign upon reflection. This forces all the other coefficients to be zero. The opposite is true for the functional form of z. Here all the $c_{2,k}$ are forced to be zero due to the fact that they change sign upon reflection.

Now we pick $n = 3$ and randomly generate coefficients to obtain different dynamical matrices of parameters β_1 and β_2. The coefficients are chosen with a uniform distribution in the $[-1/2, +1/2]$ interval. Then we find the location of the Weyl-points using an iterative method which is described in Ref..[1] This iterative search is started from 100 random points in the configuration space and these converge to the degeneracy points in the spectrum. We identify degeneracy points which are close to each other as being the same. Then we calculate the charge of each Weyl-point for the given system. To do this we simply take a small discretized loop around the degeneracy point and measure the winding of the vector field defined by the dynamical matrix. We get rid of numerical errors by rounding the winding numbers to integers. Then we check the total charge of the system and the number of Weyl-points found. We throw away those systems in which the total charge is nonzero. Then, if the system has 4 or 2 Weyl-points we save the σ_x and σ_z components of its dynamical matrix so that those can be used later on. An example for such a random system with Weyl-points can be seen on Fig. 1.

With this method implemented the generation of 2000 random matrices takes about 10 minutes. For this method, with $n = 3$, one dataset of such 2000 random matrices contained 71 systems with 4 Weyl-points and 32 systems with 2 Weyl-points. In what follows we linearly interpolate between these systems and investigate how the number of Weyl-points change during this interpolation.

III. THREE POINT PROCESS

In this section we investigate what happens with the Weyl-points in the configuration space when we linearly interpolate between two systems with 4 and 2 Weyl-points in the spectrum.

That is, from the previously generated datasets we take randomly a system with 4 Weyl-points and a system with 2 Weyl-points and define the following system

$$t \in [0, 1] : t \to D(t) = (1 - t) \cdot D_1 + t \cdot D_2. \tag{5}$$

In the above equation D_1 and D_2 represents the systems with 4 and 2 Weyl-points. It is clear that for $t = 0$ the configuration space contains 4 Weyl-points and for $t = 1$ the configuration space contains 2 Weyl-points. What happens for other t values is not clear. An example for the interpolation can be seen on Fig. 2. We can see that

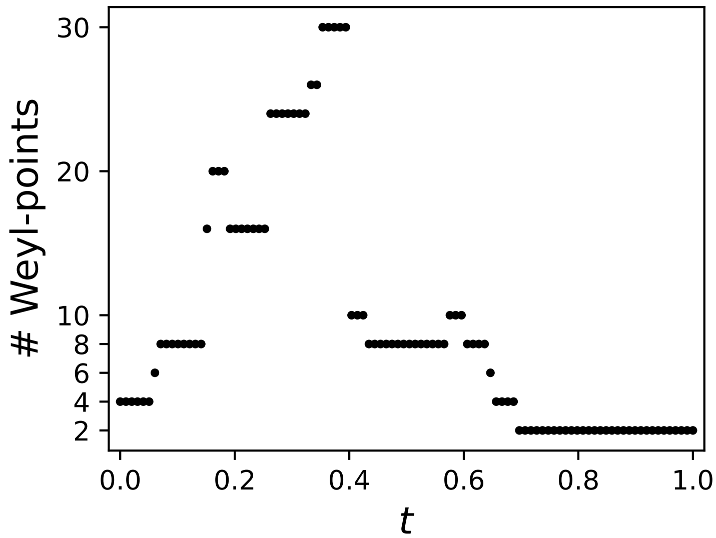

Figure 2. t dependence of the total number of Weyl-points in the system. We can see that instead of the expected $4 \to 2$ transition the number of Weyl-points increases up to 30 before decreasing to 2. By investigating how the number of Weyl-points changes we can see that the number of points changes by two during the whole interpolation.

instead of the expected $4 \to 2$ transition, the number of Weyl-points changes in a rather wild way. As already mentioned, we want to demonstrate that the process $4 \to 3^* \to 2$[2] is impossible. By observing the way

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[1] G. Frank, D. Varjas, G. Pintér, and A. Pályi, "Weyl-point teleportation," (2021).

[2] Here 3^* represents the scenario when there are 3 degeneracy points in the configuration space out of which there are 2 Weyl-points and 1 doubly-charged degeneracy point (which is not a Weyl-point).