Application of Singularity Theory to Material Sciences

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Abstract

We classify Hamiltonians in a neighborhood of a crossing between their eigenvalues from a viewpoint of differential topology [1, 2] and construct a normal form for each class. We provide several examples that appear in quantum chemistry and solid-state physics.

1 Settings

Here, we provide the most generic settings but we can also take symmetries of systems into account. Let $M_m(\mathbb{C})$ be a set of m-by-m complex matrices ($m \in \mathbb{N}$),

$$\mathrm{Herm}_0(m) = \left\{ X \in M_m(\mathbb{C}) \middle| X^\dagger = X,\ \mathrm{Trace}X = 0 \right\} \tag{1}$$

be a set of m-by-m traceless Hermite matrices,

$$SU(m) = \left\{ X \in M_m(\mathbb{C}) \middle| X^\dagger X = XX^\dagger = I_m,\ \det X = 1 \right\} \tag{2}$$

be a set of m-by-m special unitary matrices, where $X^\dagger$ is the Hermite conjugate of the matrix X, I_m is the m-by-m unit matrix, $\mathrm{Trace}X$ and $\det X$ are the trace and the determinant of the matrix X, respectively. Let $H, H' : (\mathbb{R}^n, 0) \to (\mathrm{Herm}_0(m), O_m)$ be C^∞ map germs where $n \in \mathbb{N}$ and O_m is the m-by-m zero matrix. We say that H and H' are $\mathcal{SU}(m)$-equivalent if there exist a map germ $U : (\mathbb{R}^n, 0) \to (SU(m), U(0))$ and a diffeomorphism germ $s : (\mathbb{R}^n, 0) \to (\mathbb{R}^n, 0)$ such that $H(s(x)) = U(x) H'(x) U^\dagger(x)$ for $x \in \mathbb{R}^n$. In what follows, we consider map germs of class C^∞ unless otherwise stated.

2 Results

Here, we classify map germ $H : (\mathbb{R}^n, 0) \to (\mathrm{Herm}_0(m), O_m)$ with respect to $\mathcal{SU}(m)$-equivalence for $n = 3$ and $m = 2$. For example, this case appears in a classification of Hamiltonians in a neighborhood of a crossing between two bands in a bulk of material. In this example, two-by-two Hamiltonians are defined on a three-dimensional Bloch wavenumber spaces such as $H(\mathbf{k}) = \beta(\mathbf{k})\,\sigma_1 + \gamma(\mathbf{k})\,\sigma_2 + \gamma(\mathbf{k})\,\sigma_3$ where $\beta, \gamma, \delta : (\mathbb{R}^3, 0) \to (\mathbb{R}, 0)$ are map germs, $\mathbf{k} = (k_1, k_2, k_3) \in \mathbb{R}^3$ is a Bloch wavenumber, and

$$\sigma_1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3}$$

are three Pauli matrices. We write such a Hamiltonian as $H(\mathbf{k}) = (\beta(\mathbf{k}), \gamma(\mathbf{k}), \gamma(\mathbf{k})) \cdot \sigma$ in what follows, where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$.

In this classification, we classify Hamiltonians starting from generic cases to less generic cases. In order to quantify how generic each Hamiltonian is, we define the codimension of each Hamiltonian as the minimum number of parameters that are necessary to construct a universal unfolding of the Hamiltonian (For a precise definition of codimension, see [1].). We start the classification from the Hamiltonian of codimension 0 up to that of codimension 7. In principle, it is possible to continue the classification up to an arbitrary codimension but it becomes more and more difficult to do that as the codimension increases. Therefore, we restrict ourselves to the cases of codimensions less than 8. As a result of the classification, we obtain the following list of Hamiltonians that represent the classes. If the codimension of a Hamiltonian is less than 8, the Hamiltonian is $\mathcal{SU}(2)$-equivalent to one of the Hamiltonians listed in Table 1. The class of Hamiltonians of codimension 0 in Table 1 corresponds to that of Hamiltonians having a Weyl point at the origin, which is persistent against an arbitrary smooth and small perturbation [3] and is recently observed experimentally [4, 5]. The other classes have codimensions larger than 0 and can appear on verges of quantum phase transitions. To control material properties, not only the class of codimension 0 but also ones of higher codimensions are essential and Table 1 provides a complete list of the classes up to the codimension 7.

$\hat{H}(\mathbf{k})$	ranges	codimension
$(k_1, k_2, k_3) \cdot \sigma$		0
$\left(k_1, k_2, k_3^\ell\right) \cdot \sigma$	$\ell = 2, 3, \cdots, 8$	$\ell - 1$
$\left(k_1, k_2^2, k_3^2 + r k_2^2\right) \cdot \sigma$	$r \in [0, \infty)$	5
$\left(k_1, k_2 k_3, \frac{r}{2}\left(k_2^2 - k_3^2\right)\right) \cdot \sigma$	$r \in (0, 1)$	5
$\left(k_1, k_2^2 + k_3^2, r\left(k_2^3 + k_3^3\right)\right) \cdot \sigma$	$r \in (0, \infty)$	7
$\left(k_1, k_2 k_3, r\left(k_2^3 + k_3^3\right)\right) \cdot \sigma$	$r \in (0, \infty)$	7
$\hat{H}_r(\mathbf{k})$	$r \in (0, \infty)$	7

Table 1: List of Hamiltonian in each class of codimension less than 8 where $\hat{H}_r(\mathbf{k}) = \left(k_1, k_2 k_3 + \frac{r}{2} k_2\left(k_2^2 - k_3^2\right), \frac{1}{2}\left(k_2^2 - k_3^2\right)(1 + r k_3)\right) \cdot \sigma$.

References

[1] H. Teramoto, K. Kondo, S. Izumiya, M. Toda, and T. Komatsuzaki. Classification of Hamiltonians in neighborhoods of band crossings in terms of the theory of

singularities. *J. Math. Phys.*, 58:073502, 2017.

[2] S. Izumiya, M. Takahashi, and H. Teramoto. Geometric equivalence among smooth section-germs of vector bundles with respect to structure groups. *in preparation*.

[3] O. Vafek and A. Vishwanath. Dirac Fermions in Solids: From High-T_c Cuprates and Graphene to Topological Insulators and Weyl Semimetals. *Ann. Rev. Condens. Matter Phys.*, 5:83, 2014.

[4] B. Q. Lv, H. M. Weng, B. B. Fu, X. P. Wang, H. Miao, J. Ma, P. Richard, X. C. Huang, L. X. Zhao, G. F. Chen, Z. Fang, X. Dai, T. Qian, and H. Ding. Experimental Discovery of Weyl Semimetal TaAs. *Phys. Rev. X.*, 5:031013, 2015.

[5] S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee, S.-M. Huang, H. Zheng, J. Ma, D. S. Sanchez, B. Wang, A. Bansil, F. Chou, P. P. Shibayev, H. Lin, S. Jia, and M. Z. Hasan. Discovery of a Weyl fermion seminetal and topological Fermi arcs. *Science*, 349:613, 2015.