High order VHS in quasicrystalline Moiré superlattice

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1 Background: Superpotential on the surface of a TI

Moire superlattices have been a large focus in recent condensed matter research. These lattices display many interesting properties including having flat bands, superconductivity, topological effects and interesting surface states, and more [1], [2]. Specifically, we focus on the surface states of a 3D topological insulator (TI), and explore high-order divergences in the density of states at certain energies.

This involves the Dirac cone on the surface of the TI,

$$H_0(\vec{k}) = v\vec{k} \cdot \vec{\sigma} \tag{1}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ is the fermion spin-basis. This has eigenvalues $E(\vec{k}) = \pm v|\vec{k}|$. We arbitrarily choose a dot product instead of e.g. a cross product.

We also select as our N-fold symmetric potential

$$U(\vec{r}) \equiv 2W \sum_{n=0}^{N-1} \cos(\vec{Q}_n \cdot \vec{r}) \tag{2}$$

$$\vec{Q}_n \equiv Q(\cos(2\pi n/N), \sin(2\pi n/N)) \tag{3}$$

The potential will be periodic for $N = 1, 2, 3, 4, 6$, and will be quasicrystal-like for all other values of N. There are N fundamental reciprocal lattice vectors, $\vec{Q}_0, \vec{Q}_1, ..., \vec{Q}_{N-1}$. $U(\vec{r})$ contributes symmetrically to both spins and so in spin-basis is $H \sim U(\vec{r})\sigma_0$

Given this system, our goal is to determine the conditions required for a high-order Van Hove Singularity (HOVHS), where the density of states (DOS) diverges to high order. The 2D DOS for some dispersion $E \sim k^\nu$ is $g(E) \sim E^{2/\nu-1}$. We see that divergences in the DOS occur when the energy expansion has a leading term of $\nu > 2$.

More concretely, the energy dispersion of about some point $\vec{K}$ is $E_{\vec{K}+\vec{k}} - E_{\vec{K}} = \Omega \cdot O(k) + \alpha \cdot O(k^2) + \beta \cdot O(k^3) + \gamma \cdot O(k^4) + ...$; One possible condition for divergent DOS is then $\Omega = \alpha = 0$. Note this only applies in the absence of time reversal (TR) symmetry, since TR symmetric points are at least doubly degenerate (no direct gap) and will not have divergent DOS.

Divergent DOS are realized experimentally by tuning physical parameters. For instance, each coefficient is a function of the physical parameters, i.e. $\alpha = \alpha(W, v, Q)$. By tuning W, v, or Q, we can allow α to vanish.

To formalize this, a HOVHS is present at $\vec{K}$ if $\vec{\nabla}E|_{\vec{K}} = \vec{0}$ (it is a regular VHS) and also if $det(D = 0)$, where $D_{ij} = \partial_i\partial_j E|_{\vec{K}}$.

$$\vec{\nabla}E|_{\vec{K}} = \vec{0} \tag{4}$$

$$det(D = 0) \tag{5}$$

In the remainder of the paper, we study the location and order of HOVHS for potentials of various N (both lattice-like and quasilattice-like values of N!). Using the above definition of a HOVHS, we will see that it is helpful to search for HOVHS on lines of high symmetry. In the later part of this paper, we will demonstrate that as symmetry N of the superpotential increases, we expect the HOVHS order to also increase (see Section 4.3). For instance, one might expect a superpotential with infinite rotational symmetry to have an arbitrarily large leading order dispersion in k.

2 Analytical analysis of HOVHS

2.1 Location of HOVHS

It is helpful to expand our energy dispersion about a symmetric line or point. This constrains the dispersion to depend on fewer parameters, and will allow us to satisfy (4) and (5) more easily.

This is best demonstrated by example. One begins with the arbitrary dispersion

$$E_{\vec{K}+\vec{k}} - E_{\vec{K}} = a_x k_x + a_y k_y + b_{xx} k_x^2 + b_{yy} k_y^2 + b_{xy} k_x k_y + c_{xxx} k_x^3 + c_{yyy} k_y^3 + c_{xxy} k_x^2 k_y + c_{xyy} k_x k_y^2 + ... \quad (6)$$

Consider the case of $N = 3$, and expand about the K point (Figure 1b), where 3-fold rotational symmetry is present. Reflection symmetry is also present, and we can choose the k_x to be mirror-symmetric, and k_y perpendicular. The constraints are

$$E(k_x, k_y) = E(k_x, -k_y) \quad (7)$$

$$E(\vec{k}) = E(\hat{R}_{(2\pi n/N)} \cdot \vec{k}) \quad (8)$$

Yielding

$$E_{\vec{K}+\vec{k}} - E_{\vec{K}} = ak^2 + b(k_x^3 - 3k_x k_y^2) + \gamma k^4 ... \quad (9)$$

Of course, here $k^2 = k_x^2 + k_y^2$.

Using (4) and (5), it is easy to see a HOVHS exists at $\vec{K}$ if $a = 0$ (Appendix A). We can tune 1 coefficient to get a HOVHS. As a result, this likely requires tuning only one parameter (the potential strength W is the easiest parameter to tune).

More generally, consider the dispersion at some point $\vec{P}$ on a mirror-symmetric line. Our system will always have a mirror-symmetric contour available to do this expansion. Now, (7) is the constraint so the dispersion only has even powers of k_y. The analysis using (4) and (5) is not as straightforward as before. One simple solution is that all first and at least one second order term vanishes (tune two parameters). Using this analysis, it is difficult to determine whether tuning just one parameter will lead to a HOVHS. (See Appendix A for details)

2.2 Analytic dispersion

We must compute the hamiltonian to determine the HOVHS:

The superlattice potential from (2) is

$$\hat{H}_{pot} = \int_{allspace} d^2\vec{r}\, U(\vec{r})(\sigma_0)_{\sigma,\sigma'} \; |\vec{r},\sigma\rangle \langle \vec{r},\sigma'| = \int_{allspace} d^2\vec{r}\, U(\vec{r}) \, |\vec{r},\sigma\rangle \langle \vec{r},\sigma| \quad (10)$$

$$= \int_{allspace} \frac{d^2\vec{k}}{(2\pi)^2} \frac{d^2\vec{k}'}{(2\pi)^2} \, |\vec{k}',\sigma\rangle \langle \vec{k},\sigma| \sum_{\vec{Q}=\vec{Q}_0}^{\vec{Q}_N} W \left[\frac{1}{V} \int_{allspace} d^2\vec{r}\, e^{-i\vec{Q}\cdot\vec{r}} e^{i(\vec{k}'-\vec{k})\cdot\vec{r}} \right] + \quad H.c. \quad (11)$$

$$= \int_{allspace} \frac{d^2\vec{k}}{(2\pi)^2} \left[W \sum_{\vec{Q}} |\vec{k}+\vec{Q},\sigma\rangle \langle \vec{k},\sigma| \right] \quad + H.c. \quad (12)$$

$$= \int_{(pseudo)unitcell} \frac{d^2\vec{k}}{(2\pi)^2} \left[W \sum_{\vec{Q},\,\vec{G}} |\vec{k}+\vec{Q}+\vec{G},\sigma\rangle \langle \vec{k}+\vec{G},\sigma| \right] + \quad H.c. \quad (13)$$

Where $\vec{G}$ is the reciprocal lattice $\sum_i n_i \vec{Q}_i$ and n_i are all integers, and a sum over repeated σ implied. We identify the integrand in the final line to be the density $H_{pot}(\vec{k})$, whose eigenenergies are the dispersion at $\vec{k}$.

Similarly, the term from the massless Dirac fermion (1) is

$$\hat{H}_{TI} = \int_{allspace} \frac{d^2\vec{k}}{(2\pi)^2} (H_0(\vec{k}))_{\sigma,\sigma'} \left|\vec{k}\ \sigma\right\rangle \left\langle\vec{k}\ \sigma'\right| \tag{14}$$

$$= \int_{(pseudo)unitcell} \frac{d^2\vec{k}}{(2\pi)^2} \left[\sum_{\vec{G}} (H_0(\vec{k}+\vec{G}))_{\sigma,\sigma'} \left|\vec{k}+\vec{G},\sigma\right\rangle \left\langle\vec{k}+\vec{G},\sigma'\right| \right] \tag{15}$$

Similar to before, the integrand is the density $H_{TI}(\vec{k})$. We then have

$$H(\vec{k}) = H_{TI}(\vec{k}) + H_{pot}(\vec{k}) \tag{16}$$

which has eigenenergies $\{E_{\vec{k}}\}$.

We now know the energy dispersion. Next, we look for HOVHS for $N = 3, 4, 5$, using python to compute these eigenenergies at various $\vec{k}$.

3 Computation approach

In this section, I search for HOVHS computationally, by computing the eigenvalues of (16) with python. I analyze systems of various N-symmetry. For a system of a given N, I tune only the superpotential strength W to create a HOVHS (natural units are used, so that $\hbar = v = L = 1$, where L is the real lattice spacing).

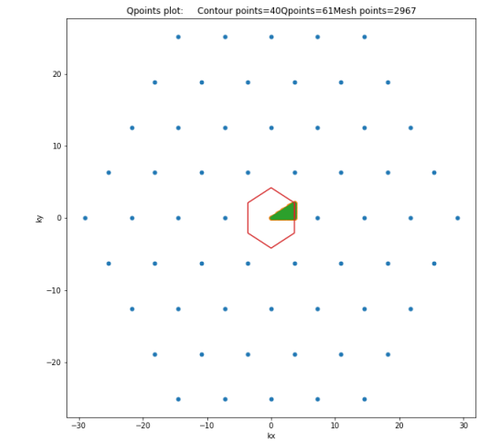
To compute (16) exactly, one must use an infinite sum over the set of reciprocal lattice vectors $\vec{G} = \{\sum_{i=1}^{N} n_i \vec{Q}_i, n_i \in Z\}$. This is not possible computationally and we must impose a cutoff on the n_i. To do this, I consider only tuples of $(n_1, n_2, ..., n_N)$ such that $\sum_{i=1}^{N} |n_i| \leq R$. Thus, we only consider reciprocal lattice vectors up to R 'steps' (or 'rings') of size $|\vec{Q}_i| = Q$ away from the origin. As $R \to \infty$, the computation becomes exact. Our definition for a stable ring size R is then $E_{R+1} - E_R \ll 1$.

See Figures 1, 2, and 3 for our results. Our $N = 3, 4$ cases match well with results found in [2] and we hope to find HOVHS in other $N = 5, 7, 8, ...$

3.1 Computation process

For lattice-generating N, one can construct the Brillouin zone (BZ) naturally, which is just a Wigner–Seitz cell (indicated by red lines). We extend this construction to systems with quasilattice-generating values of N. This BZ helps us define relevant contours and meshes to compute over.

Our process is 1) choose an N and W 2) choose appropriate details relevant to the computation, which are the number of rings R (indicated by blue points), the mesh of k points for computing the DOS (indicated by green points), and the contour for computing the band structure (indicated by orange points).



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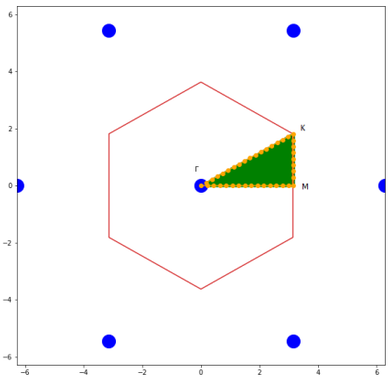

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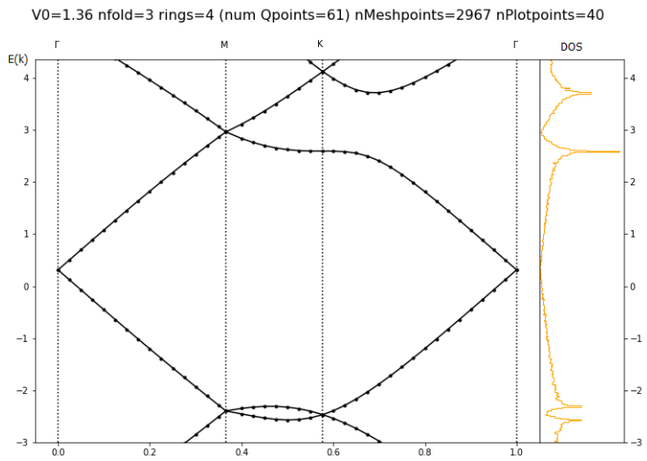

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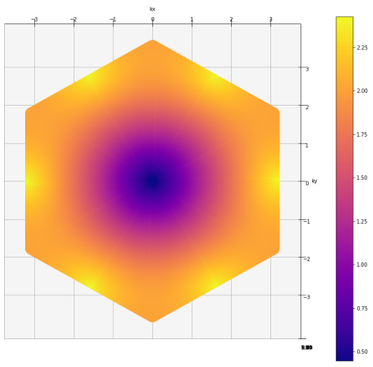


(d)

Figure 1: Here we find a HOVHS with $N = 3$ and $W = 1.36$. a) Setup of $N = 3$, $R = 4$ calculation b) Close-up of (a). HOVHS should be on lines of high symmetry (ΓM or $K\Gamma$), so we look for flat bands on these contours. c) Band calculation for the setup shown in (a), (b). At $W = 1.36$, the band is flat at K, and high-order divergence of the DOS at $E(K)$. d) Fermi surface calculated at $W = 1.36$. Note with units $W = 1.36\hbar v/L$, and $Q \equiv 2\pi/\tilde{L}$, where $\tilde{L}$ is some multiple of the real lattice spacing L. In the $N = 3$ case, $\tilde{L} = \frac{\sqrt{3}}{2}L$.

3.2 $N = 5$ issues

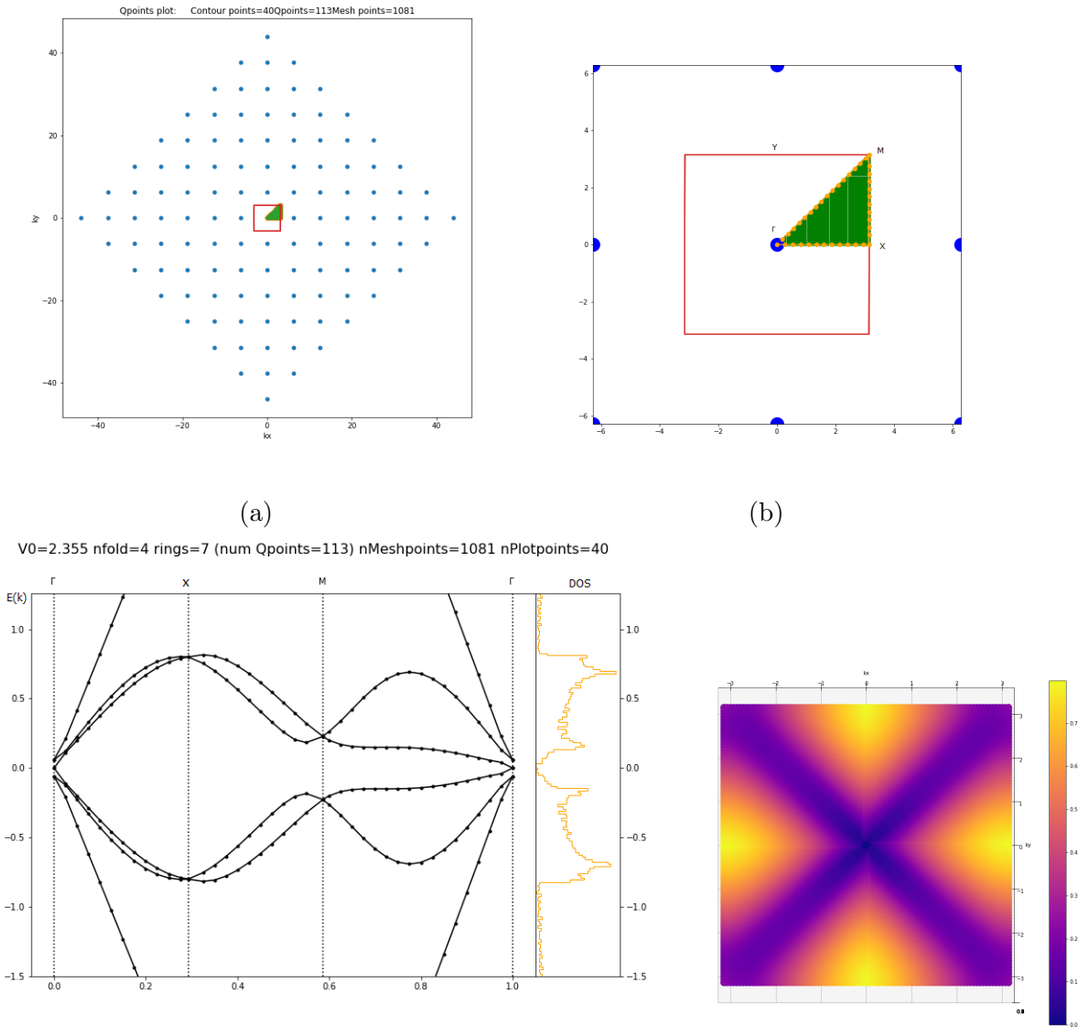
From Figure 3, our perturbation starts to break down before a HOVHS forms. However, there are many possible issues including:

1) Building in rings is too inefficient. For instance, $N = 4$ requires a high number of cutoff $\vec{G}$ points (6 rings), but there are other definitions of the cutoff that require fewer points. The number of points grows exponentially with the number of rings for $N = 5$ and it is not viable to use more than a few rings.

2) It is possible our architecture of building 'rings' poorly represents quasilattices. The quasilattice set $\vec{G}$ densely fills all space, and we are only tiling some finite subset. Deeper analysis such as [3],[4] may be needed.

3) We may need to sample k-points differently when computing DOS. The Wigner-Seitz construction may not be appropriate.

There are a lot of possible computation issues, and so we move to perturbation theory.



(a) (b)

(c) (d)

Figure 2: Here we find a HOVHS with $N = 4$, $W = 4.71/2 = 2.355$ (half the potential found by [2]), since we twice the amount of Q's. This is just a detail). a) Setup of $N = 4$, $R = 7$. I needed at least 6 rings for the calculation to stabilize. b) Close-up of (a). c) Band calculation for $W = 2.355$. There are 4 divergences of the DOS, and on the $M\Gamma$ line is a HOVHS. d) Fermi surface.

4 Perturbative analysis

4.1 Background

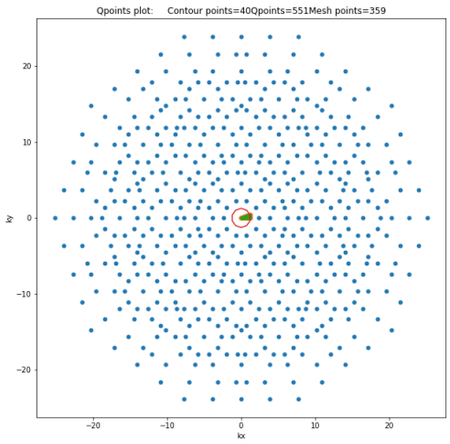
Let us look at our system (16) from the lens of degenerate perturbation theory. We have a Dirac cone which will produce rings of degenerate points. At certain distances from the origin, these degenerate points will be separated by the fundamental reciprocal lattice vectors $\vec{Q}_n$. This is a great use for degenerate PT.

The eigenstates of the Dirac hamiltonian (1) are

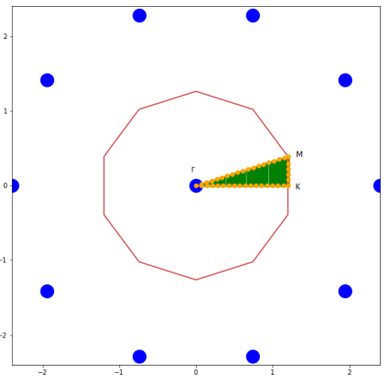
$$|k, \pm\rangle = |\vec{k}\rangle \times \frac{1}{\sqrt{2}}(1, \pm e^{i\phi_{\vec{k}}}) \tag{17}$$

We consider positive energy states for simplicity.

Each N-fold degeneracy is an N-polygon with edges $\vec{k}_n = k_0(\cos(2\pi n/N), \sin(2\pi n/N))$ that



(a)



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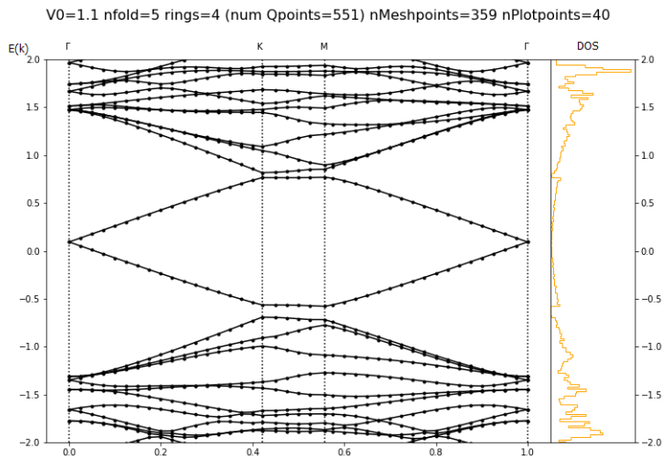

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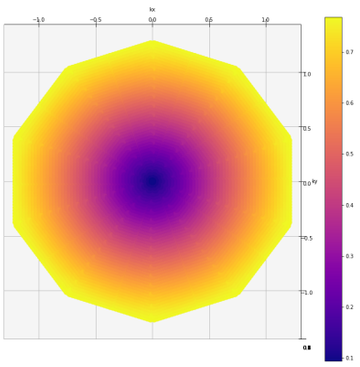

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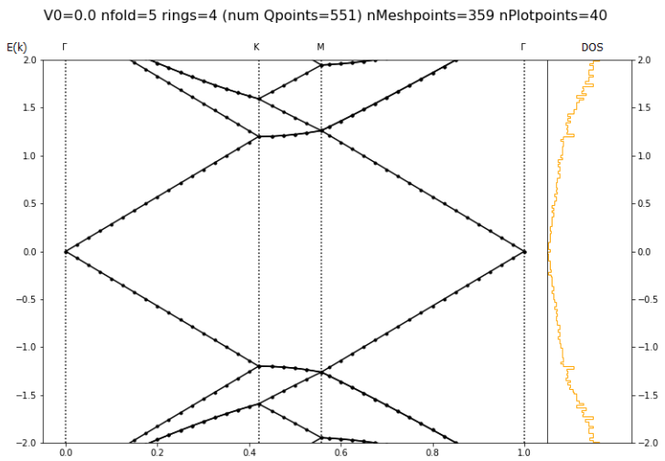

(e)

Figure 3: Here we unsuccessfully look for HOVHS with $N = 5$, $R = 4$. This is our first quasicrystal-like example. a) Setup of $N = 5$, $R = 4$. There are many more unique $\vec{G}$ points than before, since $\vec{Q}_i + \vec{Q}_j \neq \vec{Q}_k$ where $i \neq j \neq k$. b) Close-up of (a). As a result of two Q's not adding to some third Q, the innermost ring is not of distance Q to the origin, but instead of some smaller distance $\min |\sum_i n_i \vec{Q}_i|$. We base our BZ on this innermost ring (dependent on the computational parameter R which has no physical relevance!). In (c-d) I consider $W = 1.1$ c) I slowly increased the potential W to see if the DOS would contain divergences as before. Note that the band structure of a quasilattice is not well-defined, but can be used to gain intuition. The first significant change from Dirac-cone occured at $W = 1.1$. However, we see that there is no flattening of bands. Instead, a gap opens up, which violates TR symmetry and indicates that our perturbation is no longer valid. d) Fermi surface, with fairly trivial behavior. e) Band structure and DOS with zero potential strength ($N = 5$, $W = 0$).

differ by $\vec{Q}_n$. These states are clearly

$$|n\rangle = |\vec{k}_n, +\rangle = |\vec{k}_n\rangle \times |e^{i\phi_n}\rangle \tag{18}$$

$$|e^{i\phi_n}\rangle \equiv \frac{1}{\sqrt{2}}(1, e^{i\phi_n}) \tag{19}$$

$$\phi_n \equiv 2\pi n/N \tag{20}$$

We now perturb in potential strength W. For an N-fold degeneracy, we need to consider contributions from (1) and (2). Let us consider one term at a time, so that $H_{tot} = H^1 + H^2$. We start with the Dirac cone (1).

$$H^1_N = v \sum_{n=0}^{N-1} |\vec{k}_n| \ \langle n|n\rangle \, |n\rangle \langle n| \tag{21}$$

$$= v \sum_{n} |\vec{k}_n| \ |n\rangle \langle n| \tag{22}$$

Let us now consider the contribution from a potential with N-fold rotational symmetry (2).

$$H^2_N = \sum_{n=0}^{N-1} V_{(\vec{k}_{n+1} - \vec{k}_n)} \ \langle n+1|n\rangle \, |n+1\rangle \langle n| + H.c. \tag{23}$$

$$= W \sum_{n} \ e^{-i\frac{(\phi_{n+1}-\phi_n)}{2}} \cos\frac{(\phi_{n+1}-\phi_n)}{2} \, |n+1\rangle \langle n| + H.c. \tag{24}$$

I didn't evaluate further as these forms are useful later on. One can simplify using $|\vec{k}_n| = k_0$ and $\phi_a - \phi_b = \phi_{a-b}$.

Let us now expand in a small region surrounding the $\vec{k}_n$. We expand with $\vec{k} = k(\cos(\phi_{\vec{k}}), \sin(\phi_{\vec{k}}))$, and of course $k \ll |\vec{k}_n| = k_0$.

$$|n'\rangle = |\vec{k}_n + \vec{k}, +\rangle = |\vec{k}_n + \vec{k}\rangle \times |e^{i\phi'_n}\rangle \tag{25}$$

$$\phi_n \to \phi'_n = \arctan\left(\frac{k_0 \sin(\phi_n) + k\sin(\phi_{\vec{k}})}{k_0\cos(\phi_n) + k\cos(\phi_{\vec{k}})}\right) \tag{26}$$

$$|\vec{k}_n| \to |\vec{k}'_n| = \sqrt{(k_0\cos(\phi_n) + k\cos(\phi_{\vec{k}}))^2 + (k_0\sin(\phi_n) + k\sin(\phi_{\vec{k}}))^2} \tag{27}$$

One substitutes (26) into (24) and (27) into (22) to compute this perturbation.

Expanding in small k, we find the exact result (See Appendix B),

$$H^1_N = vk_0 \sum_{n=0}^{N-1} \sum_{m=0}^{\infty} \sum_{l=0}^{m} (C_{m,l}) \cos^l(\phi_k - \phi_n) (\frac{k}{k_0})^{2m-l} \, |n\rangle \langle n| \tag{28}$$

$$C_{m,l} \equiv \binom{m}{l} \text{FactorialPow}[\frac{1}{2}, m]/m! \tag{29}$$

$$H^2_N = W \sum_{n=0}^{N-1} \left(e^{-\frac{\pi i}{N}} \cos(\frac{\pi}{N}) + \frac{e^{-\frac{2\pi i}{N}}}{2} \sum_{x=1}^{\infty} \text{coeffs}_n(x) (\frac{k}{k_0})^x \right) |n+1\rangle \langle n| + H.c. \tag{30}$$

$$\text{coeffs}_n(x) \equiv \sum_{\substack{\text{all } a\vec{r}g, p\vec{o}w \\ \text{s.t. } arg_i,\ pow_i \in Z>0 \\ \sum_i arg_i \, pow_i = x}} \frac{(dim(p\vec{o}w))!}{\prod_{pow_i \in p\vec{o}w}(pow_i)!} D_{(dim(p\vec{o}w))} \prod_i \left[\lambda_{(arg_i)} \, c_n(arg_i)\right]^{pow_i} \tag{31}$$

$$c(m) \equiv c_n(m) = \cos\left(m(\phi_{\vec{k}} - \phi_n - \frac{\pi}{N})\right) \tag{32}$$

$$\lambda_m \equiv \frac{(-1)^{m+1}}{m} \sin(\frac{m\pi}{N}) \tag{33}$$

$$D_l \equiv \frac{(2i)^l}{l!} \tag{34}$$

coeffs(x) is computed using partitions of x (see Appendix B). For example, coeffs(4)$\sim c(1)^4 + c(4) + c(2)^2 + c(1)c(3) + c(1)^2c(2)$ from the five summands, $a\vec{r}g = (1)$ $p\vec{o}w = (4)$; $a\vec{r}g = (4)$ $p\vec{o}w = (1)$; $a\vec{r}g = (2)$ $p\vec{o}w = (2)$; $a\vec{r}g = (1,3)$ $p\vec{o}w = (1,1)$; and $a\vec{r}g = (1,2)$ $p\vec{o}w = (2,1)$. $a\vec{r}g$ is always in increasing order to avoid extra counting.

4.2 Fourier basis

It is extremely fruitful to expand in the Fourier basis

$$|n\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N+1} e^{-2\pi i j n/N} |j\rangle \tag{35}$$

The energy of the jth state (before the perturbation in k) is

$$E_j = vk_0 + 2W\cos(\pi/N)\cos(2\pi(j+\frac{1}{2})/N) \tag{36}$$

The states $|j\rangle$ and $|-1-j\rangle$ are degenerate and protected by TR symmetry. If $W \gg k$, the bands have large spacing, and the only relevant coupling is that of degenerate states. The coupling between degenerate states should tell us which orders $(\frac{k}{k_0})$ to expect in different bands.

Before doing any analysis, we expect that the maximal order k/k_0 increases as N increases. Specifically, the order of k/k_0 might go as the difference of the degenerate state numbers $|j-(-1-j)| = 2j+1$.

4.3 Main Result

With analysis, we can get an exact result in the Fourier basis (see Appendix B for details)

$$H_N^1 = v_0 \sum_{m=0}^{\infty} \sum_{x=m}^{2m} \sum_{\substack{z=2m-x,\\ 2m-x-2,\\ 2m-x-4,\\ \dots}}^{z\geq 0} [consts1]\ (\frac{k}{k_0})^x\ e^{-i\phi_{\vec{k}} z} \sum_{j=0}^{N-1} |j+z\rangle\langle j| + H.c. \tag{37}$$

$$H_N^{2\,(x\geq 1)} = \frac{W}{2} e^{-\frac{2\pi i}{N}} \sum_{j,j'} |j'\rangle\langle j|\, e^{-\frac{2\pi i}{N} j'} \sum_{x=1}^{\infty} (\frac{k}{k_0})^x \left[\frac{1}{N}\sum_{n=0}^{N-1} \text{coeffs}_n(x)\, e^{-\frac{2\pi i}{N} n(j'-j)}\right] + H.c. \tag{38}$$

$$\left[\frac{1}{N}\sum_{n=0}^{N-1} c(M)^L\ e^{-\frac{2\pi i}{N} n(j'-j)}\right] = \sum_{\substack{z=L,\\ L-2,\\ L-4,\\ \dots}}^{z\geq 0} [consts2]\left(e^{-i(\phi_{\vec{k}}-\frac{\pi}{N})Mz}\,\delta_{[Mz=j'-j]} + [z\to -z]\right) \tag{39}$$

The leading term for the coupling between states $|j\rangle$ and $|j+z\rangle$ thus goes as their difference $(\frac{k}{k_0})^z$.

This is true for (37) since $x \leq m$, $z \leq 2m-x$, so $z \leq x$.

We show the same for (38): find the maximal coupling for a fixed x. The trick is to use the cosine rule $c(a)c(b) = (c(a+b)+c(a-b))/2$ to combine product terms in coeffs(x) into terms with a single cosine to a power, $c(M)^L$. From the orthogonality relation (39) the coupling from $c(M)^L$ is at most ML.

Now we can show the maximal coupling for a power x is x. The coefficients are $\sim c(a)^{x_1}c(b)^{x_2}c(c)^{x_3}...$ s.t. $x = ax_1 + bx_2 + cx_3 + ...$ We notice only $c(a)c(b) = c(a+b)/2$ contributes to maximal coupling since the other $c(a-b)/2$ term has a lower M but the same L. The algebra for this is $c(a) \sim e^a$. Using this algebra, the coefficients that give maximal coupling are $c(ax_1+bx_2+cx_3+...) = c(x) = c(M_{max})^{L_{max}}$. Coupling is at most $M_{max}L_{max} = x$ and we are done.

4.4 Analysis

Let us check that as N increases, we expect to see higher order VHS. For the first term (37), $x \leq m$, $z \leq 2m-x$, so $z \leq x$. The leading term for the coupling between states $|j\rangle$ and

$|j+z\rangle$ goes as $(\frac{k}{k_0})^z$, as we guessed before. We see the same result for H_N^2, and thus the whole system.

Another application of perturbation theory is finding the dependencies of the coefficients in the dispersion (6).

Let us consider $N = 3$. We find that the singlet dispersion is

$$\begin{aligned} E(\vec{k}) = &\left(-\frac{3W}{8\mathrm{k}0^2} + \frac{v}{2\mathrm{k}0} - \frac{v^2}{3W}\right)k^2 + \left(\frac{v^3}{9W^2} - \frac{v}{4\mathrm{k}0^2}\right)(k_x^3 - 3k_x k_y^2) \\ &+ \left(-\frac{v}{4\mathrm{k}0^3} + \frac{3v^2}{8\mathrm{k}0^2 W} - \frac{5v^3}{18\mathrm{k}0W^2} + \frac{v^4}{27W^3}\right)(k^4) + ... \end{aligned} \tag{40}$$

This is consistent with (9). Note that this was an early result where the sum in (37) was only evauluated for $m \leq 1, x = z = 1$. However, there is no real solution of W to make the second-order coefficient vanish. If we include all the terms in both sums, I expect to fix this and be able to tune W to make a HOVHS. Terms in H_N^2 rely on partition functions which are computational and not analytical (I think they must be computed).

5 Conclusion and Future

We have seen that one might expect very high order VHS to be present on the surface of TIs when a quasilattice-like superpotential is present. We have studied two approaches to finding such HOVHS: computational and perturbation theory. We hope to confirm these HOVHS are possible, and find their locations.

Next steps are to continue with our perturbative approach. We hope to replicate the known results of $N = 3, 4$ with this method, and then move on to $N = 5, 7, 8, ...$ We may continue with the computation approach when we have more intuition on best next steps.

6 Acknowledgements

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7 Appendix A

For an expansion about the 3-fold symmetric point K (see Figure 1), we have

$$E(K_x + k_x, K_y + k_y) - E(k_x, k_y) = a(k_x^2 + k_y^2) + b(k_x^3 - 3k_x k_y^2) + gk^4 + ... \tag{41}$$

$$\frac{\partial E}{\partial k_x} = 0 = 2akx + b(3kx^2 - 3ky^2) + 4gkx(kx^2 + ky^2) + ... \tag{42}$$

$$\frac{\partial E}{\partial k_y} = 0 = 2aky - 6bkxky + 4gky(kx^2 + ky^2) + ... \tag{43}$$

$$\det(D) = 0 = 4a^2 + (-36b^2 + 32ag)kx^2 - 48bgkx^3 + 48g^2kx^4 + ... \tag{44}$$

One solution is $a = k_x = k_y = 0$. Clearly there a HOVHS at K requires tuning one coefficient a, thus likely one parameter W.

For an expansion about P mirror-symmetric line with k_x parallel and k_y perpendicular to

the line, we have

$$E(P_x+k_x,P_y+k_y)-E(k_x,k_y)=ak_x+bk_x^2+ck_y^2+dk_x^3+ek_xk_y^2+fk_x^4+gk_x^2k_y^2+hk_y^4+... \tag{45}$$

$$\frac{\partial E}{\partial k_x}|_{k_y=0}=0=a+2bk_x+3dk_x^2+4fk_x^3+... \tag{46}$$

$$\frac{\partial E}{\partial k_y}|_{k_y=0}=0=0 \text{ (always holds)} \tag{47}$$

$$\begin{aligned}\det(D)|_{k_y=0}=0=4bc+(12cd+4be)k_x+(12de+24cf+4bg)k_x^2\\ +(24ef+12dg)k_x^3+24fgk_x^4+...\end{aligned} \tag{48}$$

We assume $k_y=0$ because we want a VHS on the mirror-symmetric line. Clearly setting $a=b=0$ or $a=c=0$ and $k=k_x$ is a solution. However, the conditions for a solution for roots of k_x is complicated and may not be real. It is not clear if tuning just 1 coefficient (or harder yet, 1 parameter) will satisfy the 3 HOVHS conditions.

8 Appendix B

8.1 H_N^2 derivation

The second Hamiltonian term after expanding the arctan and simplifying is,

$$H_N^2=W\sum_{n=0}^{N-1}\left[e^{-\frac{\pi i}{N}}\cos(\frac{\pi}{N})+\frac{e^{-\frac{2\pi i}{N}}}{2}\sum_{l=1}^{\infty}(D_l)(\Lambda)^l\right]|n+1\rangle\langle n|+H.c. \tag{49}$$

$$\Lambda\equiv\sum_{m=1}^{\infty}(\lambda_m)\cos\Big(m(\phi_k-\phi_n-\frac{\pi}{N})\Big)(\frac{k}{k_0})^m \tag{50}$$

Where the constants are given in the text. The sum over Λ^l is hard to deal with so we simplify it.

It is convenient to use

$$c(m)\equiv\cos\Big(m(\phi_{\vec{k}}-\phi_n-\frac{\pi}{N})\Big) \tag{51}$$

$$b(m)\equiv\lambda_m c(m) \tag{52}$$

To simplify, we solve for coeffs(x) in the following,

$$\sum_{x=1}^{\infty}\text{coeffs}(x)(\frac{k}{k_0})^x=\sum_{l=1}^{\infty}D_l(\Lambda)^l=\sum_{l=1}^{\infty}D_l\Big(\sum_{m=1}^{\infty}b(m)(\frac{k}{k_0})^m\Big)^l \tag{53}$$

$$=\sum_{l=1}^{\infty}D_l\bigg(b(1)(\frac{k}{k_0})+b(2)(\frac{k}{k_0})^2+b(3)(\frac{k}{k_0})^3+...\bigg)^l \tag{54}$$

In trying to find coeffs(x), one realizes the connection to (mathematical) partitions from number theory, or all the ways of breaking a positive integer into other positive integers. This is best shown by example. All the partitions of the number 4 are: 1+1+1+1, 1+1+2, 1+3, 2+2, and 4. A "part" in a partition are the pieces. For instance, 1+1+2 has three parts, two of "length" 1 and one of length 2.

We apply this terminology to the above. In (54) the power l contributes all terms $(b(1)\frac{k}{k_0})^{pow_1}$ $(b(2)\frac{k}{k_0}^2)^{pow_2}(b(3)\frac{k}{k_0}^3)^{pow_3}...$ constrained to 1) $\sum_i pow_i=l$ and 2) $pow_1+2pow_2+3pow_3+...=x$. There is also an easy factor to account for in multiplying out the terms. From 2, $b(arg_i)$ gives a factor arg_i in the partition of x, so arg_i is the part of length i. From 1, we are dealing with partitions of x with l parts, so pow_i corresponds to the number of parts of length i. We are considering an infinite sum over l, so we get partitions of any number of parts.

Using all of this,

$$\text{coeffs}(x) = \sum_{\substack{\text{partition}_i \in \\ \text{all partitions of } x}} D_{(\substack{\#\text{ of parts} \\ \text{in partition}_i})} \frac{(\#\text{ of parts in partition}_i)!}{\prod_{\substack{\text{part length}_j \\ \in \text{partition}_i}} (\text{degeneracy of length}_j)!} \cdot \left(\prod_{\substack{\text{part length j} \in \\ \text{partition}_i}} b(\text{length j})^{\text{degeneracy of length}_j} \right) \tag{55}$$

Here by "degeneracy of part j" I mean "number of parts with length j".

It is not hard to see that this is the same as the form given in the paper (31).

8.2 Orthogonality derivation

I begin with

$$\frac{1}{N} \sum_n \cos^L \left(M(\phi_{\vec{k}} - \phi_n - \frac{\pi}{N}) \right) e^{-\frac{2\pi i}{N}(j'-j)} \tag{56}$$

Expanding the cosine and using binomial expansion over dummy variable q, we get

$$= (\frac{1}{2})^L \sum_{q=0}^{L} \binom{L}{q} e^{-i(\phi_k - \frac{\pi}{N})M(L-2q)} \left[\frac{1}{N} \sum_n e^{\frac{2\pi i}{N} nM(L-2q)} e^{-\frac{2\pi i}{N} n(j'-j)} \right] \tag{57}$$

Where the term in brackets is $\delta_{[M(L-2q)=j'-j]}$.

We need to find a hermitian conjugate somewhere. We see that $L-2q$ goes from $-L, -L+2, -L+4, ..., L-4, L-2, L$. Let us define $z = L-2q$ and consider only positive z. This should do the trick.

$$= (\frac{1}{2})^L \left(\sum_{q=0}^{\text{floor}(L/2)} + \sum_{\text{floor}(L/2)+1}^{L} \right) \tag{58}$$

$$= (\frac{1}{2})^L \sum_{z=L,L-2,...}^{z \geq 0} \binom{L}{(L-z)/2} [1 - \frac{1}{2}\delta_{z=0}] \left[e^{-i(\phi_k - \frac{\pi}{N})Mz} \delta_{Mz=j'-j} + e^{i(\phi_k - \frac{\pi}{N})Mz} \delta_{-Mz=j'-j} \right] \tag{59}$$

I account for double counting at 0 with the $[1 - \frac{1}{2}\delta_{z=0}]$ term.

8.3 Values of constants

I computed that

$$[consts1] = C_m \binom{m}{2m-x} \binom{2m-x}{m-\frac{x+z}{2}} [1 - \frac{1}{2}\delta_{z=0}] \tag{60}$$

$$[consts2] = (\frac{1}{2})^L \binom{L}{(L-z)/2} [1 - \frac{1}{2}\delta_{z=0}] \tag{61}$$

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