How to detect higher order Van Hove singularities in multi-band Hamiltonians in practice

Anirudh Chandrasekaran *, Joseph J. Betouras **

Department of Physics and Centre for the Science of Materials, Loughborough University, Loughborough LE11 3TU, UK.
* a.chandrasekaran@lboro.ac.uk, **J.Betouras@lboro.ac.uk,
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Abstract

We present a practical method to detect and diagnose higher order Van Hove singularities in multiband systems, with no restrictions on number of bands and hopping terms. The method allows us to directly compute the Taylor expansion of the dispersion of any band at arbitrary k points, using an extension of the Feynman Hellmann theorem. Being fairly general in scope, it also allows us to incorporate and analyse the effect of tuning parameters on the low energy dispersions, which can greatly aid the search for higher order Van Hove singularities. A restricted class of degenerate bands can be handled within this framework, which can be readily computationally implemented. Subsequently, we demonstrate the use of the method, taking the Haldane model as an example.

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1 Introduction

Nearly a century after its introduction, band theoretic modelling of crystalline solids continues to play a significant role in our understanding of real materials. Much progress has been made, both in the realm of techniques for the calculation of band structures, and the analysis of non-trivial band features. Progress in the latter is particularly epitomized by the rapid advances made in recent times, in the areas of band topology and geometry. The investigation of unusual band topologies and their physical importance was initiated by Lifshitz and Van Hove [1, 2]. Their work led to the discovery of Fermi surface topological transitions (FSTT), where the Fermi surface geometry changes suddenly when some parameters in the system are tuned. In his pioneering early work, Lifshitz identified two types of Fermi surface topological transitions, namely the pocket appearing/disappearing type and the neck formation/collapse type [1]. In both these cases, and also more generally in FSTTs, the transition happens through a situation wherein the Fermi surface hosts one or more critical points of the dispersion.

Critical points are accompanied by a vanishing gradient of the energy dispersion, and typically correspond to either a maximum, a minimum or a saddle point of the dispersion. The canonical form of the Taylor expansion of the dispersion at a critical point to quadratic order, is normally given by \( \pm k_x^2 \pm k_y^2 \). Such a form of the dispersion leads to a logarithmic divergence in the density of states (DOS) [2] at the critical energy. Sometimes however, we need to expand the dispersion beyond quadratic order to adequately capture the low energy features. These are situations where the determinant of the Hessian matrix of the dispersion, evaluated at the critical point, also vanishes. In such a scenario, the critical point is referred to as a higher order critical point, and the dispersion is said to have a higher order Van Hove singularity (HOVHS). A simple and commonly reported example of HOVHS is the cusp singularity with dispersion \( k_x^4 - k_y^2 \) [3–5].

In the case of HOVHS, the divergence of the DOS is enhanced to a much stronger power law divergence, often with asymmetric prefactors above and below the critical energy. [3, 6]. This is expected to strengthen electronic correlations in the vicinity of the HOVHS. The consequences of this could be potentially dramatic [7], and may lead to novel quantum phases. The fundamental reason is that due to the vanishing gradient of the energy dispersion in the vicinity of those points, the fermions get heavy and interaction effects become important.

Ordinary Van Hove singularities have been observed in the context of Lifshitz transitions in many materials including cuprate and iron based superconductors, cobaltates, \( \text{Sr}_2\text{RuO}_4 \) and heavy fermion systems [8–17]. With the recent advances in the experimental methods of tuning materials and improved resolutions of various spectroscopic probes (including angle resolved photoemission spectroscopy (ARPES)), there is both an increasing interest and emerging avenues for the investigation of the presence and consequence of exotic band geometry in real materials. This is particularly true for HOVHS, which have been linked with the unusual magnetic and thermodynamic behaviour of \( \text{Sr}_3\text{Ru}_2\text{O}_7 \) [4], twisted bilayer graphene near magic angle, close to half filling [18–20], the recently proposed unusual quantum phase referred to as ‘supermetal’, which has diverging susceptibilities without the presence of any long range order [21], the distinct Landau level spectrum of biased bilayer graphene [5] and the ‘extended’ Van Hove singularity in both doped graphene [22] and highly overdoped graphene [23]. More recently, HOVHS have been reported in the kagome superconductors [25–28], and may be relevant to the observed phases of doped Bernal bilayer graphene [24].

It is important to note that while a regular VHS is simply an ordinary saddle point singularity (having canonical dispersion \( k_x^2 - k_y^2 \)), HOVHS are, in contrast, a large class of distinct singularities. Although in principle there are infinitely many of them, we need to consider only a finite subset of
singularity when studying two dimensional and layered materials (see Ref [3] for a justification, and Refs [3, 6] for a thorough classification of these relevant singularities). Apart from this, another complication that arises in the context of HOVHS is that they are somewhat elusive compared to regular VHS, i.e., they typically require a fine tuning of parameters in the system (by the application of strain, pressure, twist, bias voltage, doping, etc). A slightly different manifestation of this problem is that the HOVHS already present may be sensitive to impurities and changes in the parameters, upon which the higher order critical point could split into a number of ordinary critical points. Fortunately, as a recent study of the effect of impurities on HOVHS [29] shows, for a low concentration of impurities, the distinct quantitative signatures of the HOVHS do survive.

As already noted above, there has been a renewed interest and improved ability to experimentally tune real materials in recent times. This renders a sound theoretical analysis of HOVHS a relevant and necessary programme. To this end, in this work, we address the question of how we can detect a HOVHS given a k-space Hamiltonian, even when the description is detailed (in the sense of number of terms, hopping parameters, etc.) and involves multiple bands. The HOVHS can be diagnosed from the Taylor expansion of the band in question, at the chosen k point. Low energy theories determined either by polynomial fits or purely symmetry considerations are often also a stepping stone for further analysis, such as diagrammatic many-body treatment of electronic correlations and transport studies [7, 29, 30]. But the full and correct Taylor expansion to a given order is needed for the unambiguous diagnosis of a HOVHS (see Ref [3] for an illustration of how relying purely on symmetry considerations can lead to a misdiagnosis of the HOVHS, the DOS divergence exponent and the ratio of prefactors).

In this paper, we provide a technique based on an extension of the Feynman Hellmann theorem, to directly compute the Taylor expansion to any order, of band dispersion given the k-space Hamiltonian, with no restriction on number of bands and hopping terms. We present the method and treat a particular case of degenerate bands. An explicit proof of the method, up to cubic degree of Taylor expansion is provided in the appendix. The general proof along with an extension to other non-trivial band degeneracies will be presented in a future paper. In the following sections we first define precisely the issue which we tackle in section 2, then we deal with multi-band models in section 3 and provide the method and some general formulae. It is worth emphasizing that the method can be applied to any Hamiltonian $H(k)$. In section 4 we apply the method and the generic results to the case of the Haldane model and we conclude in section 5. For clarity and to facilitate the flow, details of the calculations are presented in the appendix.

2 Defining the problem: Identifying and diagnosing higher order singularities

While HOVHS have been increasingly reported in real materials and theoretical models, detecting their presence and diagnosing their precise nature is not a straightforward task. Even when the Taylor expansion of the band at the critical point is available, naive inspection or even scaling arguments may not help us identify the correct singularity, and its associated power law exponents and ratio of prefactors (see Ref [3] for a discussion of the issue with an illustrative example). Nevertheless, a straightforward algorithm exists, which, given the Taylor expansion, can be used to exactly pinpoint the singularity that is present [3]. To this end it becomes necessary for us to compute the Taylor expansion of the bands in tight-binding and Wannierised models, particularly when these models are able to account for experiments on materials (such as angle resolved photoemission spectroscopy and
quasiparticle interference measurements).

A technique that is widely used in this context is polynomial fits to the band along some directions in k-space. While this may indeed reveal some aspects of the Taylor expansion, it may at times altogether miss the presence of a higher order singularity if the directions of the fits do not coincide with the ‘principal’ directions of the singularity. For example, the singularity with dispersion relation:

$$\varepsilon(k) \propto (k_x + k_y)^4 - (k_x - k_y)^2$$

(1)

will not be revealed as a higher order saddle by polynomial fits of the dispersion along the $k_x$ and $k_y$ directions. Even in the cases where the polynomial fit reveals a higher order singularity, by virtue of absence or smallness of the quadratic part of the fit, the full Taylor expansion to a specified order may not be revealed by polynomial fits along some chosen directions. Therefore, given a tight-binding model, we need a general technique for extracting the Taylor expansion of bands at arbitrary k-points unambiguously. In the next section, we discuss another aspect of this problem before proceeding to provide the solution for it.

3 Multi-band tight binding models

As described in the preceding sections, the active bands near the Fermi level of many real materials can be captured by complicated tight binding models that might, in practice, require a large number of Wannier functions or orbitals and several hopping terms to be able to adequately reproduce DFT and ARPES bands. This can often make the analysis of low energy theory around some k point quite difficult, especially if we want to avoid resorting to polynomial fits or if we are interested in tracking the effect of changing tuning parameters on the dispersion. Since the characteristic equation has a degree equal to the dimension of the Hamiltonian matrix (i.e the total number of bands), any analytic solution to the eigenvalue problem for general $k$, is possible only up to the four band case (with some exceptions). Already for cubic and quartic polynomials, the general solutions are quite complicated. We therefore need a more practical method to obtain the Taylor expansion around a particular $k$ point in a specified band. In the next section we describe such a method that can handle large and detailed k-space Hamiltonians (including those based on TBMs) and can be readily implemented numerically.

3.1 Preliminaries

To compute the Taylor expansion to order $N$ at $k_0$, in principle we need to compute all the mixed partial derivatives $\partial_{l_1} \partial_{l_2} \cdots \partial_{l_d} \varepsilon_n(k)|_{k_0}$ for $1 \leq l_1 + l_2 + \cdots + l_d \leq N$ in a $d$-dimensional system. However, computing all these mixed partial derivatives within the Feynman Hellmann method will be rather involved. We can simplify this procedure considerably by computing instead, the derivatives with respect to a single variable $\lambda$, taking the form $\partial^M \varepsilon_n(k_0 + \lambda k)/\partial \lambda^M$ and setting $\lambda$ to zero at the end. By repeated application of the chain rule for differentiation, it can be shown that

$$\left. \frac{\partial^M \varepsilon_n(k_0 + \lambda k)}{\partial \lambda^M} \right|_{\lambda=0} = \sum_{1 \leq l_1, l_2, \ldots, l_d < M} \frac{M!}{l_1! l_2! \cdots l_d!} \frac{\partial^M \varepsilon_n(k)}{\partial k_1^{l_1} \partial k_2^{l_2} \cdots \partial k_d^{l_d}} \bigg|_{k=k_0} k_1^{l_1} k_2^{l_2} \cdots k_d^{l_d}.$$

(2)
Thus, \( \frac{1}{M!} \left. \frac{\partial^M}{\partial \lambda^M} \varepsilon_n(k_0 + \lambda k) \right|_{\lambda=0} \) is the sum of all the monomials of degree \( M \) in the Taylor expansion of \( \varepsilon_n(k) \) at \( k_0 \). The full Taylor expansion to order \( N \) is then given by

\[
\varepsilon_n(k_0 + k) = \sum_{M=1}^{N} \frac{1}{M!} \left. \frac{\partial^M \varepsilon_n(k_0 + \lambda k)}{\partial \lambda^M} \right|_{\lambda=0} + \mathcal{O}(k^{N+1}).
\]

To compute the Taylor expansion of the band dispersion, it is sufficient to use this trick along with the Feynman Hellmann formula.

Before proceeding to the method, we state the important assumptions. The Hamiltonian is a finite dimensional matrix that is a smooth function of \( k \). This is of course always the case with tight-binding models, however large and complicated they may be. We allow for the band in question to be degenerate with some other bands but demand that its Taylor expansion to order \( N \) also coincides with the other bands. This is a restrictive assumption that we will relax in part II of the paper, where we shall treat the more complicated scenarios of bands touching and intersecting each other in complicated ways (like a linear band crossing for example. Such multi-band intersections, sometimes collectively referred to as multi-fold fermions, can involve several bands and may be stabilized by symmetries. [31]).

### 3.2 The method

We are interested in computing the Taylor expansion at \( k_0 \) to order \( N \), of the \( n \)th band (denoted by \( \varepsilon_n(k) \)) arising from the Hamiltonian matrix \( \hat{H}(k) \). The method proceeds to compute the terms order by order.

1. Compute numerically, all the eigenvalues and eigenvectors of \( \hat{H}(k) \) at the chosen point \( k_0 \). Let us order these eigenvalues and denote them by \( \varepsilon_1, \varepsilon_2, ..., \varepsilon_N \). The corresponding eigenvectors are arranged into the columns of a matrix \( \hat{E} \).

2. Perform a change of basis from the orbital basis to the eigenbasis at \( k_0 \) by transforming the Hamiltonian: \( \hat{H}(k) \rightarrow \hat{E}^\dagger \hat{H}(k) \hat{E} \). (Note that we are transforming the Hamiltonian as a function of \( k \), not just the Hamiltonian at the chosen \( k_0 \). The eigenvectors that constitute the new basis are however the numerically computed ones at \( k_0 \). Technically this change of basis is not needed. But it makes the algorithm more efficient since we will not have to repeatedly compute matrix elements of the form \( \langle m_1 | \partial^M \hat{H} | m_2 \rangle \) with respect to the eigenvectors \( |m_1\rangle \) and \( |m_2\rangle \) by matrix multiplication, and can instead directly read off the corresponding matrix elements).

3. Compute the following matrices analytically by directly differentiating the basis transformed Hamiltonian:

\[
\partial \hat{H} := \left. \frac{\partial \hat{H}(k_0 + \lambda k)}{\partial \lambda} \right|_{\lambda=0}, \quad \partial^2 \hat{H} := \left. \frac{\partial^2 \hat{H}(k_0 + \lambda k)}{\partial \lambda^2} \right|_{\lambda=0}, \quad \ldots
\]

\[
\ldots, \quad \partial^N \hat{H} := \left. \frac{\partial^N \hat{H}(k_0 + \lambda k)}{\partial \lambda^N} \right|_{\lambda=0}.
\]

(These matrices when divided by the appropriate factorial weights and assembled together make up the Taylor expansion of the Hamiltonian at \( k_0 \) to order \( N \)).
4. To compute the Taylor expansion, we shall now outline the procedure to compute the following polynomials and assemble them into the Taylor series as in Eq 3:

$$\partial \varepsilon_n := \left. \frac{\partial \varepsilon_n(k_0 + \lambda k)}{\partial \lambda} \right|_{\lambda=0}, \quad \partial^2 \varepsilon_n := \left. \frac{\partial^2 \varepsilon_n(k_0 + \lambda k)}{\partial \lambda^2} \right|_{\lambda=0}, \ldots$$

$$\ldots, \partial^N \varepsilon_n := \left. \frac{\partial^N \varepsilon_n(k_0 + \lambda k)}{\partial \lambda^N} \right|_{\lambda=0}. \quad (5)$$

5. Before computing each of the above polynomials, we formally define the following recursive lemma, with \(\varepsilon_m \neq \varepsilon_n\) and \(1 \leq \kappa \leq N\):

$$f(\kappa, m, n) = \left[ \frac{\partial^\kappa \hat{H}}{n-m} \right] + \sum_{\kappa=1}^{\kappa-1} \binom{\kappa}{\kappa} \sum_{|m| \notin D(n)} \left[ \frac{\partial^{\kappa-\kappa} \hat{H}}{m-m} \right] \varepsilon_m \varepsilon_m f(\kappa, m, n), \quad (6)$$

where \([\partial^\kappa \hat{H}]_{m,n}\) is a shorthand for \((m)|\partial^\kappa \hat{H}|n\), a matrix element of the matrix \(\partial^\kappa \hat{H}\), while \(D(n)\) is the set of all the eigenstates that are degenerate to \(|n\rangle\) (including itself) and the combinatoric factor is defined by

$$\binom{\kappa}{\kappa} = \frac{\kappa!}{(\kappa-\kappa)!\kappa!}.$$  

(7)

Obviously, since this is a recursive definition, we will obtain a sequence of product of the function \(f\) evaluated at different \(\kappa\) and decreasing \(\kappa\) in the full expansion of the right hand side. We list the explicit expression for \(f(\kappa, m, n)\) for \(\kappa = 1, 2\)

$$f(1, m, n) = \frac{\left[ \partial \hat{H} \right]_{m,n}}{\varepsilon_m - \varepsilon_m}, \quad (8a)$$

$$f(2, m, n) = \frac{\left[ \partial^2 \hat{H} \right]_{m,n}}{\varepsilon_n - \varepsilon_m} + 2 \sum_{|m| \notin D(n)} \frac{\left[ \partial \hat{H} \right]_{n,m}}{\varepsilon_n - \varepsilon_m} \varepsilon_m \left[ \partial \hat{H} \right]_{n,m} - 2 \frac{\varepsilon_n \left[ \partial \hat{H} \right]_{m,n}}{\left( \varepsilon_n - \varepsilon_m \right)^2}. \quad (8b)$$

The sequence \(f\)’s always terminates when \(\kappa = 1\), and we have in that case \(f(\kappa = 1, m, n) = \left[ \partial \hat{H} \right]_{m,n}/(\varepsilon_n - \varepsilon_m)\). For any \(\kappa > 1\) and given \(m\) and \(n\), to evaluate \(f(\kappa, m, n)\), we need to know all the lower derivatives of the dispersion of band \(n\), denoted by \(\partial \varepsilon_n, \partial^2 \varepsilon_n, \ldots, \partial^{\kappa-1} \varepsilon_n\). But since we know the first derivative from Feynman - Hellmann lemma, \(\partial \varepsilon_n = \left[ \partial \hat{H} \right]_{n,n}\), we can explicitly evaluate all the higher derivatives from \(\partial^2 \varepsilon_n\) onwards order by order using the formula:

$$\partial^M \varepsilon_n = \left[ \partial^M \hat{H} \right]_{n,n} + \sum_{\kappa=1}^{M-1} \binom{M}{\kappa} \sum_{|m| \notin D(n)} \left[ \partial^{M-\kappa} \hat{H} \right]_{n,m} f(\kappa, m, n). \quad (9)$$

6. Having computed \(\partial \varepsilon_n\) through \(\partial^N \varepsilon_n\), we assemble them into the Taylor polynomial of degree \(N\) at \(k_0\):

$$j^N(\varepsilon_n)|_{k_0} = \varepsilon_n + \frac{\partial \varepsilon_n}{1!} + \frac{\partial^2 \varepsilon_n}{2!} + \cdots + \frac{\partial^N \varepsilon_n}{N!}. \quad (10)$$
Before we proceed further, it is important to emphasize that the method can be also used to track the changes in the dispersion due to small changes in the tuning parameters. This can be achieved by simply redefining $\partial^N \widetilde{H}$ in Eq 4. For example, consider the case where we have the Hamiltonian of the system parametrized for changes in some hopping term $t$ around a critical value $t_0$ (this could be the result of twist, strain, pressure etc). To obtain the effect of the tuning directly in the Taylor expansion of the dispersion, we redefine Eq 4 as follows and apply the rest of the algorithm

$$\partial \widetilde{H} := \left. \frac{\partial \widetilde{H}(k_0 + \lambda k, t_0 + \lambda \delta t)}{\partial \lambda} \right|_{\lambda=0}, \partial^2 \widetilde{H} := \left. \frac{\partial^2 \widetilde{H}(k_0 + \lambda k, t_0 + \lambda \delta t)}{\partial \lambda^2} \right|_{\lambda=0}, \ldots, \partial^N \widetilde{H} := \left. \frac{\partial^N \widetilde{H}(k_0 + \lambda k, t_0 + \lambda \delta t)}{\partial \lambda^N} \right|_{\lambda=0} . \quad (11)$$

This will then yield terms in the Taylor expansion that contain $\delta t, \delta t^2, \ldots$ which will track the changes in the dispersion under the tuning of parameters. This procedure is, by no means, restricted to a single tuning parameter. If we search for unusual band geometries under tuning, this procedure can be very helpful. All this is illustrated using an example in section 4.

### 3.3 Unpacking the formula

Before proceeding with the application, we need to state the explicit form of the linear, quadratic and cubic derivatives arising from Eqs 6 and 9 which will be used later. The detailed derivations are included in the Appendix.

\begin{align}
\partial \varepsilon_n &= \langle n | \partial \widetilde{H} | n \rangle , \quad (12a) \\
\partial^2 \varepsilon_n &= \langle n | \partial^2 \widetilde{H} | n \rangle + 2 \sum_{|m_1| \notin D(n)} \frac{\langle n | \partial \widetilde{H} | m_1 \rangle \langle m_1 | \partial \widetilde{H} | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} , \quad (12b) \\
\partial^3 \varepsilon_n &= \langle n | \partial^3 \widetilde{H} | n \rangle + 3 \sum_{|m_1| \notin D(n)} \frac{\langle n | \partial^2 \widetilde{H} | m_1 \rangle \langle m_1 | \partial \widetilde{H} | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \\
&\quad + 3 \sum_{|m_1| \notin D(n)} \frac{\langle n | \partial \widetilde{H} | m_1 \rangle \langle m_1 | \partial^2 \widetilde{H} | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \\
&\quad + 6 \sum_{|m_1| \notin D(n)} \sum_{|m_2| \notin D(n)} \frac{\langle n | \partial \widetilde{H} | m_1 \rangle \langle m_1 | \partial \widetilde{H} | m_2 \rangle \langle m_2 | \partial \widetilde{H} | n \rangle}{(\varepsilon_n - \varepsilon_{m_1})(\varepsilon_n - \varepsilon_{m_2})} \\
&\quad - 6 \partial \varepsilon_n \sum_{|m_1| \notin D(n)} \frac{\langle n | \partial \widetilde{H} | m_1 \rangle \langle m_1 | \partial \widetilde{H} | n \rangle}{(\varepsilon_n - \varepsilon_{m_1})^2} . \quad (12c)
\end{align}

Note that the formulae listed above only require us to be able to numerically diagonalize the Hamiltonian $\widetilde{H}(k)$ at a chosen $k_0$, and be able to differentiate $\widetilde{H}(k)$ analytically a finite number of times, all of which can be readily and quickly done using a computer algebra system (such as Mathematica [32] or Maple [33]). Knowing the eigenvalues at $k_0$ and the matrix elements of various derivatives of $\widetilde{H}(k)$, we shall be able to compute the Taylor expansion order by order, with each higher order depending upon the lower order terms. The first order term (Eq 12a) is of course the familiar Fenyman-Hellmann result.
4 Application of the method: Haldane model

In this section, we benchmark the method against the Haldane model [34]. An extension of the Haldane model can be tuned to host the monkey saddle singularity having dispersion $k_y^3 - 3k_x^2k_y$ [29]. Although the method can more generally be applied to larger systems that require numerical diagonalization, we choose the Haldane model for its simplicity and analytic tractability, so that it may serve as a pedagogical example. The underlying lattice for the Haldane model is a honeycomb lattice similar to graphene, with two triangular sublattices A and B. The nearest neighbor unit vectors originating from the A sublattice onto the B sublattice are given by

$$a_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad a_2 = \begin{pmatrix} -\frac{1}{2} \\ \sqrt{3}/2 \end{pmatrix}, \quad a_3 = \begin{pmatrix} -\frac{1}{2} \\ -\sqrt{3}/2 \end{pmatrix}. \quad (13)$$

The next nearest neighbor vectors are given by $b_1 = a_2 - a_3$, $b_2 = a_3 - a_1$ and $b_3 = a_1 - a_2$. The full $k$-space Hamiltonian is then the sum of nearest neighbor, staggered chemical potential and next nearest neighbor terms:

$$\hat{H}(k) = \hat{H}_0(k) + M \sigma_z + 2t_2 \sum_i \sin(k \cdot b_i) \sigma_z,$$

where $\sigma_z$ is the familiar Pauli matrix and

$$\hat{H}_0(k) = \begin{pmatrix} 0 & t_1 \sum_i e^{i k \cdot a_i} \\ t_1 \sum_i e^{-i k \cdot a_i} & 0 \end{pmatrix}. \quad (14)$$

Since the Hamiltonian is two-dimensional, it can be diagonalized exactly to give two bands indexed by $n = 1, 2$

$$\varepsilon_n(k) = (-1)^n \left[ \left( M + 2t_2 \sum_i \sin(k \cdot b_i) \right)^2 + t_1^2 \sum_i e^{i k \cdot a_i} \right]^\frac{1}{2}. \quad (15)$$

Consider the following point of three-fold rotation symmetry

$$K_- = \frac{4\pi}{3\sqrt{3}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (16)$$

Let us define a critical value for the staggered chemical potential

$$M_0 = \frac{t_1^2 - 18t_2}{2\sqrt{3}t_2}. \quad (17)$$

We can analytically derive the Taylor expansion for the upper band ($n = 2$) dispersion, which around the $K_-$ point reads

$$\varepsilon_2(k + K_-) \approx \left| M - 3\sqrt{3}t_2 \right| + \frac{9\sqrt{3}t_2(M + M_0)}{4 \left| M - 3\sqrt{3}t_2 \right|} \left( k_x^2 + k_y^2 \right)$$

$$+ \frac{6t_2 (\sqrt{3}M - 9t_2) - 9t_1^2}{16 \left| M - 3\sqrt{3}t_2 \right|} \left( k_y^2 - 3k_y k_x^2 \right) + \mathcal{O}(k^4). \quad (18)$$

When we tune $M \to -M_0$

$$\varepsilon_2(k + K_-) \approx \frac{t_1^2}{2\sqrt{3}t_2} - \frac{3\sqrt{3}|t_2|}{2} \left( k_y^2 - 3k_y k_x^2 \right) + \mathcal{O}(k^4). \quad (19)$$
Thus we have obtained a monkey saddle. Let us examine what happens when $M$ is close to but not equal to $-M_0$, i.e. $M = -M_0 + \delta M$. Assuming $t_2 > 0$, for very small $\delta M$, the Taylor expansion gets modified as

$$
\varepsilon_2(k + K_{\perp}) \approx -\frac{t_1^2}{2\sqrt{3}t_2} + \delta M + \frac{27t_2^2}{4t_1^2}\delta M \left( k_x^2 + k_y^2 \right) - \left( \frac{3\sqrt{3}t_2}{4} + \frac{27}{16}\delta M \right) \left( k_y^3 - 3k_yk_x^2 \right) + \mathcal{O}(k^4,\delta M^2).
$$

(20)

Using the numerical values: $t = 1$ and $t = 1/2$:

$$
\varepsilon_2(k + K_{\perp}) \approx \frac{1}{\sqrt{3}} - \delta M + \frac{27}{8}\delta M \left( k_x^2 + k_y^2 \right) - \left( \frac{3\sqrt{3}}{4} + \frac{27}{16}\delta M \right) \left( k_y^3 - 3k_yk_x^2 \right) + \mathcal{O}(k^4,\delta M^2).
$$

(21)

We will now attempt to reproduce this Taylor expansion using the method illustrated above. Firstly we calculate the eigenvalues and eigenvectors at $K_{\perp}$ for the critical tuning (since $\delta M$ is treated here as a perturbation, we are computing eigenvalues and eigenvectors of $H(K_{\perp} + \lambda k; -M_0 + \lambda \delta M)$ at $\lambda = 0$, which is the same as computing them for the critical tuning). The Hamiltonian takes the value

$$
\tilde{H}(K_{\perp}) = \begin{pmatrix}
-\frac{1}{\sqrt{3}} & 0 \\
0 & \frac{1}{\sqrt{3}}
\end{pmatrix}
$$

(22)

Thus it is already diagonal. The eigenvalues and eigenvectors are then given by

$$
\varepsilon_1(K_{\perp}) = -\frac{1}{\sqrt{3}}, \quad |E_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix},
$$

$$
\varepsilon_2(K_{\perp}) = \frac{1}{\sqrt{3}}, \quad |E_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
$$

(23)

We now compute the matrices $\partial \tilde{H}$, $\partial^2 \tilde{H}$ and $\partial^3 \tilde{H}$, defined in Eq 4, in the eigenbasis:

$$
\partial \tilde{H} = \begin{pmatrix}
\delta M & \frac{3}{2}i(k_x + ik_y) \\
-\frac{3}{2}i(k_x - ik_y) & -\delta M
\end{pmatrix}
$$

(24a)

$$
\partial^2 \tilde{H} = \begin{pmatrix}
\frac{9}{4}\sqrt{3}(k_x^2 + k_y^2) & -\frac{3}{4}(k_x - ik_y)^2 \\
-\frac{3}{4}(k_x + ik_y)^2 & -\frac{9}{4}\sqrt{3}(k_x^2 + k_y^2)
\end{pmatrix}
$$

(24b)

$$
\partial^3 \tilde{H} = \begin{pmatrix}
\frac{9}{8}\sqrt{3}k_y(k_y^3 - 3k_x^2) & -\frac{9}{8}i(k_x - ik_y)(k_x + ik_y)^2 \\
\frac{9}{8}i(k_x - ik_y)^2(k_x + ik_y) & -\frac{9}{8}\sqrt{3}k_y(k_y^3 - 3k_x^2)
\end{pmatrix}
$$

(24c)

The derivatives $\partial^N \varepsilon_2$ for $N = 1, 2, 3$ are then given by

$$
\partial \varepsilon_2 = \langle E_2 | \partial \tilde{H} | E_2 \rangle = -\delta M,
$$

$$
\partial^2 \varepsilon_2 = \langle E_2 | \partial^2 \tilde{H} | E_2 \rangle
$$

$$
\partial^3 \varepsilon_2 = \langle E_2 | \partial^3 \tilde{H} | E_2 \rangle.
$$
\[\begin{align*}
\partial^2 \epsilon_n &= \langle E_2 | \partial^2 \hat{H} | E_2 \rangle + 2 \frac{\langle E_2 | \partial \hat{H} | E_1 \rangle \langle E_1 | \partial \hat{H} | E_2 \rangle}{\epsilon_2(K_-) - \epsilon_1(K_-)} \\
&= - \frac{9\sqrt{3}}{4} (k_x^2 + k_y^2) + 2 \left( \frac{3\epsilon}{2} (k_x - ik_y) \times \frac{3\epsilon}{2} (k_x + ik_y) \right) \\
&= 0,
\end{align*}\]

\[\begin{align*}
\partial^3 \epsilon_n &= \langle E_2 | \partial^3 \hat{H} | E_2 \rangle + 3 \frac{\langle E_2 | \partial^2 \hat{H} | E_1 \rangle \langle E_1 | \partial \hat{H} | E_2 \rangle}{\epsilon_2(K_-) - \epsilon_1(K_-)} + 3 \frac{\langle E_2 | \partial \hat{H} | E_1 \rangle \langle E_1 | \partial^2 \hat{H} | E_2 \rangle}{\epsilon_2(K_-) - \epsilon_1(K_-)} \\
&+ 6 \frac{\langle E_2 | \partial \hat{H} | E_1 \rangle \langle E_1 | \partial \hat{H} | E_1 \rangle \langle E_1 | \partial \hat{H} | E_2 \rangle}{(\epsilon_2(K_-) - \epsilon_1(K_-))^2} \\
&- 6 \partial \epsilon_n \frac{\langle E_2 | \partial \hat{H} | E_1 \rangle \langle E_1 | \partial \hat{H} | E_2 \rangle}{(\epsilon_2(K_-) - \epsilon_1(K_-))^2} \\
&= - \frac{9\sqrt{3}}{8} (k_y^3 - 3k_x^2k_y) + 3 \left( \frac{2\Re \left[ -\frac{3\epsilon}{4} (k_x + ik_y)^2 \times \frac{3\epsilon}{2} (k_x + ik_y) \right]}{\frac{\sqrt{3}}{2} - \left( -\frac{1}{\sqrt{3}} \right)^2} + \frac{3\epsilon}{2} (k_x - ik_y) \times \frac{3\epsilon}{2} (k_x + ik_y) \right) \\
&- \frac{9\sqrt{3}}{8} (k_y^3 - 3k_x^2k_y) \left( \frac{27\sqrt{3}}{8} (k_y^3 - 3k_x^2k_y) + \frac{81}{8} \delta M \left( k_x^2 + k_y^2 \right) \right) \\
&+ \frac{81}{8} \delta M \left( k_x^2 + k_y^2 \right) \\
&= - \frac{9\sqrt{3}}{2} (k_y^3 - 3k_x^2k_y) + \frac{81}{4} \delta M \left( k_x^2 + k_y^2 \right). \tag{25}
\end{align*}\]

We can assemble these into the Taylor expansion using Eq 10:
\[\begin{align*}
\epsilon_2(k + K_-) &\approx \frac{1}{\sqrt{3}} - \delta M + \frac{27}{8} \delta M \left( k_x^2 + k_y^2 \right) - \frac{3\sqrt{3}}{4} \left( k_y^3 - 3k_x^2k_y \right) + \cdots \tag{26}
\end{align*}\]

As it is evident, the Taylor expansion matches with the one we obtained by directly Taylor expanding the band dispersion, except for the extra \(\delta M\) modulation of the coefficient of the cubic term. The reason why we did not obtain that term is that it arises from the expansion to fourth order in the auxiliary parameter \(\lambda\) (basically from a term of the form \(\lambda^4 \delta M \left( k_y^3 - 3k_x^2k_y \right)\)), and here we have expanded only up to cubic order for the sake of brevity. Nevertheless, the main feature, which is the appearance of the small quadratic part that perturbs the monkey saddle when we tune off the critical value of the staggered chemical potential, is quite manifest here.

5 Conclusion

In this paper, we set in detail the method to find HOVHS in practice, when the Hamiltonian \(H(k)\) is known. The knowledge of \(H(k)\) can come from tight-binding models or ab-initio calculations or
even motivated by experimental results. The fundamental idea outlined above was to use the Feynman Hellmann theorem to compute the various derivatives of the dispersion of any specified band using the technique explained in Sec 3.2. These derivatives were then used to assemble the Taylor expansion of the band to any specified order, at arbitrary \( k \) points, with the added possibility of incorporating the influence of tuning of any parameters in the Hamiltonian. The latter result is particularly timely, given the increasing interest and recent remarkable progress of experimental methods to engineer exotic phases in materials by tuning them (via stress, twist, pressure, bias voltage, etc).

In the case of a non-trivial degeneracy at a point in \( k \)-space (such as band crossing, band touching etc.), the process of the computation of the derivatives and terms in the series expansion becomes more complicated since the procedure outlined above is not directly applicable. This is beyond the scope of the present work and will be presented in future in part II of the work.

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Note  A readily usable implementation of the algorithm in Wolfram Mathematica is available and can be shared upon reasonable request.

A  Proof of the expressions

In this section, we explicitly prove the formula in Eq 9 for linear, quadratic and cubic derivatives of the band. For the sake of convenience of notation, we drop the ‘hats’ on the Hamiltonian \( \hat{H} \) and write it simply as \( H \).

A.0.1 First derivative

The eigenvalue equation reads

\[ H\ket{n} = \varepsilon_n \ket{n}. \]  \hspace{1cm} (27)

Differentiating this once and applying the product rule for derivatives, we get

\[ \partial H\ket{n} + H\partial\ket{n} = \partial \varepsilon_n \ket{n} + \varepsilon_n \partial \ket{n}. \]  \hspace{1cm} (28)

(There is no problem with applying product rule since we are working with a finite dimensional vector space where all the terms in the eigenvalue equation are simply finite sums of product of vector and matrix coefficients in some basis). Now we take inner product of this equation with \( \ket{n} \)

\[ \braket{n|\partial H|n} + \braket{n|H|\partial n} = \partial \varepsilon_n \braket{n|n} + \varepsilon_n \braket{n|\partial n}, \]

\[ \implies \partial \varepsilon_n = \braket{n|\partial H|n}. \]  \hspace{1cm} (29)

This is of course the familiar Feynman Hellmann result. We now take inner product of Eq 28 with another eigenstate \( \ket{m} \) that is not degenerate to \( \ket{n} \):

\[ \braket{m|\partial H|n} + \braket{m|H|\partial n} = \partial \varepsilon_n \braket{m|n} + \varepsilon_n \braket{m|\partial n}, \]
\[ \langle m | \partial n \rangle = \frac{\langle m | \partial H | n \rangle}{\varepsilon_n - \varepsilon_m}. \]  

(30)

Thus, we can find the overlap of the derivative of the eigenvector \(|n\rangle\), denoted by \(|\partial n\rangle\) with the other eigenvectors not degenerate to it. It is not possible within this framework to compute \(\langle n | \partial n \rangle\) or even overlap with eigenvectors degenerate to it. We can however differentiate \(\langle n | n \rangle = 1\) to obtain \(\text{Re} \langle n | \partial n \rangle = 0\). The imaginary part is of course the famous Berry connection that cannot be gauged out in general (specifically when we have topological bands). The fact that we cannot precisely compute \(\langle n | \partial n \rangle\) will not be an impediment to computing the higher derivatives of the band, as we shall show below. We also compute the overlap of Eq 28 with respect to another eigenstate that is degenerate to \(|n\rangle\), denoted by \(|n_1\rangle \in D(n)\) (where \(D(n)\) is the set of eigenvectors degenerate to \(n\))

\[ \langle n_1 | \partial H | n \rangle + \langle n_1 | H | \partial n \rangle = \partial \varepsilon_n \langle n_1 | n \rangle + \varepsilon_n \langle n_1 | \partial n \rangle, \]

\[ \implies \langle n_1 | \partial H | n \rangle = 0, \text{ for } \varepsilon_{n_1} = \varepsilon_n \text{ but } |n_1\rangle \neq |n\rangle. \]  

(31)

In practice, however, we may find the projection of the first derivative of Hamiltonian matrix \(\partial H\) to the degenerate subspace to be non-diagonal. That is, we may find \(\langle n_1 | \partial H | n_2 \rangle \neq 0\), for distinct but degenerate \(|n_1\rangle\) and \(|n_2\rangle\). In such situations, we diagonalise the projection of \(\partial H\) in this subspace, and replace the original set of \(|n_i\rangle\) with the new eigenbasis, so that Eq 31 is automatically satisfied.

**A.0.2 Second derivative**

Differentiating Eq 28 once again, we get

\[ \partial^2 H |n\rangle + 2 \partial H |\partial n\rangle + H |\partial^2 n\rangle = \partial^2 \varepsilon_n |n\rangle + 2 \partial \varepsilon_n |\partial n\rangle + \varepsilon_n |\partial^2 n\rangle. \]  

(32)

Taking inner product with \(|n\rangle\), we get

\[ \langle n | \partial^2 H |n\rangle + 2 \langle n | \partial H |\partial n\rangle + \langle n | H |\partial^2 n\rangle = \partial^2 \varepsilon_n \langle n | n\rangle + 2 \partial \varepsilon_n \langle n | \partial n\rangle + \varepsilon_n \langle n | \partial^2 n\rangle \]  

(33)

On rearranging and inserting a resolution of identity, this becomes

\[
\begin{align*}
\partial^2 \varepsilon_n &= \langle n | \partial^2 H |n\rangle + 2 \langle n | \partial H |\partial n\rangle - 2 \partial \varepsilon_n \langle n | \partial n\rangle \\
&= \langle n | \partial^2 H |n\rangle + 2 \sum_{|m\rangle \notin D(n)} \langle n | \partial H |m\rangle \langle m | \partial n\rangle + 2 \sum_{|n_1\rangle \in D(n)} \langle n | \partial H |n_1\rangle \langle n_1 | \partial n\rangle \\
&\quad - 2 \partial \varepsilon_n \langle n | \partial n\rangle \\
&= \langle n | \partial^2 H |n\rangle + 2 \sum_{|m\rangle \notin D(n)} \frac{\langle n | \partial H |m\rangle \langle m | \partial H |n\rangle}{\varepsilon_n - \varepsilon_m},
\end{align*}
\]

(34)

where we have used \(\langle n | \partial H |n\rangle = \partial \varepsilon_n\) and \(\langle n | \partial H |n_1\rangle = 0\) when \(|n_1\rangle \neq |n\rangle\) in going to the last line.

We now compute the overlap of the terms in Eq 32 with \(|m\rangle \notin D(n)\):

\[ \langle m_1 | \partial^2 H |n\rangle + 2 \langle m_1 | \partial H |\partial n\rangle + \langle m_1 | H |\partial^2 n\rangle = \partial^2 \varepsilon_n \langle m_1 | n\rangle + 2 \partial \varepsilon_n \langle m_1 | \partial n\rangle + \varepsilon_n \langle m_1 | \partial^2 n\rangle. \]  

(35)

Simplifying this further by rearranging terms and introducing another resolution of identity:

\[ \langle m_1 | \partial^2 n\rangle = \frac{1}{\varepsilon_n - \varepsilon_{m_1}} [\langle m_1 | \partial^2 H |n\rangle + 2 \langle m_1 | \partial H |\partial n\rangle - 2 \partial \varepsilon_n \langle m_1 | \partial n\rangle] \]
\[
\frac{1}{\varepsilon_n - \varepsilon_m} \left[ \langle m_1 | \partial^2 H | n \rangle + 2 \sum_{|m_2| \notin D(n)} \langle m_1 | \partial H | m_2 \rangle \langle m_2 | \partial n \rangle - 2 \partial \varepsilon_n \langle m_1 | \partial n \rangle + 2 \sum_{|m_2| \notin D(n)} \langle m_1 | \partial H | m_2 \rangle \langle m_2 | \partial n \rangle - 2 \partial \varepsilon_n \langle m_1 | \partial H | n \rangle \right] = 0.
\]

This will be used in the computation of the third derivative below. Note that once again we are not able to explicitly evaluate the overlap with \(|n\rangle\). Lastly, we compute the overlap of Eq 34 with \(|n_1\rangle \in D(n)\) and \(|n_1\rangle \neq |n\rangle\)

\[
\langle n_1 | \partial^2 H | n \rangle + 2 \langle n_1 | \partial H | \partial n \rangle + \langle n_1 | H | \partial^2 n \rangle = \partial^2 \varepsilon_n \langle n_1 | n \rangle + 2 \partial \varepsilon_n \langle n_1 | \partial n \rangle + \varepsilon_n \langle n_1 | \partial^2 n \rangle.
\]

Using \(\langle n_1 | H = \varepsilon_n \langle n_1 | \rangle\), introducing resolution of identity and simplifying

\[
\langle n_1 | \partial^2 H | n \rangle + 2 \sum_{|m_1| \notin D(n)} \langle n_1 | \partial H | m_1 \rangle \langle m_1 | \partial n \rangle + 2 \sum_{|m_2| \notin D(n)} \langle n_1 | \partial H | m_2 \rangle \langle m_2 | \partial n \rangle
\]

\[
\Rightarrow \langle n_1 | \partial^2 H | n \rangle + 2 \sum_{|m_1| \notin D(n)} \frac{\langle n_1 | \partial H | m_1 \rangle \langle m_1 | \partial H | n \rangle}{\varepsilon_n - \varepsilon_m} = 0.
\]

The expression on the left hand side resembles the expression for \(\partial^2 \varepsilon_n\), with the difference that the leftmost bra in each of the terms is \(|n_1\rangle\) instead of \(|n\rangle\).

### A.0.3 Third derivative

The third derivative of the eigenvalue equation reads

\[
\partial^3 H |n\rangle + 3 \partial^2 H |\partial n\rangle + 3 \partial H |\partial^2 n\rangle + H |\partial^3 n\rangle = \partial^3 \varepsilon_n |n\rangle + 3 \partial^2 \varepsilon_n |\partial n\rangle + 3 \partial \varepsilon_n |\partial^2 n\rangle + \varepsilon_n |\partial^3 n\rangle.
\]

We compute the overlap of this equation with \(|n\rangle\), rearrange terms, introduce resolutions of identity and do some simplifications

\[
\partial^3 \varepsilon_n = \langle n | \partial^3 H | n \rangle + 3 \langle n | \partial^2 H | \partial n \rangle + 3 \langle n | \partial H | \partial^2 n \rangle + 3 \partial^2 \varepsilon_n \langle n | \partial n \rangle - 3 \partial \varepsilon_n \langle n | \partial^2 n \rangle
\]

\[
= \langle n | \partial^3 H | n \rangle + 3 \sum_{|m_1| \notin D(n)} \langle n | \partial^2 H | m_1 \rangle \langle m_1 | \partial n \rangle + 3 \sum_{|m_1| \notin D(n)} \langle n | \partial H | m_1 \rangle \langle m_1 | \partial^2 n \rangle
\]

\[
+ 3 \sum_{|n_1| \in D(n)} \langle n | \partial^2 H | n_1 \rangle \langle n_1 | \partial n \rangle + 3 \sum_{|n_1| \in D(n)} \langle n | \partial H | n_1 \rangle \langle n_1 | \partial^2 n \rangle
\]

\[
- 3 \partial^2 \varepsilon_n \langle n | \partial n \rangle - 3 \partial \varepsilon_n \langle n | \partial^2 n \rangle
\]

(40)

We can substitute for \(\langle m_1 | \partial n \rangle\) and \(\langle m_1 | \partial^2 n \rangle\) from Eqs 30 and 36 respectively to obtain
\[ \partial^3 \varepsilon_n = \langle n | \partial^3 H | n \rangle + 3 \sum_{|m_1\rangle \notin D(n)} \frac{\langle n | \partial^2 H | m_1 \rangle \langle m_1 | \partial H | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \]
\[ + 3 \sum_{|m_1\rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial^2 H | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \]
\[ + 6 \sum_{|m_1\rangle \notin D(n)} \sum_{|m_2\rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | m_2 \rangle \langle m_2 | \partial H | n \rangle}{(\varepsilon_n - \varepsilon_{m_1})(\varepsilon_n - \varepsilon_{m_2})} \]
\[ - 6 \partial \varepsilon_n \sum_{|m_1\rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | n \rangle}{(\varepsilon_n - \varepsilon_{m_1})^2} \]
\[ + (\ast 1) 6 \sum_{|n_1\rangle \in D(n)} \sum_{|m_1\rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \langle n_1 | \partial n \rangle \]
\[ + (\ast 2) 3 \sum_{|n_1\rangle \in D(n)} \langle n | \partial^2 H | n_1 \rangle \langle n_1 | \partial n \rangle \]
\[ + (\ast 3) 3 \sum_{|n_1\rangle \in D(n)} \langle n | \partial H | n_1 \rangle \langle n_1 | \partial^2 n \rangle \]
\[ - 3 \partial^2 \varepsilon_n \langle n | \partial n \rangle - 3 \partial \varepsilon_n \langle n | \partial^2 n \rangle. \tag{41} \]

Now let us look at some of the terms marked with a \( \ast \). To simplify them, we pull out the term containing \( |n\rangle \) from the sum over \( |n_1\rangle \in D(n) \) and substitute the expression for \( \partial^2 \varepsilon_n \):

\((\ast 2) + (\ast 1)\)
\[ = 3 \sum_{|n_1\rangle \in D(n)} \langle n | \partial^2 H | n_1 \rangle \langle n_1 | \partial n \rangle \]
\[ + 6 \sum_{|n_1\rangle \in D(n)} \sum_{|m_1\rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | n_1 \rangle}{\varepsilon_n - \varepsilon_{m_1}} \langle n_1 | \partial n \rangle \]
\[ = 3 \left( \langle n | \partial^2 H | n \rangle + 2 \sum_{|m_1\rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \right) \langle n | \partial n \rangle \]
\[ + 3 \sum_{|n_1\rangle \in D(n)} \sum_{|m_1\rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | n_1 \rangle}{\varepsilon_n - \varepsilon_{m_1}} \langle n_1 | \partial n \rangle \]
\[ = 3 \partial^2 \varepsilon_n \langle n | \partial n \rangle, \tag{42} \]

where we substitute from Eq 34 for the terms within parenthesis, while the terms within [ ] vanish due to Eq 38 (since \( |n_1\rangle \neq |n\rangle \)). Lastly, since \( \langle n | \partial H | n \rangle = \partial \varepsilon_n \) (from Eq 29) and \( \langle n | \partial H | n_1 \rangle = 0 \) for \( |n\rangle \neq |n_1\rangle \) (from Eq 31), we have

\((\ast 3) = 3 \sum_{|n_1\rangle \in D(n)} \langle n | \partial H | n_1 \rangle \langle n_1 | \partial^2 n \rangle = 3 \partial \varepsilon_n \langle n | \partial^2 n \rangle. \tag{43} \)
Therefore the sum \((\ast 1) + (\ast 2) + (\ast 3)\) cancels exactly with the last line of Eq 41 so that the expression for the third derivative of the band becomes

\[
\partial^3 \varepsilon_n = \langle n | \partial^3 H | n \rangle + 3 \sum_{|m_1 \rangle \notin D(n)} \frac{\langle n | \partial^2 H | m_1 \rangle \langle m_1 | \partial H | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \\
+ 3 \sum_{|m_1 \rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial^2 H | n \rangle}{\varepsilon_n - \varepsilon_{m_1}} \\
+ 6 \sum_{|m_1 \rangle \notin D(n)} \sum_{|m_2 \rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | m_2 \rangle \langle m_2 | \partial H | n \rangle}{(\varepsilon_n - \varepsilon_{m_1})(\varepsilon_n - \varepsilon_{m_2})} \\
- 6 \partial \varepsilon_n \sum_{|m_1 \rangle \notin D(n)} \frac{\langle n | \partial H | m_1 \rangle \langle m_1 | \partial H | n \rangle}{(\varepsilon_n - \varepsilon_{m_1})^2}. \tag{44}
\]

To obtain this, we got rid of the terms containing \(\langle n | \partial n \rangle\) and \(\langle n | \partial^2 n \rangle\) by a careful application of the results obtained for the lower derivatives \(\partial \varepsilon_n\) and \(\partial^2 \varepsilon_n\), along with the expressions involving the overlaps \(\langle n_1 | \partial H | n \rangle\) and \(\langle n_1 | \partial^2 H | n \rangle\) for \(|n_1\rangle \in D(n)\) and \(|n_1\rangle \neq |n\rangle\).

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