Towards Morse theory for dispersion relations: generic case

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+ anonym. refs.

$\mathrm{Sym}_n \equiv$ space of $n \times n$ real symm or Hermitian matrices

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \ldots \leq \lambda_n \subset \mathbb{R}$$

$\mathcal{M}$ - smooth cpt manif. $\dim \mathcal{M} = d$

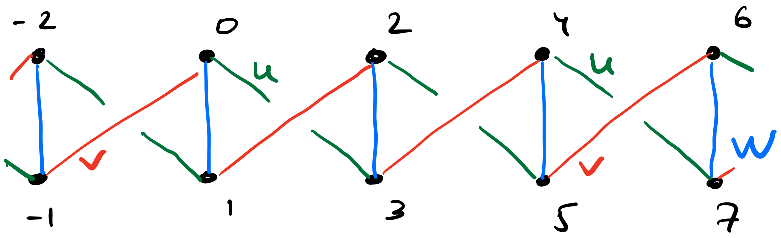
$$\mathcal{F} : \mathcal{M} \to \mathrm{Sym}_n \quad \text{smooth}$$

params

family of operators

Want: Morse theory for $\lambda_k : \mathcal{M} \to \mathbb{R}$

Example: Gener. SSH model



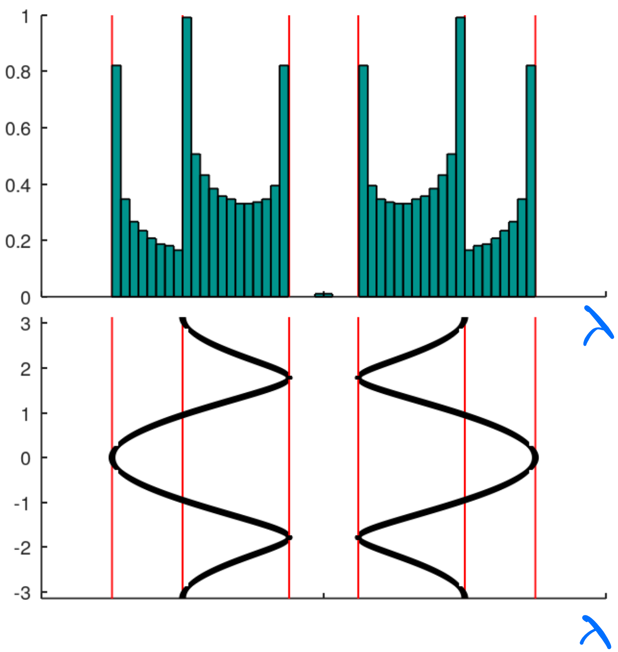
Infinite periodic graph:

$$H : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$$

$$H_{2j-1,\,2j} = H_{2j,\,2j-1} = v, \quad H_{2j,\,2j+1} = H_{2j+1,\,2j} = w, \quad H_{2j,\,2j+3} = H_{2j+3,\,2j} = u$$

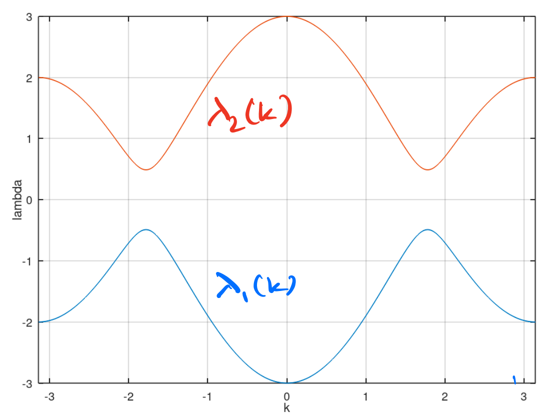
Floquet-Bloch: $\quad \mathrm{spec}(H) = \bigcup_{k\in[-\pi,\pi]} \mathrm{spec}\big(H(k)\big)$

van Hove

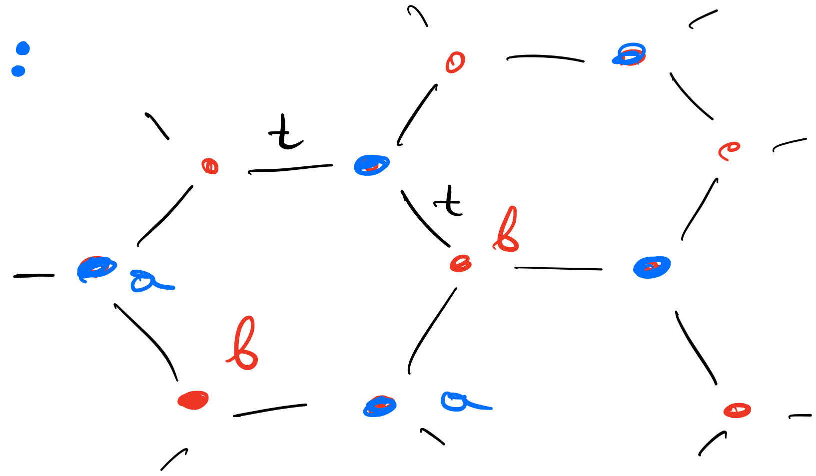


eig. density

$$H(k) = \begin{pmatrix} 0 & w+ue^{ik}+ve^{-ik} \\ w+ue^{-ik}+ve^{ik} & 0 \end{pmatrix}$$

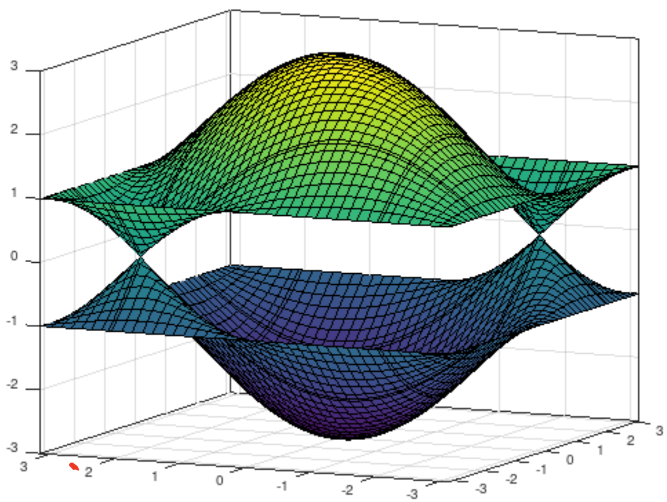


Example (Tight-binding graphene):

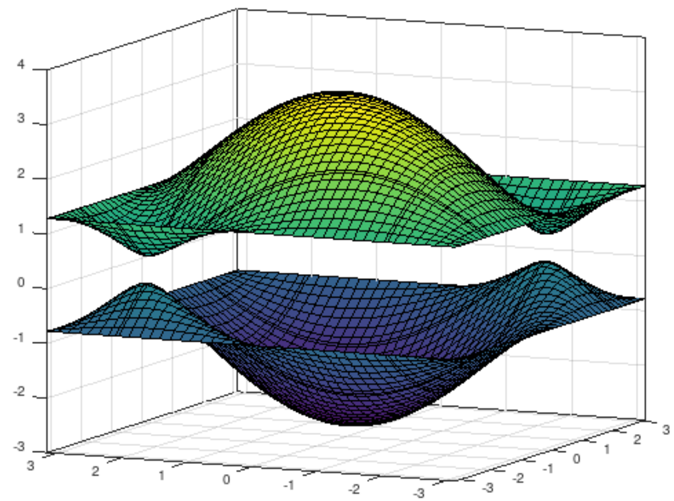


$$\mathcal{F}(\vec{k}) = \begin{pmatrix} a & -t\left(1+e^{-ik_1}+e^{-ik_2}\right) \\ -t\left(1+e^{ik_1}+e^{ik_2}\right) & b \end{pmatrix}$$

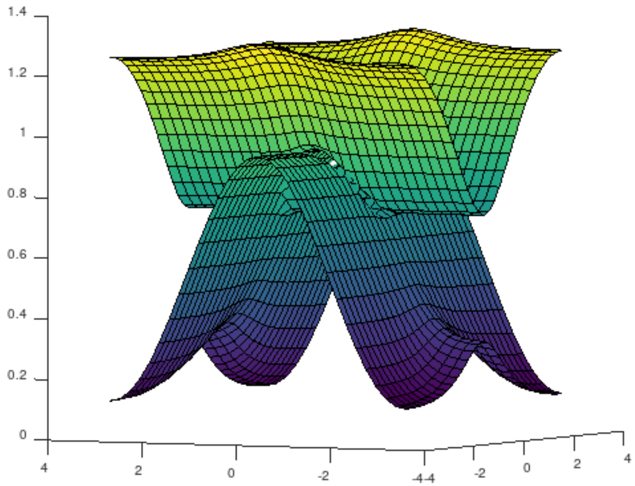
$t=1 \quad a=0 \quad b=0$

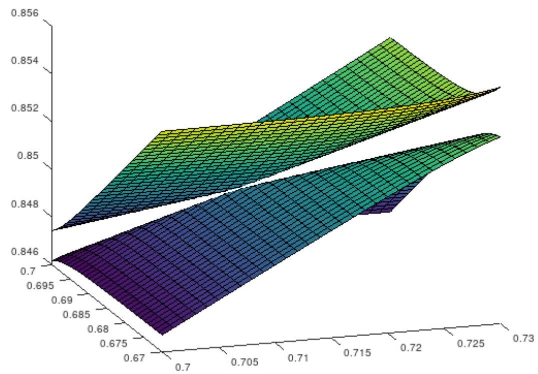


$t=1 \quad a=0.5 \quad b=0$



Motivation II: Nodal Statistics





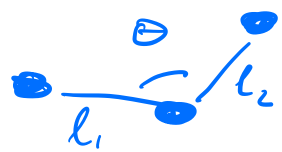
Motivation III: Minimal Spectral Partitions

Terracini, Helffer, Hoffmann-Ostenhof, ...

$\mathcal{M}$ – very complicated

Motivation IV: Quantum Chemistry

Potential Energy Surfaces (Born-Oppenheimer)

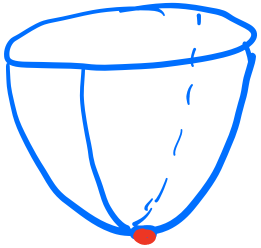


$\mathcal{F}(x)$ – electronic Schrödinger

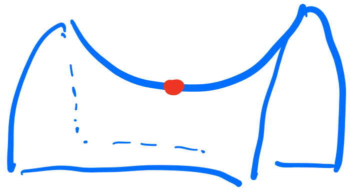
$x \in \mathcal{M}$ – molecular configurations

What is Morse theory?

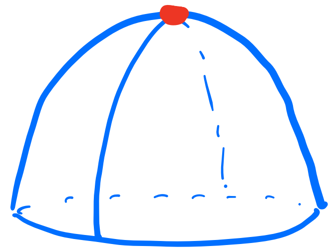
Let $F : \mathcal{M} \to \mathbb{R}$ be C^2 (If $\mathcal{M}$- surface)



C.P. $\mu = 0$



C.P. $\mu = 1$



C.P. $\mu = 2$

$$CP(F) := \{ x \in \mathcal{M} \ : \ \nabla F(x) = 0 \}$$

Morse Index $\mu(x) = \# \{ \lambda \in \text{spec}(\text{Hess}_x F) : \lambda < 0 \}$

$c_\mu := \#$ C.P. of index μ

$\beta_\mu := \operatorname{rank} H_\mu(\mathcal{M}, \mathbb{Z})$

THM (Morse Ineq.):

$\exists \, r_q \geq 0$ s.t.

$$c_0 = \beta_0 + r_0$$

$$c_1 = \beta_1 + r_1 + r_0$$

$$c_2 = \beta_2 + r_2 + r_1$$

$$\cdots$$

$$c_d = \beta_d + r_{d-1}$$

Using generating functions

$$P_F(t) := \sum_{x \in CP(F)} t^{\mu(x)} \qquad P_{\mathcal{M}} := \sum \beta_\mu t^\mu$$

THM (Morse Ineq.):

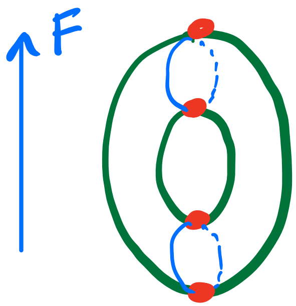
$$P_F(t) - P_{\mathcal{M}}(t) = (1+t)\, R(t)$$

where $R(t) = r_0 + r_1 t + \dots + r_{d-1} t^{d-1}, \quad r_q \geq 0$

Examples:

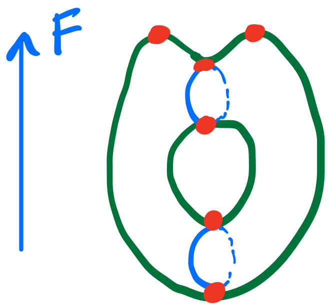
$\mathcal{M} = \mathbb{T}^2 \to P_{\mathcal{M}}(t) = (1+t)^2$

$\beta_0 = 1 \quad \beta_1 = 2 \quad \beta_2 = 1$



$c_0 = \beta_0 = 1$
$c_1 = \beta_1 = 2$
$c_2 = \beta_2 = 1$

$P_F - P_{\mathcal{M}} = 0$



$c_0 = \beta_0$
$c_1 = \beta_1 + 1$
$c_2 = \beta_2 + 1$

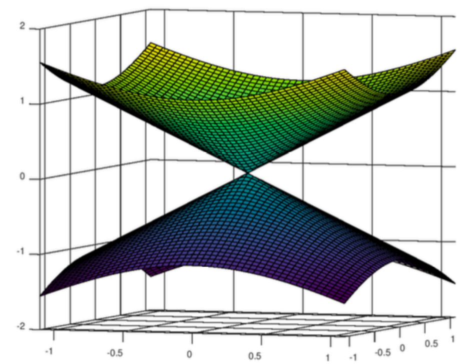
$P_F = 1 + 3t + 2t^2$

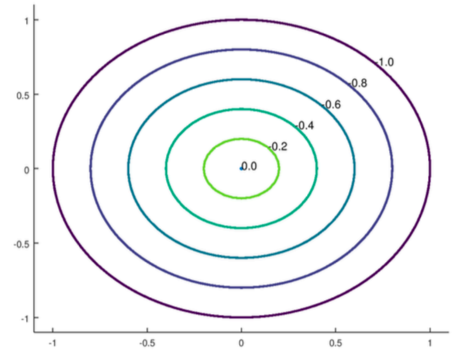
$P_F - P_{\mathcal{M}} = t + t^2$
$= (1+t)\,t$

Difficulty: Lack of smoothness of $\lambda_k(\mathcal{F}(x))$ around points of multiplicity

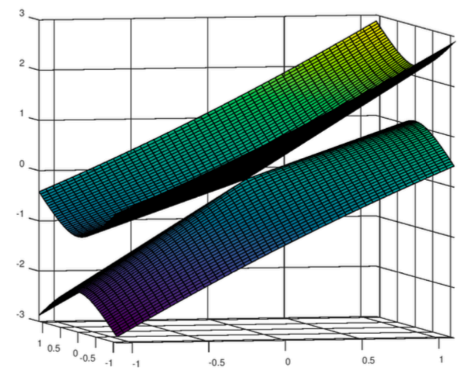
Example:

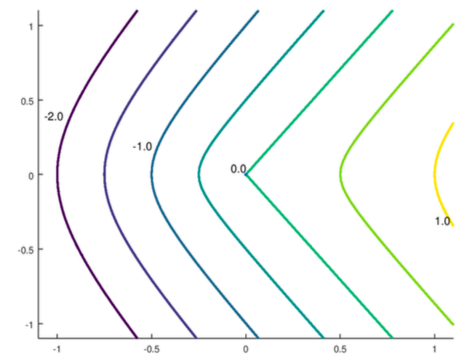
$$\mathcal{F}_1(\vec{x}) = \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix}$$





$$\mathcal{F}_2(\vec{x}) = \begin{pmatrix} x_1 & x_2 \\ x_2 & 2x_1 \end{pmatrix}$$





How to distinguish looking at $\mathcal{F}$?

Main Results

$\mathrm{Sym}_\nu^{++} :=$ positive def. matrices in Sym_ν

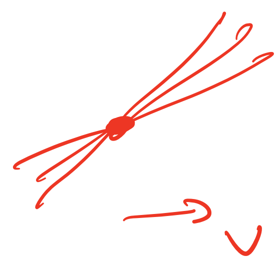
Let $x \in \mathcal{M}$, λ_k of $\mathcal{F}(x) \in \mathrm{Sym}_n$ have mult. ν

U – $n \times \nu$ matrix of eigenvectors of λ_k $\quad U: \mathbb{R}^\nu \to E_{\lambda_k}$

$\mathcal{H}_x : T_x\mathcal{M} \to \mathrm{Sym}_\nu \qquad \vec{v} \mapsto U^*\left(D_{\vec{v}}\mathcal{F}(x)\right)U$

$\nu = 1 \qquad \dot{\lambda}_k = (\psi_k, \dot{\mathcal{F}}\psi_k)$

Thm I (First derivative test):



* If $\exists B \in \mathrm{Sym}_\nu^{++}$ $\quad B \in \mathrm{Ran}\,\mathcal{H}_x$

then x is a regular point.

* If $\exists B \in \mathrm{Sym}_\nu^{++}$

$$(\mathrm{Ran}\,\mathcal{H}_x)^\perp = \mathrm{span}(B)$$

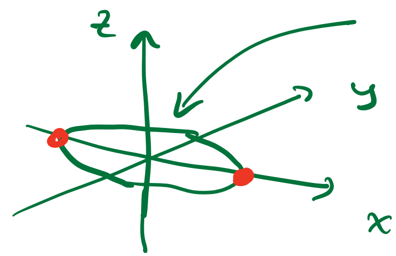
then x is a critical point.

Example: $$\tilde{F}_c(x,y,z) = \begin{pmatrix} x+z & \frac{1}{c}(x^2+y^2-1) \\ \frac{1}{c}(x^2+y^2-1) & x-z \end{pmatrix}$$

Example: $\mathcal{F}_c(x,y,z) = \begin{pmatrix} x+z & \frac{1}{c}(x^2+y^2-1) \\ \frac{1}{c}(x^2+y^2-1) & x-z \end{pmatrix}$

Look for $\nu = 2$ C.P.

$\Rightarrow \mathcal{F}_c = \lambda I \Rightarrow \{x^2+y^2=1,\ z=0\}$



multiplicity 2 submanif.

$$\frac{\partial F}{\partial x} = \begin{pmatrix} 1 & \frac{2}{c}x \\ \frac{2}{c}x & 1 \end{pmatrix} \qquad \frac{\partial F}{\partial y} = \begin{pmatrix} 0 & \frac{2}{c}y \\ \frac{2}{c}y & 0 \end{pmatrix} \qquad \frac{\partial F}{\partial z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

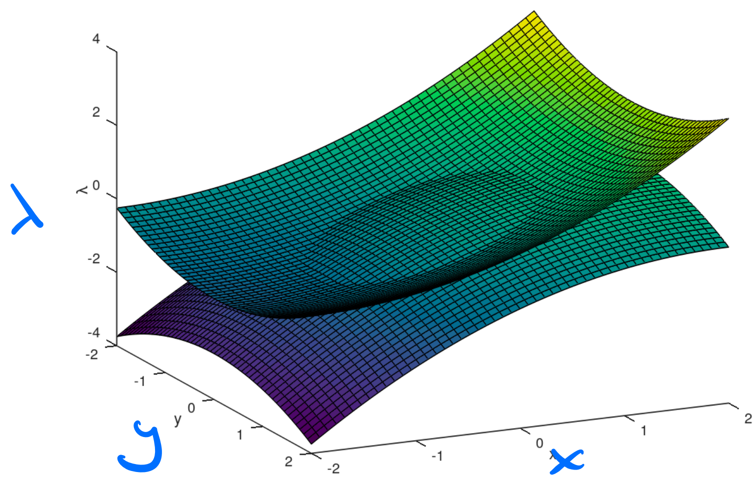
$$\dim \operatorname{span}\left\{\frac{\partial F}{\partial x}, \frac{\partial F}{\partial y}, \frac{\partial F}{\partial z}\right\} = 3$$

unless $y=0$: possible C.P.

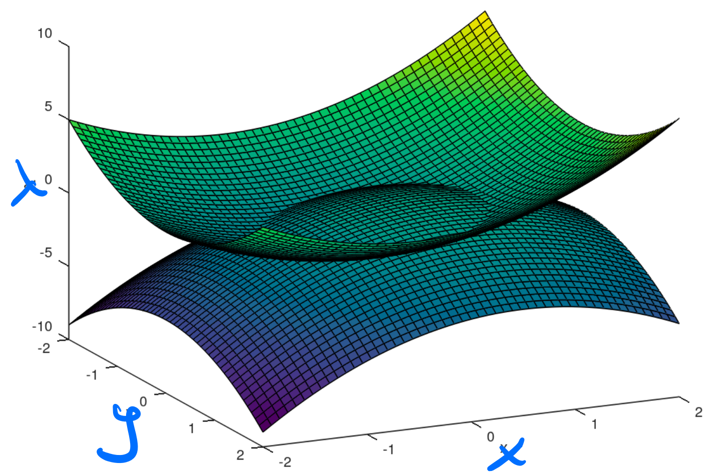
If $y=0$ $\quad (\operatorname{Ran} \mathcal{H})^{\perp} = \left\{ \begin{pmatrix} 1 & \frac{2}{c}x \\ \frac{2}{c}x & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}^{\perp}$

$x = \pm 1$ $\qquad = \begin{pmatrix} 2x/c & -1 \\ -1 & 2x/c \end{pmatrix} \in \mathrm{Sym}_2^{++}$ if $c < 2$

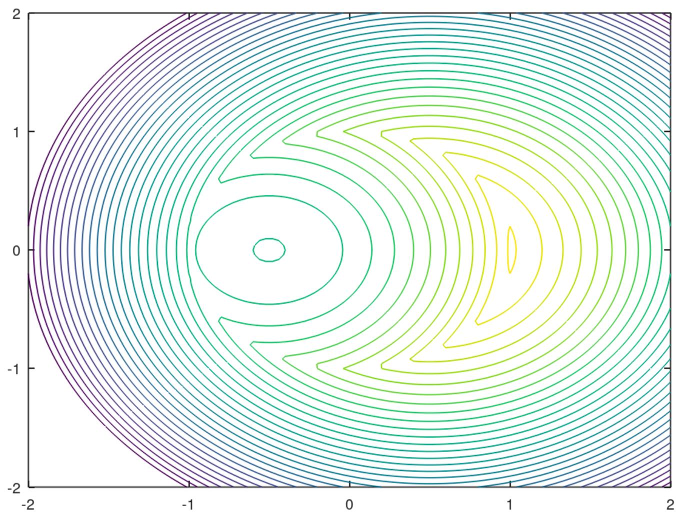
$c = 1$ $z = 0$ $c = 4$



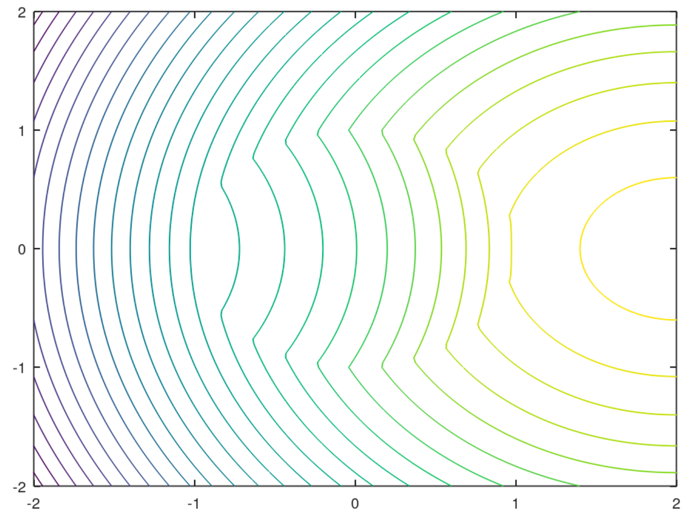
4
2
λ 0
-2
-4
λ
-2
-1
y 0
1
2
y
-2
-1
0
1
2
x



10
5
0
-5
-10
λ
-2
-1
0
1
2
y
-2
-1
0
1
2
x

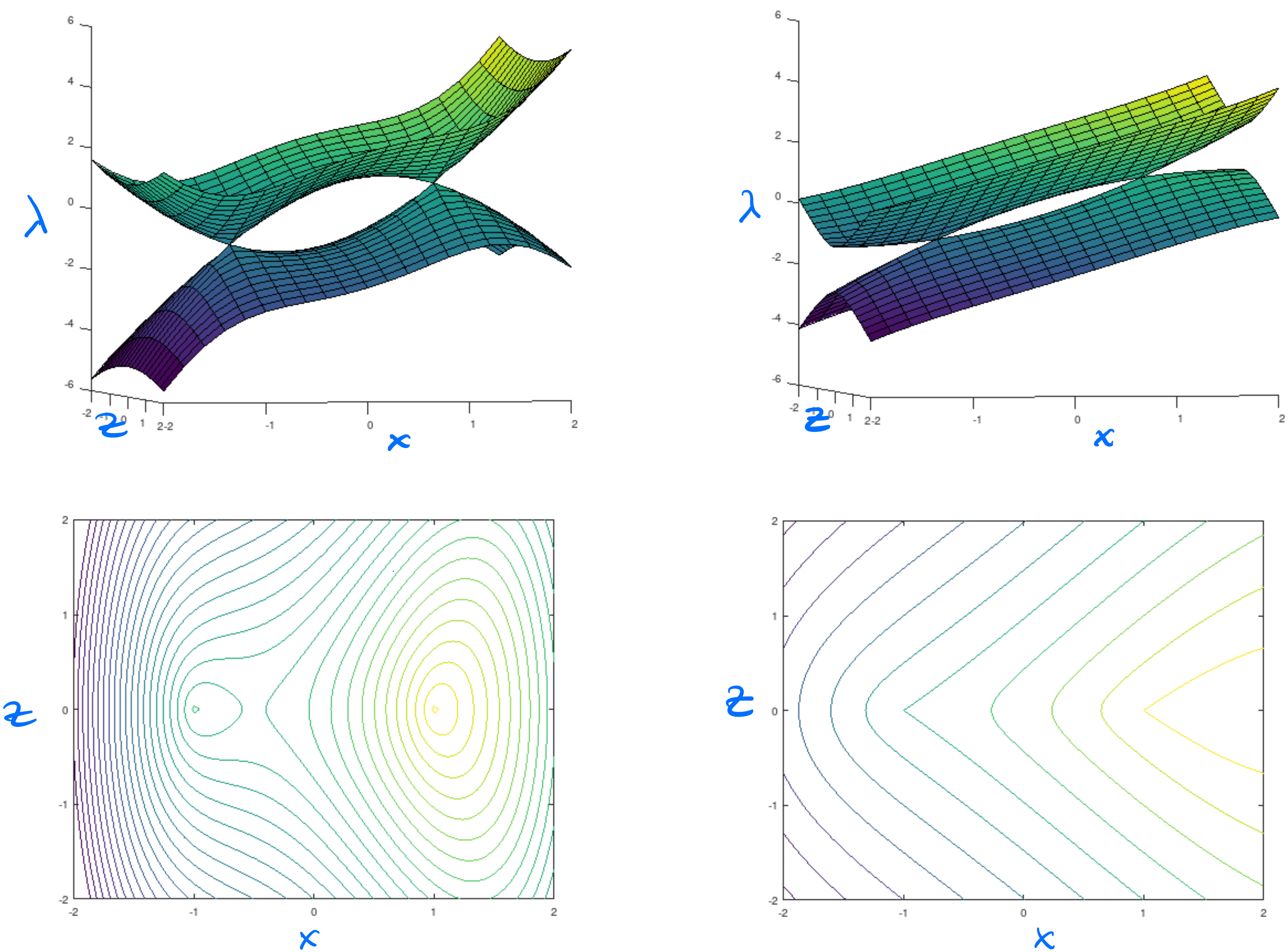


2
1
0
-1
-2
-2
-1
0
1
2



2
1
0
-1
-2
-2
-1
0
1
2

$c = 1$ $\quad$ $y = 0$ $\quad$ $c = 4$

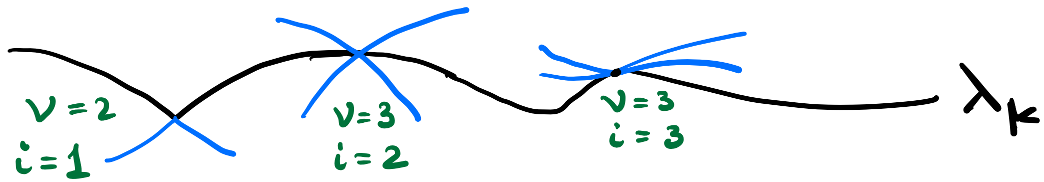


Morse Inequalities

Contribution of a Critical Point of Multiplicity

$\nu = \nu(x,k)$ = multiplicity of λ_k at x

$i = i(x,k)$ = relative index of λ_k at x

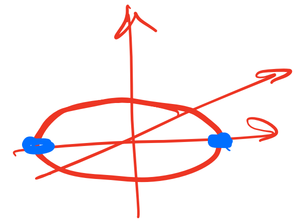


$$S(i) = \begin{cases} \frac{1}{2} i(i+1) - 1 & \text{if } \mathbb{R} \\ i^2 - 1 & \text{if } \mathbb{C} \end{cases}$$

"codimension of matrices with an i-deg. eigenvalue"

$$\operatorname{codim}_{\mathcal{M}} S_x = \mathcal{H}(\nu)$$

$$\binom{n}{k}_q := \frac{(1-q)(1-q^2)\cdots(1-q^n)}{(1-q)\cdots(1-q^k)\,(1-q)\cdots(1-q^{n-k})}$$



Thm II ("second deriv. test")

Morse inequalities remain valid with

$$P_{\mathcal{F}}(t) = \sum_{x \in C.P.} P(t;x)$$

these inequalities remain

$$P(t;x) = t^{\mu + s(i)} \begin{cases} \binom{\lfloor (\nu-1)/2 \rfloor}{(i-1)/2}_{t^4} & \mathbb{R}, \quad i \text{ odd} \\ 0 & \mathbb{R}, \quad i \text{ even } \nu \text{ odd} \\ t^{\nu - i} \binom{\nu/2 - 1}{i/2 - 1}_{t^4} & \mathbb{R}, \quad i, \nu \text{ even} \\ \binom{\nu - 1}{i - 1}_{t^2} & \mathbb{C} \end{cases}$$

$\mathbb{R}$	$\nu=2$	$\nu=3$	$\nu=4$	$\nu=5$
$i=1$	1	1	1	1
$i=2$	t^2	0	t^4	0
$i=3$		t^5	t^5	t^5+t^9
$i=4$			t^9	0
$i=5$				t^{14}

$\leftarrow$ min

max (in dim $\mathcal{H}(\nu)$)

top eig is at a min

bottom eig is at a max

* the above is for "generic" $\mathcal{F}$ only.
non-generic? generic + symmetry?
10-fold way?

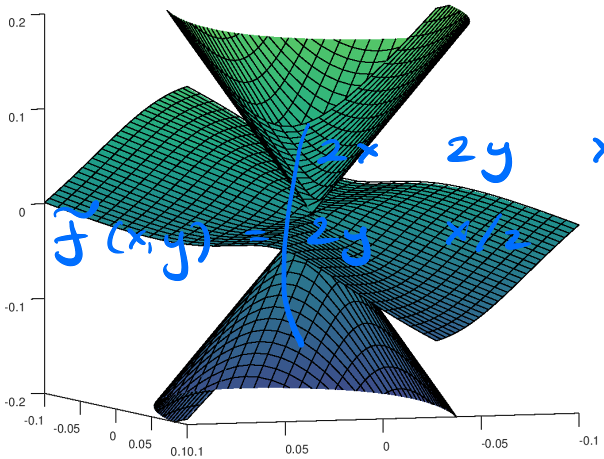
* "0" are not "completely" 0

$P(t;x)$ is the generating function of the torsion-free part of $H_r(\dots,\dots)$

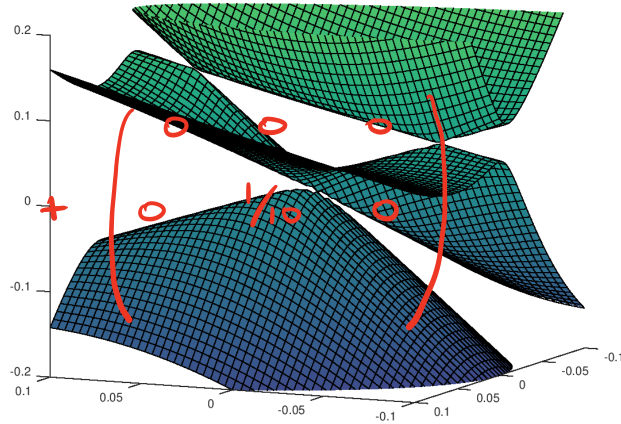
More complete info is $+\,T(s;x)$, generating function of the $\mathbb{Z}_2$ (torsion) subgroup

$\mathbb{R}$	$\nu=2$	$\nu=3$	$\nu=4$	$\nu=5$
$i=1$	1	1	1	1
$i=2$	t^2	$0+s^2$	t^4+s^2	$0+s^2+s^4$
$i=3$		t^5	t^5+s^6	$t^5+t^9+s^6+s^7$
$i=4$			t^9	$0+s^9+s^{11}$
$i=5$				t^{14}

Idea: torsion = traces of merged C.P.s



$$\tilde{J}(x,y) = \begin{pmatrix} 2x & 2y & x/1 \\ 2y & x/2 & -2 \\ & & 0 \\ & & y \\ x/10 & -2y & 2y-x \end{pmatrix}$$



$$+ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1/10 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$