UNVEILING A CRYSTALLINE TOPOLOGICAL INSULATOR IN A WEYL SEMIMETAL WITH TIME-REVERSAL SYMMETRY

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IN COLLABORATION WITH:

- Armando Aligia, CAB-Bariloche, Argentina.
- Thanks to Ruben Weht (CAC-Buenos Aires, Argentina) for many discussions.

PAUL ADRIEN MAURICE DIRAC

(1902-1984)

- I think it is a peculiarity of myself that I like to play about with equations, just looking for beautiful mathematical relations which maybe don't have any physical meaning at all. Sometimes they do.

- It seems that if one is working from the point of view of getting beauty in one's equations, and if one has really a sound insight, one is on a sure line of progress.

HERMANN KLAUS HUGO WEYL

(1885-1955)

- My work always tried to unite the truth with the beautiful, but when I had to choose one or the other, I usually chose the beautiful.

TOPOLOGY IN COND-MAT

Relativistic
quantum mechanics

Symmetry

Materials
Science

DIRAC AND WEYL EQUATIONS

DIRAC EQUATION

Quantum Mechanics & Relativity.

Masive Spin 1/2 particles

$$\mathbf{p} = -i\hbar\nabla = (p_x, p_y, p_z)$$

$$i\hbar\frac{\partial}{\partial t}\psi = \left(c\boldsymbol{\alpha}\cdot\mathbf{p} + \beta mc^2\right)\psi;$$

Spinor with 4 entries

$$\boldsymbol{\alpha} = (\tau_3\otimes\sigma_1, \tau_3\otimes\sigma_2, \tau_3\otimes\sigma_3)$$

$$\beta = -\tau_1\otimes 1$$

Pauli matrices

WEYL EQUATION

Masless Spin 1/2 particles

$$i\hbar\frac{\partial}{\partial t}\chi_{\pm} = \pm c\boldsymbol{\sigma}\cdot\mathbf{p}\chi_{\pm}.$$

Spinors with
2 entries

$$\psi = \begin{bmatrix}\chi_{+}\\ \chi_{-}\end{bmatrix}$$

True Weyl fermions: Neutrinos? No because masive

DIRAC AND WEYL EQUATIONS IN CONDENSED MATTER

Quantum non-relativistic spin 1/2 many particles

Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \mathcal{H}|\Psi\rangle$$

$$\mathcal{H} \to \mathcal{H}_0 + \mathcal{H}_{int}$$

Bloch theorem

$$\mathcal{H}_0|\phi_{n,\mathbf{k}}\rangle = E_n(\mathbf{k})|\phi_{n,\mathbf{k}}\rangle$$

band index

EFFECTIVE HAMILTONIAN FOR TWO ADJACENT BANDS

$E_+(\mathbf{k}) \ \sim \ E_-(\mathbf{k}), \quad \mathbf{k} \sim \mathbf{k}_0$ No assumption on symmetries

$|u_\mathbf{k}\rangle, \ \ |v_\mathbf{k}\rangle$ Orthogonal Bloch states consistent with symmetries of $\mathcal{H}_0$

$$\mathcal{H}_{eff} = \sum_\mathbf{k} \psi^\dagger_\mathbf{k} H(\mathbf{k}) \psi_\mathbf{k}$$

$$H(\mathbf{k}) = \begin{pmatrix} \langle u_\mathbf{k}|\mathcal{H}_0|u_\mathbf{k}\rangle & \langle u_\mathbf{k}|\mathcal{H}_0|v_\mathbf{k}\rangle \\ \langle v_\mathbf{k}|\mathcal{H}_0|u_\mathbf{k}\rangle & \langle v_\mathbf{k}|\mathcal{H}_0|v_\mathbf{k}\rangle \end{pmatrix} \equiv f(\mathbf{k})1_2 + \sum_{j=1}^{3} g_j(\mathbf{k})\sigma_j$$

BAND TOUCHING IN 3D

Eigenenergies of $\mathcal{H}_{eff}$

$$E_{\pm} = f(\mathbf{k}) \pm \sqrt{\sum_{j=1}^{3} g_j^2(\mathbf{k})}.$$

Bands touch at $\mathbf{k} = \mathbf{k}_0$ if: $g_j(\mathbf{k}_0) = 0$ (No symmetry)

In 3D: 3 eqs and 3 components

Effective Weyl Hamiltonian (No fine-tuning):

$$H(\mathbf{k}) = E_{\mathbf{k}_0} + \hbar \mathbf{v}_0 \cdot (\mathbf{k} - \mathbf{k}_0) 1_2 + \sum_{j=1}^{3} \hbar \mathbf{v}_j \cdot (\mathbf{k} - \mathbf{k}_0) \sigma_j .$$

ROLE OF T-REVERSAL SYMMETRY

Appropriate basis for $\mathcal{H}_{eff}$

$u_{1\mathbf{k}}(\mathbf{r})|\uparrow\rangle + u_{2\mathbf{k}}(\mathbf{r})|\downarrow\rangle \qquad -u^*_{1\mathbf{k}}(-\mathbf{r})|\downarrow\rangle + u^*_{2\mathbf{k}}(-\mathbf{r})|\uparrow\rangle \qquad v_{1\mathbf{k}}(\mathbf{r})|\uparrow\rangle + v_{2\mathbf{k}}(\mathbf{r})|\downarrow\rangle \qquad -v^*_{1\mathbf{k}}(-\mathbf{r})|\downarrow\rangle + v^*_{2\mathbf{k}}(-\mathbf{r})|\uparrow\rangle$

$$H(\mathbf{k}) = f(\mathbf{k})1_4 + \sum_{j=1}^{5} g_j(\mathbf{k})\Gamma_j$$

$$\Gamma_1 = \tau_3 \otimes 1,\ \Gamma_2 = \tau_1 \otimes 1,\ \Gamma_3 = \tau_2 \otimes \sigma_3,\ \Gamma_4 = \tau_2 \otimes \sigma_1,\ \Gamma_5 = \tau_2 \otimes \sigma_2$$

Eigenenergies: $E_\pm = f(\mathbf{k}) \pm \sqrt{\sum_{j=1}^{5} g_j^2(\mathbf{k})}$,

Bands touch at $\mathbf{k} = \mathbf{k}_0$ if: $g_j(\mathbf{k}_0) = 0$

In 3D: 5 eqs and 3 components → fine-tuning

WEYL SEMIMETALS

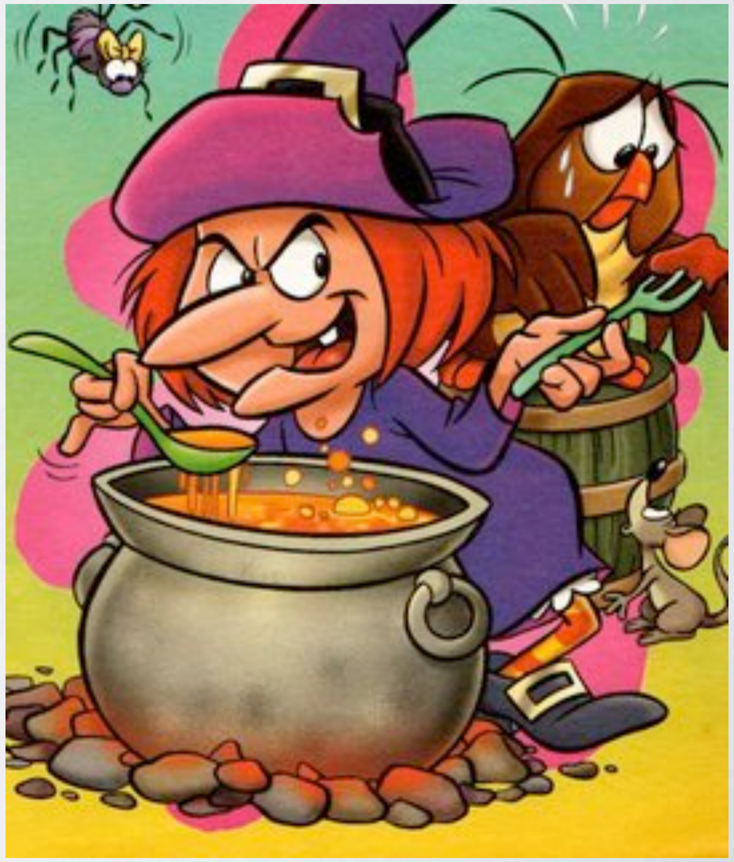
SYSTEMS WITH STABLE BAND TOUCHING IN 3D : WEYL NODES

INGREDIENTS

*No time-reversal symmetry

or

*No inversion symmetry



TOPOLOGICAL PROPERTIES

Weyl nodes exist in pairs
(no-go Nielsen-Nynomiya theorem)

Paradigmatic case: 2 Weyl nodes at $\mathbf{k}_{\pm}$

$$H_{\pm} = \pm v_F \left(p_x \sigma_1 + p_y \sigma_2 + p_z \sigma_3 \right)$$

$$\mathbf{p} = \hbar(\mathbf{k} - \mathbf{k}_{\pm})$$

Same spectrum for both nodes: $E(p) = v_F|\mathbf{p}|$

But different chiralities: ± 1 for $H_\pm$.

More generally:

$$
\begin{aligned}
\boldsymbol{A}_n(\boldsymbol{k}) &= -i\langle \boldsymbol{k}n|\nabla_{\boldsymbol{k}}|\boldsymbol{k}n\rangle, \quad \text{Berry curvature} \\
\boldsymbol{B}_n(\boldsymbol{k}) &= \nabla_{\boldsymbol{k}} \times \boldsymbol{A}_n(\boldsymbol{k}), \\
\rho_n(\boldsymbol{k}) &= \frac{1}{2\pi}\nabla_{\boldsymbol{k}} \cdot \boldsymbol{B}_n(\boldsymbol{k})
\end{aligned}
$$

Weyl nodes

$$\rho_n(\boldsymbol{k}) = \sum_l q_{ln}\delta(\boldsymbol{k}-\boldsymbol{k}_{ln})$$

Monopole charge ± 1

Fermi arcs in slab configurations

Wan X, Turner AM, Vishwanath A, Savrasov SY. 2011. *Physical Review B* 83:205101(9)

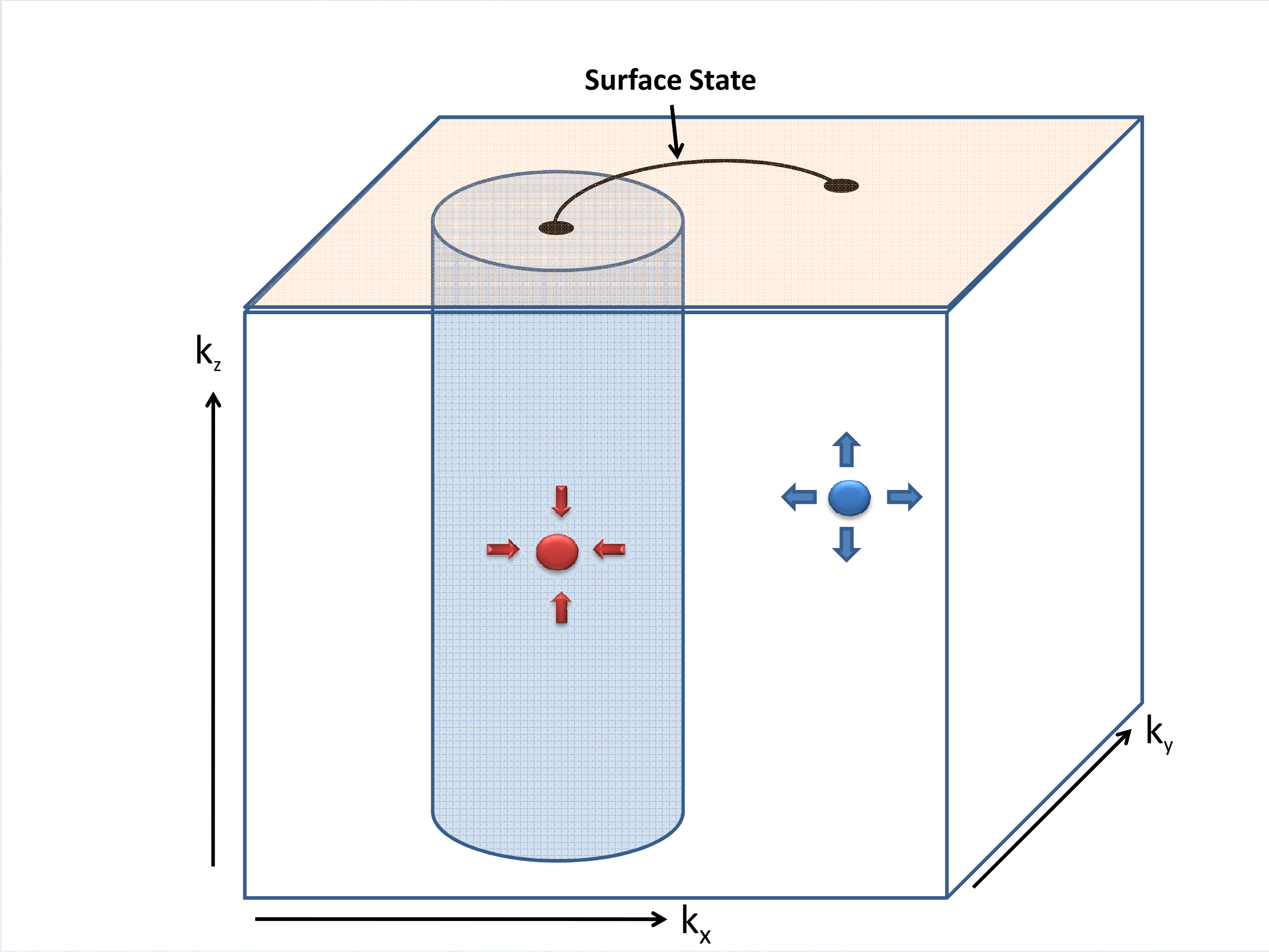


FIG. 6: Illustration of surface states arising from bulk Dirac points. For simplicity, only a pair of Dirac points with opposite chirality are shown. The imaginary cylinder in momentum space has unit Chern number, due to the Berry monopole at the Dirac point. Hence a surface state must arise, as shown schematically in the same plot. When the Fermi energy is at the Dirac point, a Fermi arc is present which connects the surface momenta of the projected bulk Dirac points of opposite chirality.

PROPOSED WEYL SEMIMETALS

Electronic Structure of Pyrochlore Iridates: From Topological Dirac Metal to Mott Insulator

Wan X, Turner AM, Vishwanath A, Savrasov SY. 2011. *Physical Review B* 83:205101(9)

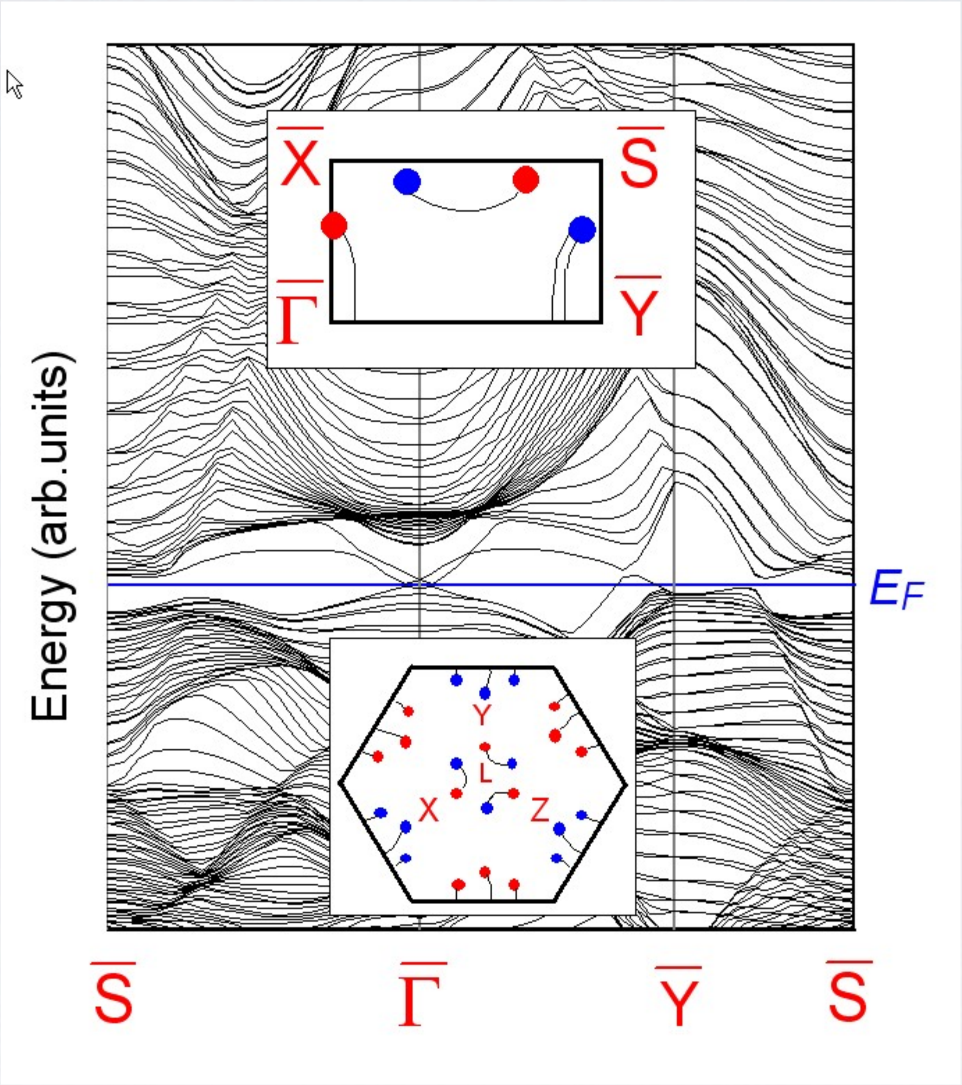


FIG. 7: Calculated surface energy bands corresponding to (110) surface of the pyrochlore iridate Y2Ir2O7. A tight binding approximation has been used to simulate the bulk band structure with 3D Dirac point as found by our LSDA+U+SO calculation. The plot corresponds to diagonalizing 128 atoms slab with two surfaces. The top inset shows the deduced Fermi arcs connecting projected bulk Dirac points of opposite chirality. The bottom inset shows a sketch how these Fermi arcs are expected to behave for the (111) surface.

Weyl Semimetal in a Topological Insulator Multilayer

A.A. Burkov[1,2] and Leon Balents[2]

PRL 107, 127205 (2011)

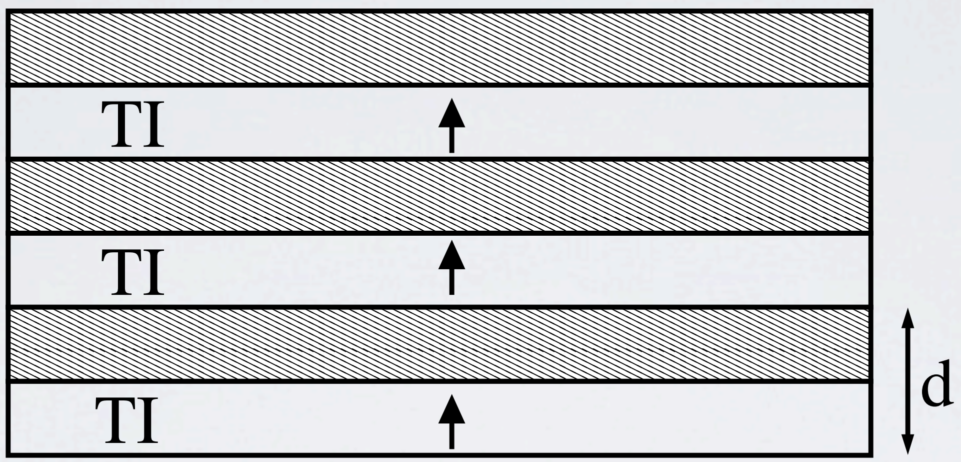


FIG. 1. Schematic drawing of the proposed multilayer structure. Unhashed layers are the TI layers, while hashed layers are the ordinary insulator spacers. Arrow in each TI layer shows the magnetization direction. Only three periods of the superlattice are shown in the figure, 20-30 unit cells can perhaps be grown realistically.

$$H = \sum_{\mathbf{k}_\perp, ij} \left[v_F \tau^z (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k}_\perp \delta_{i,j} + m\sigma^z \delta_{i,j} + \Delta_S \tau^x \delta_{i,j} + \frac{1}{2} \Delta_D \tau^+ \delta_{j,i+1} + \frac{1}{2} \Delta_D \tau^- \delta_{j,i-1} \right] c^\dagger_{\mathbf{k}_\perp i} c_{\mathbf{k}_\perp j}. \quad (2)$$

Helical Fermi arcs and surface states in time-reversal invariant Weyl semimetals

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(Dated: July 22, 2013)

Weyl semimetals are gapless three-dimensional topological materials where two bands touch at even number of points in the Brillouin zone. In this work we study a zincblende lattice model realizing a time-reversal invariant Weyl semimetal. The bulk dynamics is decribed by twelve helical Weyl nodes. Surface states form a peculiar quasi two-dimensional helical metal fundamentally different from the Dirac form typical for topological insulators. Allowed direction of velocity and spin of low-energy surface excitations are locked to the cubic symmetry axes. The studied system illustrates general properties of surface states in systems with common crystal symmetries.

PACS numbers: 03.65.Vf, 73.20.At, 73.20.-r

$$H = -\sum_{\langle i,j\rangle}(t\, c_i^\dagger c_j + \mathrm{h.c}) + \sum_i E_i\, c_i^\dagger c_i$$

$$+ i\lambda \sum_{\langle\langle i,j\rangle\rangle} (c_i^\dagger \mathbf{e}_{ij} \cdot \mathbf{s}\, c_j - \mathrm{h.c}).$$

PRB 87, 245112 (2013)

Chern semimetal and Quantized Anomalous Hall Effect in $HgCr_2Se_4$

Gang Xu, Hongming Weng, Zhijun Wang, Xi Dai, Zhong Fang
Beijing National Laboratory for Condensed Matter Physics,
and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China;

PRL 107, 186806 (2011)

Topological electronic structure and Weyl semimetal in the $TlBiSe_2$ class of semiconductors

Bahadur Singh[1], Ashutosh Sharma[1], H. Lin[2], M.Z. Hasan[3,4], R. Prasad[1] and A. Bansil[2]
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[3]*Joseph Henry Laboratory, Department of Physics,*
Princeton University, Princeton, New Jersey 08544, USA
[4]*Princeton Center for Complex Materials, Princeton University, Princeton, New Jersey 08544, USA*

PRB 86, 115208 (2012)

Weyl semimetals from noncentrosymmetric topological insulators

Jianpeng Liu[1] and David Vanderbilt[1]
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PRB 90, 155316 (2014)

Weyl Node and Spin Texture in Trigonal Tellurium and Selenium

Motoaki Hirayama,[1,2,3] Ryo Okugawa,[2] Shoji Ishibashi,[1] Shuichi Murakami,[2,3] and Takashi Miyake[1]
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arXiv:1409.7517.

Theoretical Discovery/Prediction: Weyl Semimetal states in the TaAs material (TaAs, NbAs, NbP, TaP) class

Shin-Ming Huang*,[1,2] Su-Yang Xu*,[3,†] Ilya Belopolski*,[3] Chi-Cheng Lee,[1,2]
Guoqing Chang,[1,2] BaoKai Wang,[1,2,4] Nasser Alidoust,[3] Guang Bian,[3]
Madhab Neupane,[3] Arun Bansil,[4] Hsin Lin,[1,2,‡] and M. Zahid Hasan[3,§]

Nature Comm 6, 7373 (2015)

PHYSICAL REVIEW X **5,** 011029 (2015)

Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides

Hongming Weng,[1,2,*] Chen Fang,[3] Zhong Fang,[1,2] B. Andrei Bernevig,[4] and Xi Dai[1,2]
[1]*Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
[2]*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*
[3]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
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(Received 12 January 2015; published 17 March 2015)

Based on first-principle calculations, we show that a family of nonmagnetic materials including TaAs, TaP, NbAs, and NbP are Weyl semimetals (WSM) without inversion centers. We find twelve pairs of Weyl points in the whole Brillouin zone (BZ) for each of them. In the absence of spin-orbit coupling (SOC), band inversions in mirror-invariant planes lead to gapless nodal rings in the energy-momentum dispersion. The strong SOC in these materials then opens full gaps in the mirror planes, generating nonzero mirror Chern numbers and Weyl points off the mirror planes. The resulting surface-state Fermi arc structures on both (001) and (100) surfaces are also obtained, and they show interesting shapes, pointing to fascinating playgrounds for future experimental studies.

EXPERIMENTAL EVIDENCE

Phys. Rev. X 5, 031013 (2015)

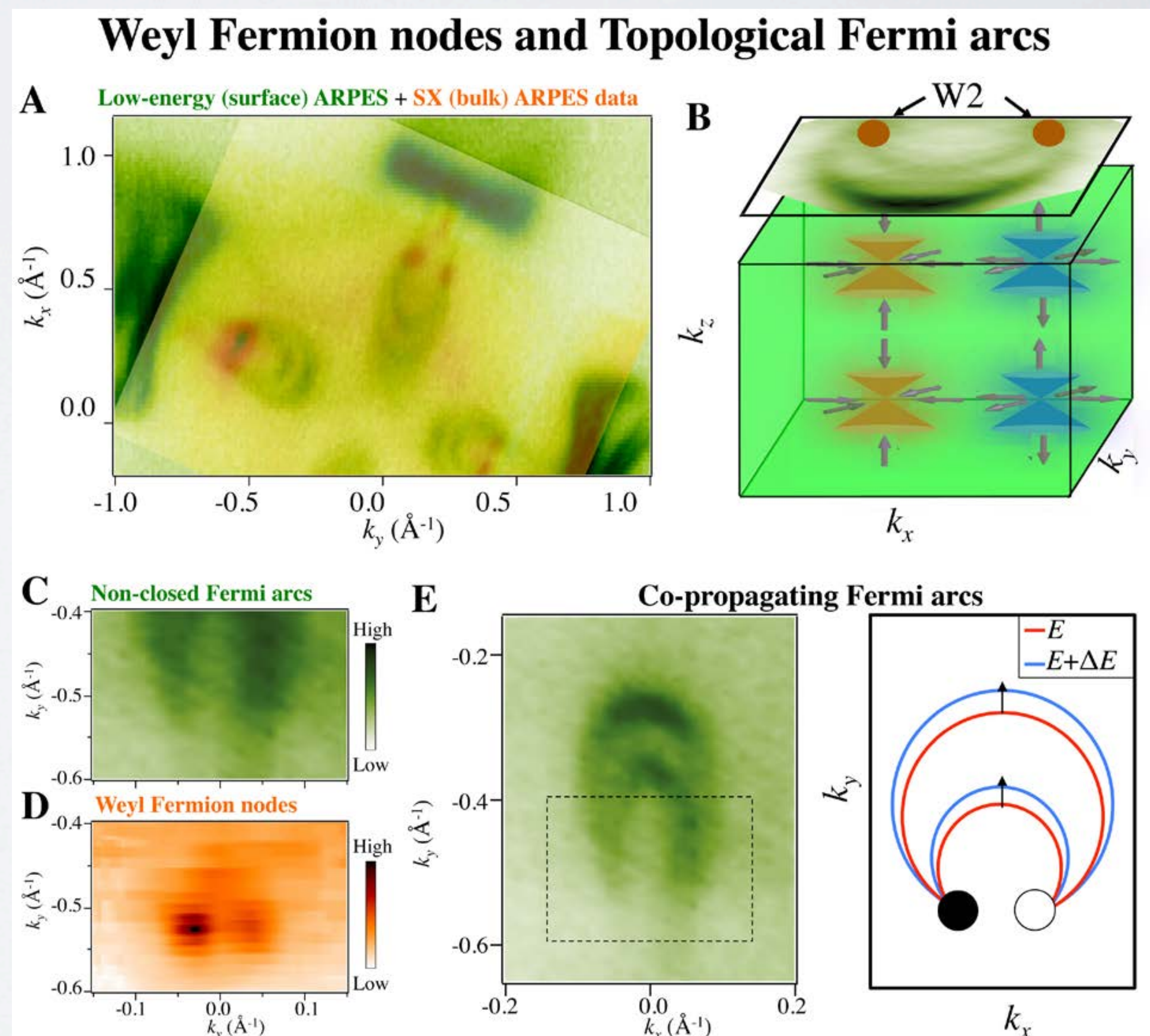
Experimental discovery of Weyl semimetal TaAs

B. Q. Lv[1,§], H. M. Weng[1,2,§], B. B. Fu[1], X. P. Wang[2,3,1], H. Miao[1], J. Ma[1], P. Richard[1,2], X. C. Huang[1], L. X. Zhao[1], G. F. Chen[1,2], Z. Fang[1,2], X. Dai[1,2], T. Qian[1,*], and H. Ding[1,2,*]

Discovery of a Weyl Fermion Semimetal and Topological Fermi Arcs

Authors: Su-Yang Xu†,[1, 2] Ilya Belopolski†,[1] Nasser Alidoust†,[1, 2] Madhab Neupane†,[1, 3] Guang Bian,[1] Chenglong Zhang,[4] Raman Sankar,[5] Guoqing Chang,[6, 7] Zhujun Yuan,[4] Chi-Cheng Lee,[6, 7] Shin-Ming Huang,[6, 7] Hao Zheng,[1] Jie Ma,[8] Daniel S. Sanchez,[1] BaoKai Wang,[6, 7, 9] Arun Bansil,[9] Fangcheng Chou,[5] Pavel P. Shibayev,[1,10] Hsin Lin,[6, 7] Shuang Jia,[4, 11] and M. Zahid Hasan*[1, 2]

Science 2015



Fermi surface interconnectivity and topology in Weyl fermion semimetals TaAs, TaP, NbAs, and NbP

Chi-Cheng Lee,[1,2] Su-Yang Xu,[3] Shin-Ming Huang,[1,2] Daniel S. Sanchez,[3] Ilya Belopolski,[3] Guoqing Chang,[1,2] Guang Bian,[3] Nasser Alidoust,[3] Hao Zheng,[3] Madhab Neupane,[3,4] Baokai Wang,[1,2,5] Arun Bansil,[5] M. Zahid Hasan,[3,6] and Hsin Lin[1,2]

PRB 92, 235104 (2015)

Unoccupied electronic structure and signatures of topological Fermi arcs in the Weyl semimetal candidate $Mo_xW_{1-x}Te_2$

arXiv:1512.09099

Ilya Belopolski*,[1,†] Su-Yang Xu*,[1] Yukiaki Ishida*,[2] Xingchen Pan*,[3] Peng Yu*,[4] Daniel S. Sanchez,[1] Madhab Neupane,[5] Nasser Alidoust,[1] Guoqing Chang,[6,7] Tay-Rong Chang,[8] Yun Wu,[9] Guang Bian,[1] Hao Zheng,[1] Shin-Ming Huang,[6,7] Chi-Cheng Lee,[6,7] Daixiang Mou,[9] Lunan Huang,[9] You Song,[10] Baigeng Wang,[3] Guanghou Wang,[3] Yao-Wen Yeh,[11] Nan Yao,[11] Julien Rault,[12] Patrick Lefevre,[12] François Bertran,[12] Horng-Tay Jeng,[8,13] Takeshi Kondo,[2] Adam Kaminski,[9] Hsin Lin,[6,7] Zheng Liu,[4,14,15,‡] Fengqi Song,[3,§] Shik Shin,[2] and M. Zahid Hasan[1,11,¶]

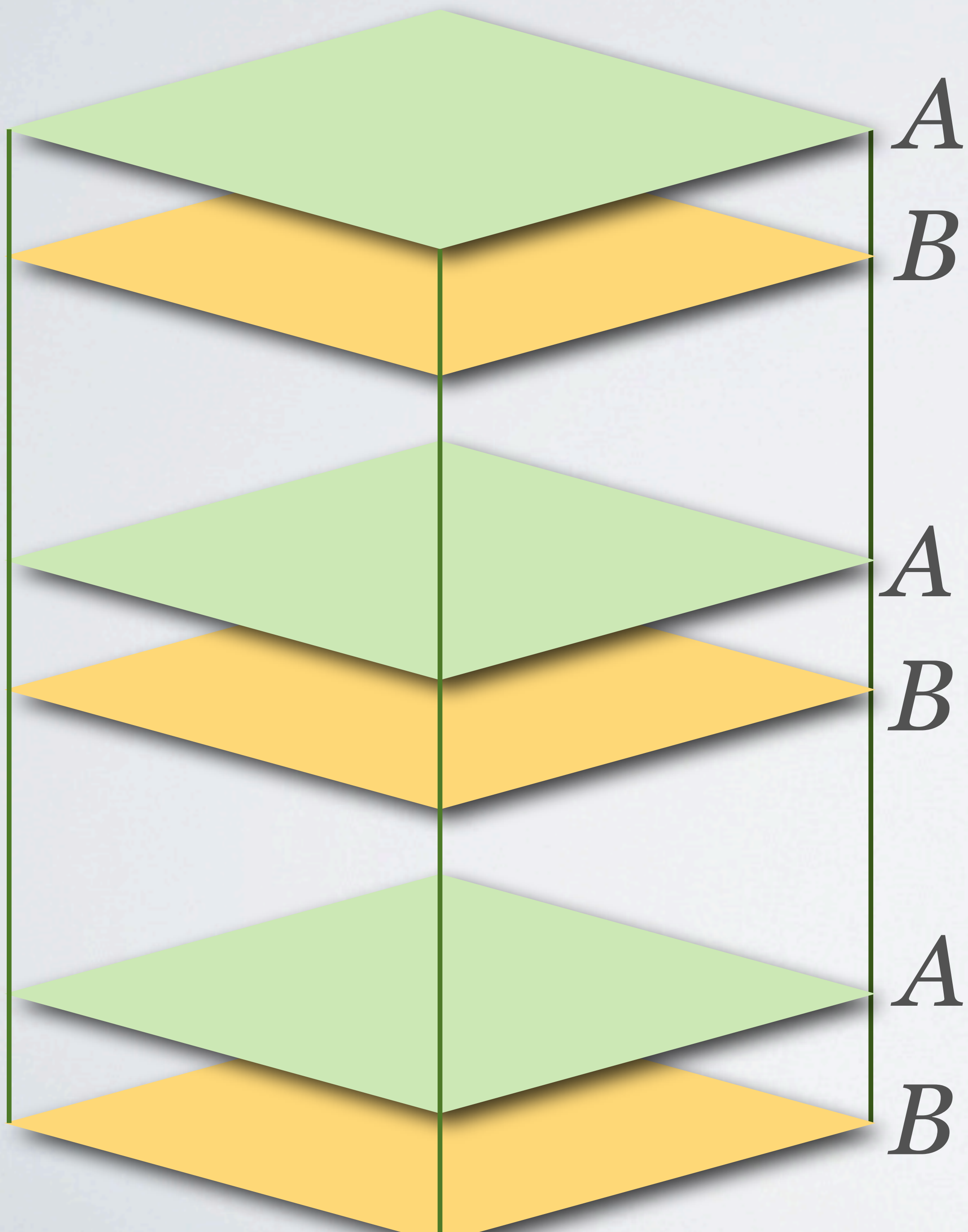
OUR PROPOSAL

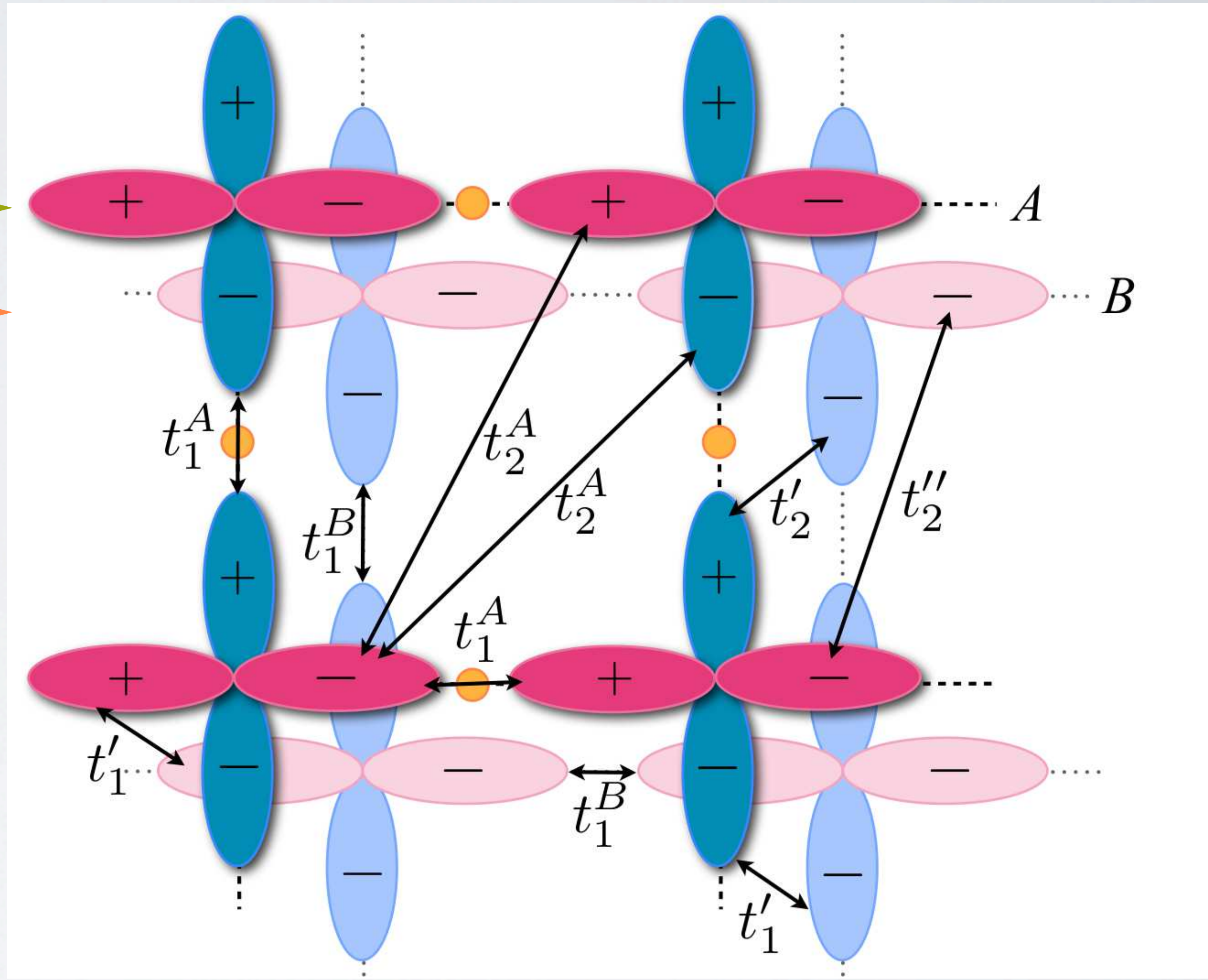
Unveiling a crystalline topological insulator in a Weyl semimetal with time-reversal symmetry

Liliana Arrachea[1] and Armando A. Aligia[2]

PRB 90, 125101 (2014)

Generalization of a model for crystalline topological insulators. L. Fu Phys. Rev. Lett. **106**, 106802 (2011)





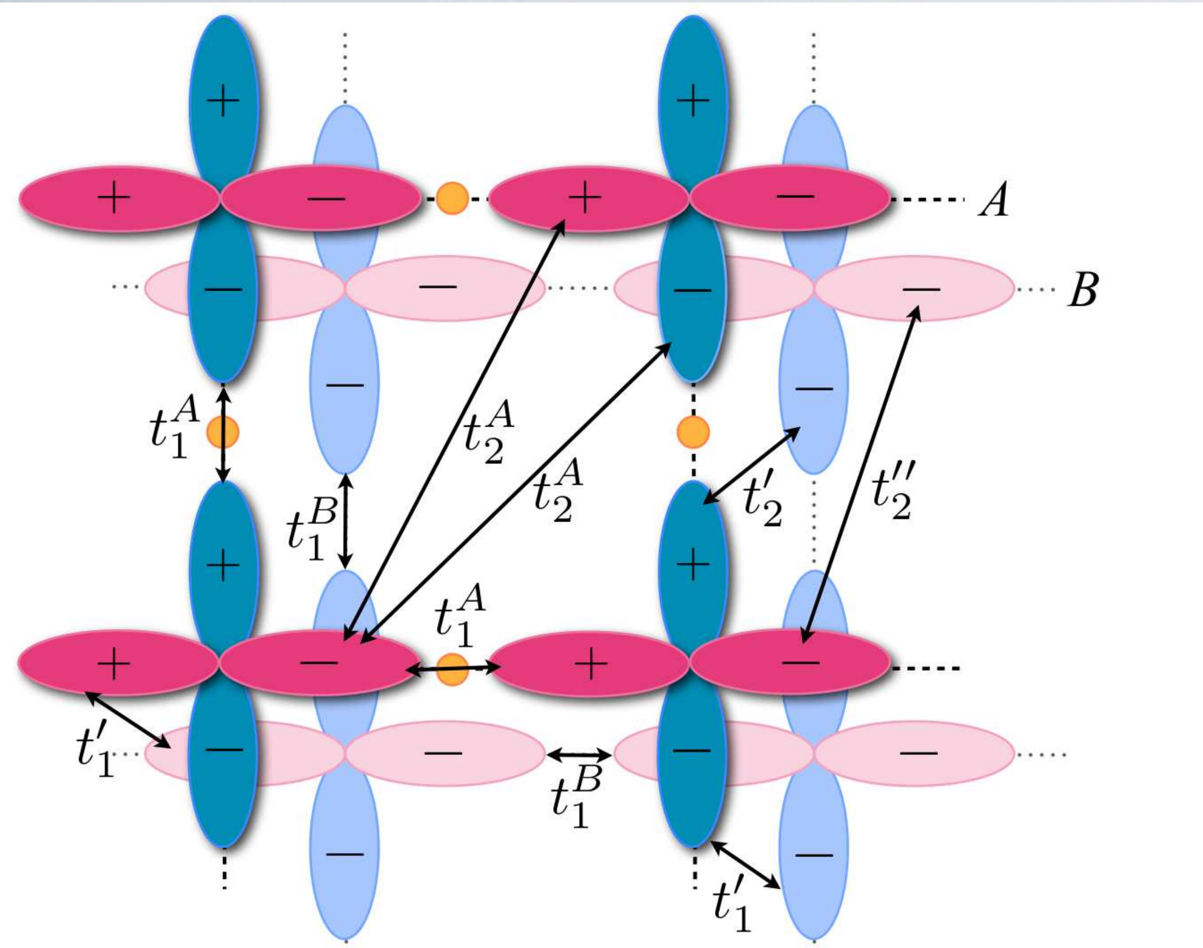
MODEL

$$H = \sum_l \left(H_l^A + H_l^B + H_l^{AB} \right) .$$

$$H_l^a = \sum_{i,j} \sum_{\alpha,\beta} c^\dagger_{a,\alpha}(\mathbf{r}_i, l) t^a_{\alpha,\beta}(\mathbf{r}_i - \mathbf{r}_j) c_{a,\beta}(\mathbf{r}_j, l), \ a = A, B$$

orbitals d_{xz} d_{yz}
or p_x and p_y

$$H_l^{AB} = \sum_{i,j} \sum_{\alpha,\beta} t'_{\alpha,\beta}(\mathbf{r}_i - \mathbf{r}_j) \left[c^\dagger_{A,\alpha}(\mathbf{r}_i, l) c_{B,\beta}(\mathbf{r}_j, l) + H.c. \right]$$
$$+ t'_z \sum_i \sum_\alpha \left[c^\dagger_{A,\alpha}(\mathbf{r}_i, l) c^\dagger_{B,\alpha}(\mathbf{r}_i, l+1) + H.c. \right] . \quad (2)$$



$$H^{AB}(\mathbf{k}) = (t_1' + t_z' e^{ik_z}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} +$$
$$2 \begin{pmatrix} t_2' \cos k_x + t_2'' \cos k_y & 0 \\ 0 & t_2' \cos k_y + t_2'' \cos k_x \end{pmatrix}$$

$$H(\mathbf{k}) = \begin{pmatrix} H^A(\mathbf{k}) & H^{AB}(\mathbf{k}) \\ H^{AB}(\mathbf{k})^\dagger & H^B(\mathbf{k}) \end{pmatrix}$$

$$H^a(\mathbf{k}) = 2t_1^a \begin{pmatrix} \cos k_x & 0 \\ 0 & \cos k_y \end{pmatrix} +$$
$$2t_2^a \begin{pmatrix} \cos k_x \cos k_y & \sin k_x \sin k_y \\ \sin k_x \sin k_y & \cos k_x \cos k_y \end{pmatrix}$$

PHASES AND SPECTRAL PROPERTIES

NORMAL INSULATOR

Gapped spectrum for bulk and surface states

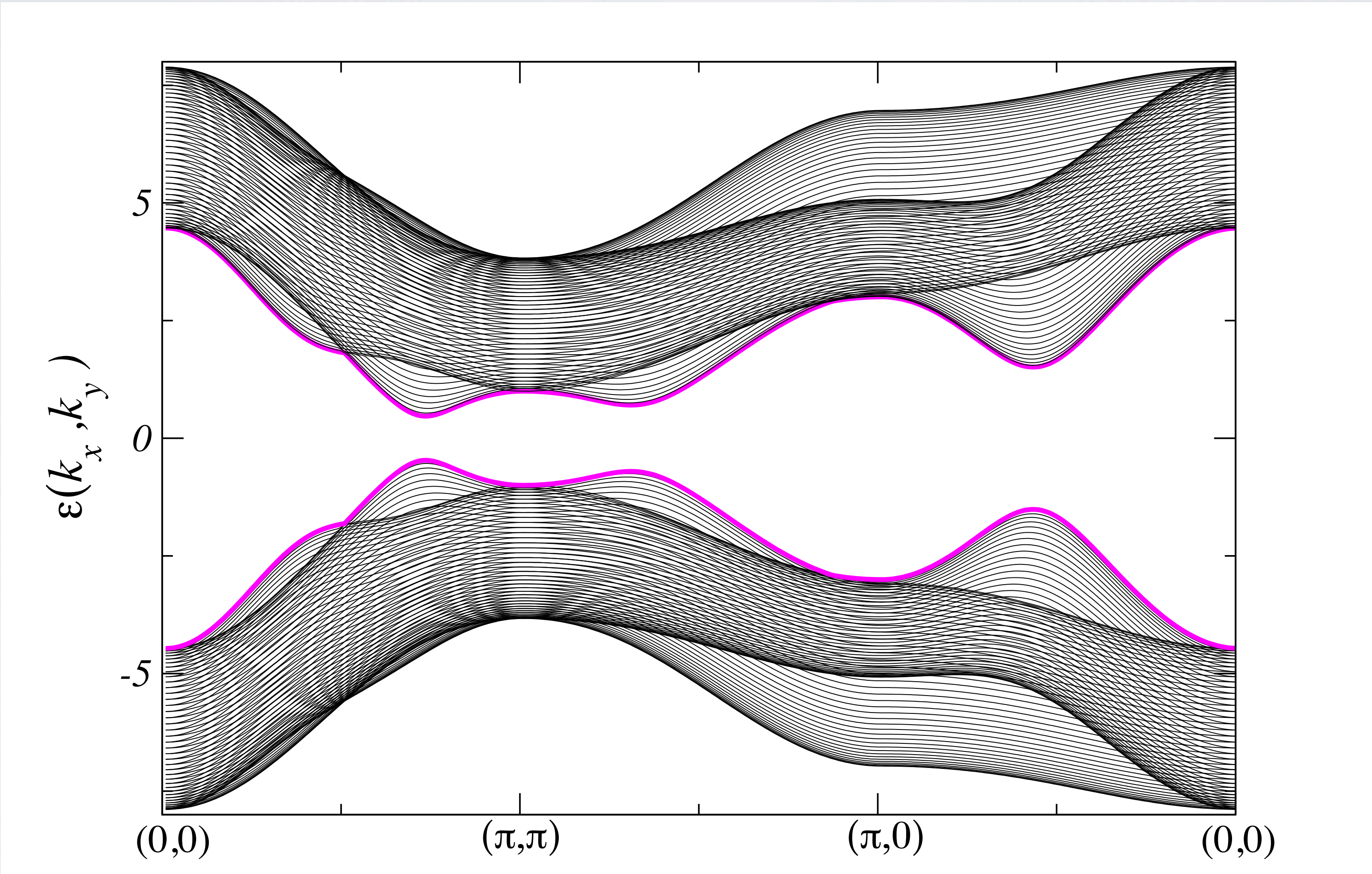
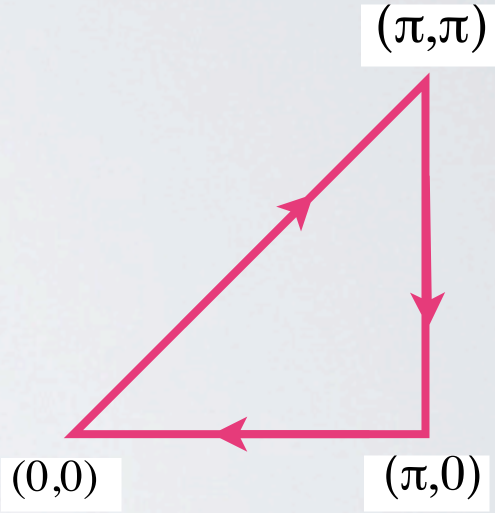


FIG. 2. (Color online) Band structure of the slab with $N = 40$ bilayers in the NI phase. Parameters are $t_1^A = 1 = -t_1^B = 1$, $t_2^A = 0.5 = -t_2^B$, $t_1' = 3.5$, $t_z' = 2$ and $t_2' = 0.8$, $t_2'' = 0.1$ States of the surfaces are shown in thick magenta lines. States of the surfaces with energies at the boundary of the gap are shown in thick magenta lines.



TOPOLOGICAL CRYSTALLINE INSULATOR

Gapped spectrum for bulk and gapless surface states

Surface states

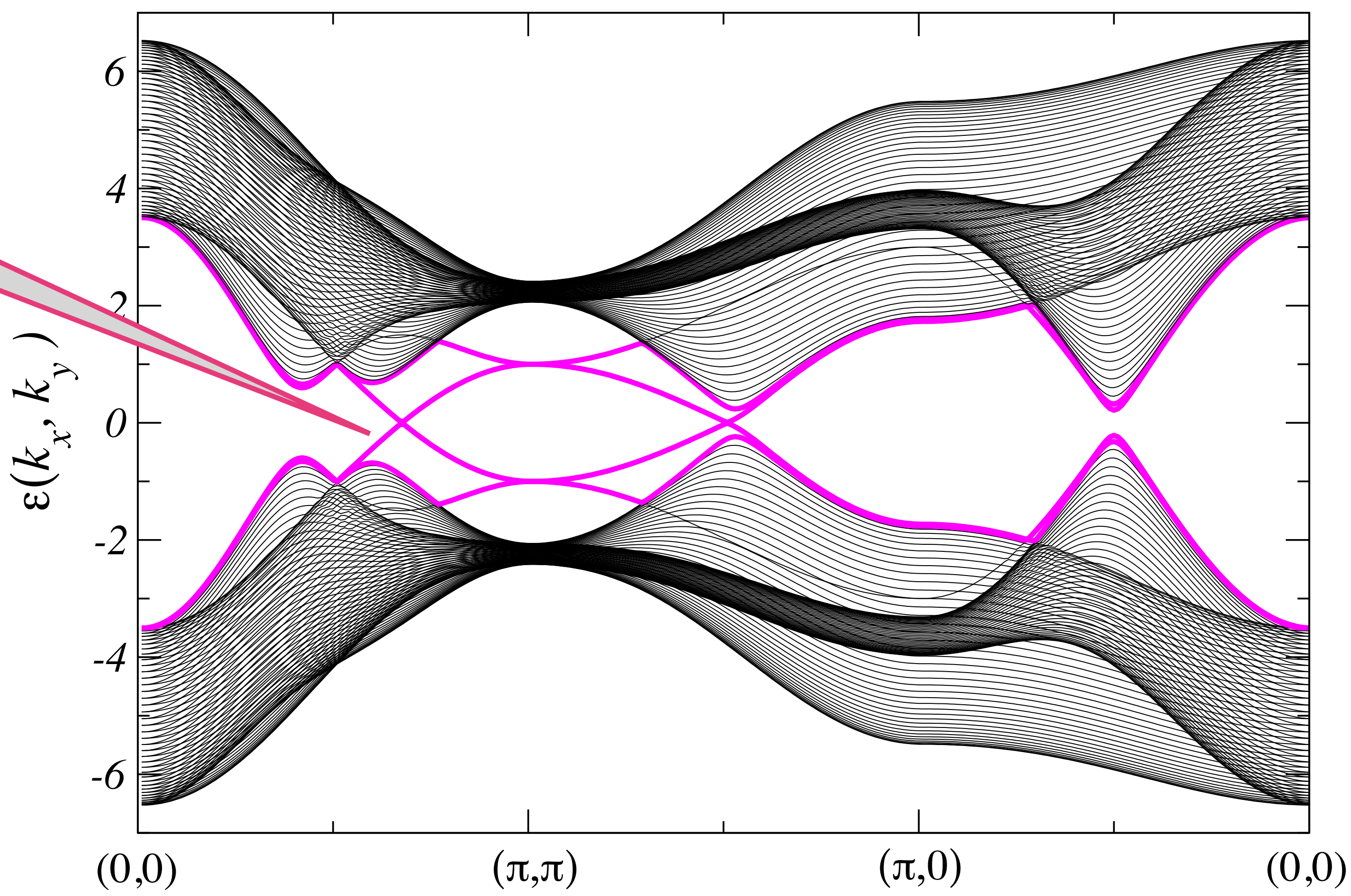
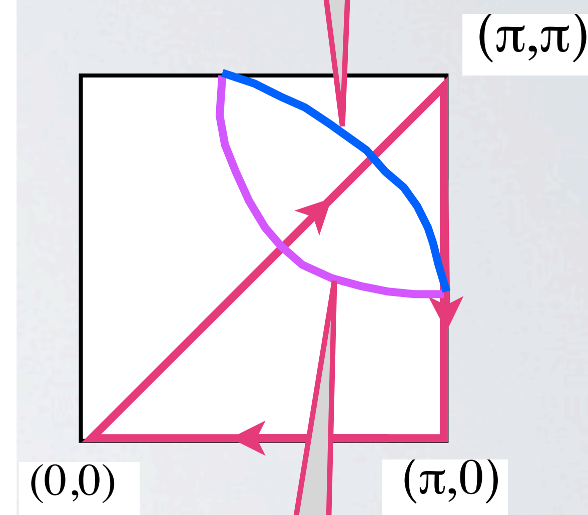


FIG. 3. (Color online) Band structure of the slab $N = 40$ bilayers in the TCI phase. Parameters are $t_1^A = 1 = -t_1^B = 1$, $t_2^A = 0.5 = -t_2^B$, $t_1' = 2.$, $t_z' = 2$ and $t_2' = 0.8$, $t_2'' = 0.1$. States of the surfaces with energies within or at the boundary of the bulk gap are shown in thick magenta lines.

Fermi surface top



Fermi surface bottom

WEYL SEMIMETAL

Nodes for bulk, gapless surface states and Fermi arcs

Surface states

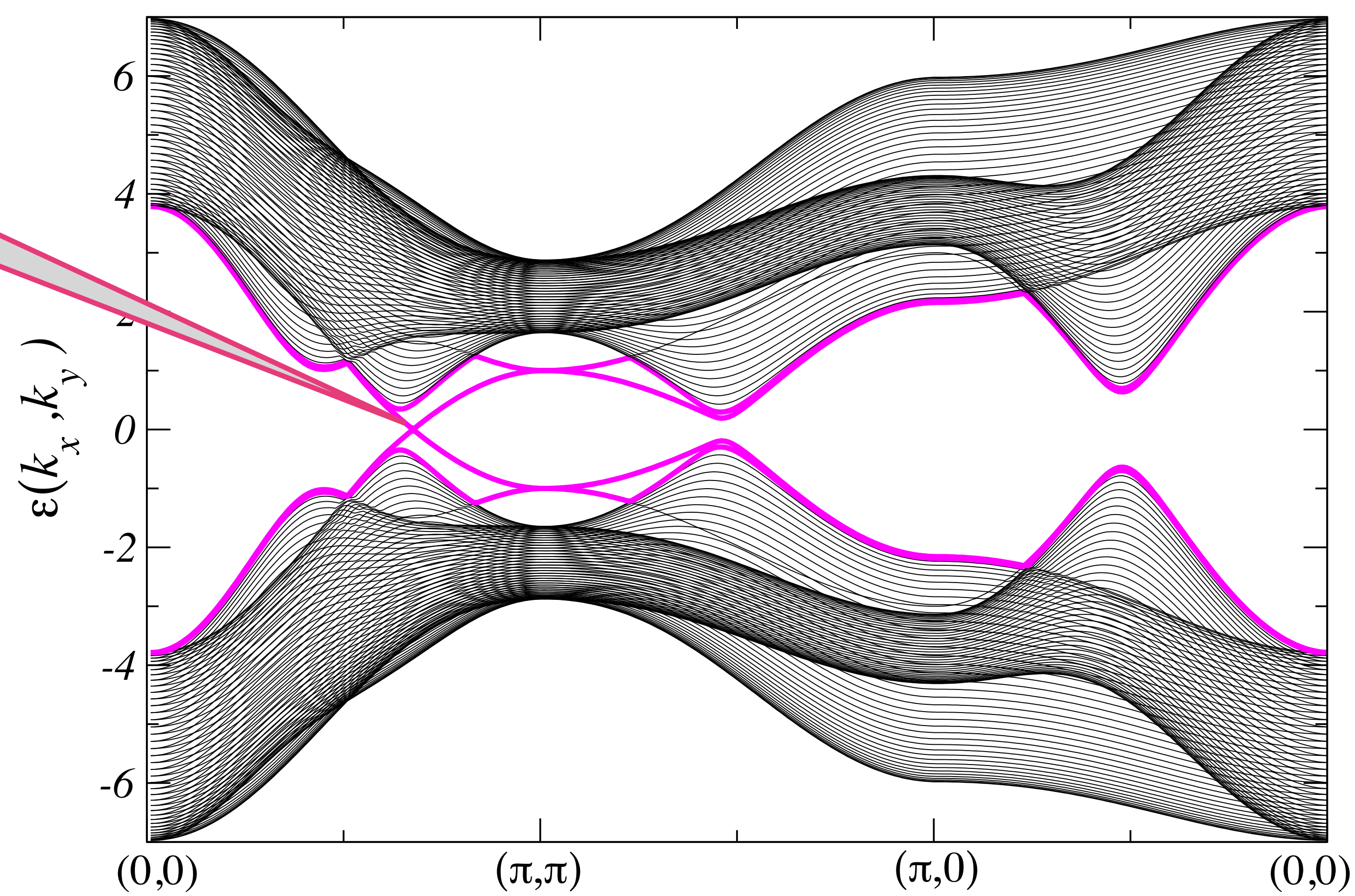
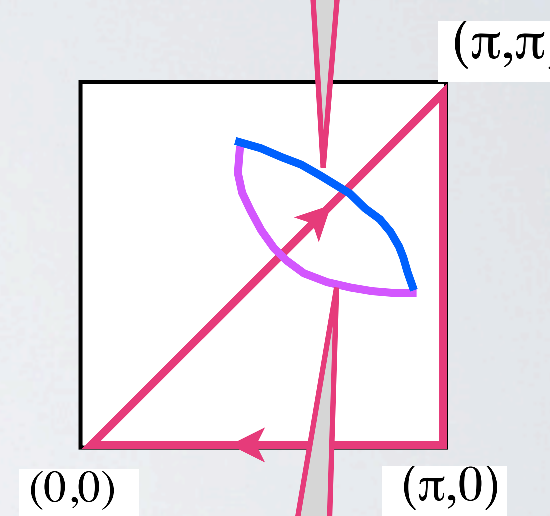


FIG. 4. (Color online) Band structure of the slab $N = 40$ bilayers in the WSM phase. Parameters are $t_1^A = 1 = -t_1^B = 1$, $t_2^A = 0.5 = -t_2^B$, $t_1' = 2.5$, $t_z' = 2$ and $t_2' = 0.8$, $t_2'' = 0.1$. States of the surfaces with energies within or at the boundary of the bulk gap are shown in thick magenta lines.

Fermi surface top



Fermi surface bottom

ANALYTICAL RESULTS

$$t_2^A = t_2^B = 0.$$

EFFECTIVE WEYL HAMILTONIAN

$$t_2^A = t_2^B = 0.$$

$$H_\alpha(\mathbf{k}) = g_x^\alpha \sigma_x + g_y^\alpha \sigma_y + g_z^\alpha \sigma_z$$

orbitals d_{xz} d_{yz}
or p_x and p_y -

$$\begin{aligned}
g_x^\alpha(\mathbf{k}) &= t_1' + t_z' \cos k_z + 2\left(t_2' \cos k_\alpha + t_2'' \cos k_{\overline{\alpha}}\right) \\
g_y^\alpha(\mathbf{k}) &= -t_z' \sin k_z, \\
g_z^\alpha(\mathbf{k}) &= 2t_1 \cos k_\alpha,
\end{aligned}$$

Eigenenergies

$$\varepsilon_\pm^\alpha(\mathbf{k}) = \pm\sqrt{(g_x^\alpha)^2 + \left(g_y^\alpha\right)^2 + (g_z^\alpha)^2}.$$

NODES ON SYMMETRY POINTS

$\mathbf{K}_1 = (\pm\pi/2, \pi, \pi)$

$$g_x^x(\mathbf{K}_1 + \mathbf{q}) = \Delta_1 - 2t_2' q_x + t_2'' q_y^2,$$
$$g_y^x(\mathbf{K}_1 + \mathbf{q}) = t_z' q_z,$$
$$g_z^x(\mathbf{K}_1 + \mathbf{q}) = -2t_1 q_x,$$

$\mathbf{K}_1' = (\pi, \pm\pi/2, \pi)$

$$g_x^y(\mathbf{K}_1' + \mathbf{q}) = \Delta_1 - 2t_2' q_y + t_2'' q_x^2,$$
$$g_y^y(\mathbf{K}_1' + \mathbf{q}) = t_z' q_z,$$
$$g_z^y(\mathbf{K}_1' + \mathbf{q}) = -2t_1 q_y,$$

Nodes for $\Delta_1 = 0$

$$\Delta_1 = t_1' - t_z' - 2t_2''$$

$\mathbf{K}_2 = (\pm\pi/2, 0, \pi)$

$\mathbf{K}_2' = (0, \pm\pi/2, \pi)$

Nodes for $\Delta_2 = 0$

$$\Delta_2 = t_1' - t_z' + 2t_2''$$

$\mathbf{K}_3 = (\pm\pi/2, \pi, 0)$

$\mathbf{K}_3' = (\pi, \pm\pi/2, 0)$

Nodes for $\Delta_3 = 0$

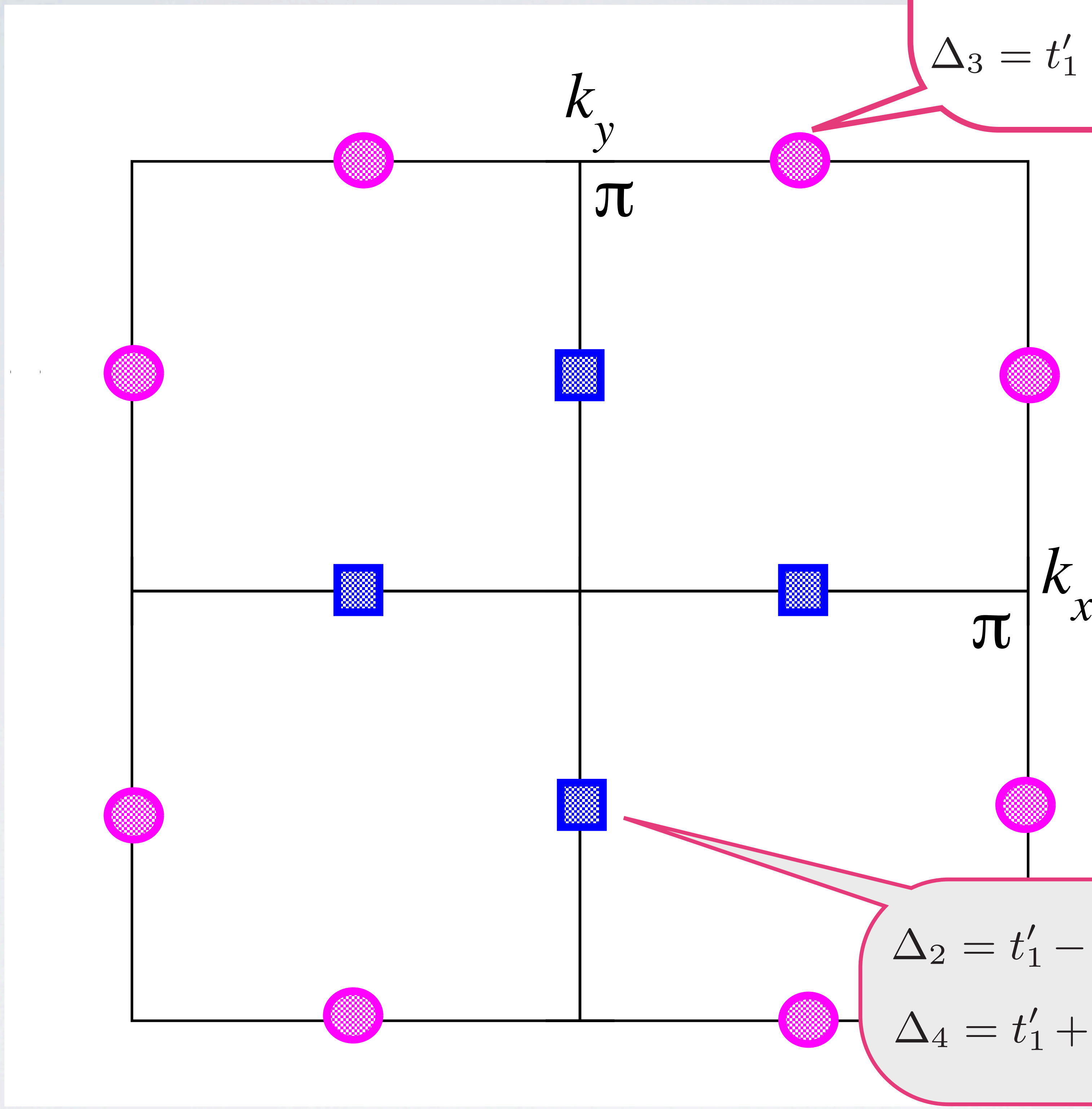
$$\Delta_3 = t_1' + t_z' - 2t_2''$$

$\mathbf{K}_4 = (\pm\pi/2, 0, 0)$

$\mathbf{K}_4' = (0, \pm\pi/2, 0)$

Nodes for $\Delta_4 = 0$

$$\Delta_4 = t_1' + t_z' + 2t_2''$$



$$\Delta_1 = t_1' - t_z' - 2t_2'' = 0 \text{ for } k_z = \pi$$

$$\Delta_3 = t_1' + t_z' - 2t_2'' = 0 \text{ for } k_z = 0$$

$$\Delta_2 = t_1' - t_z' + 2t_2'' = 0 \text{ for } k_z = \pi$$

$$\Delta_4 = t_1' + t_z' + 2t_2'' = 0 \text{ for } k_z = 0$$

NODES AWAY FROM HIGH-SYMMETRY POINTS

Node splitting $\mathbf{K}_1 \longrightarrow \mathbf{K}_{1,\pm} = (\pi/2, \pm k_1, \pi)$

$$k_1 = |\arccos[|\Delta_1/(2t_2'')| - 1]|$$

$$\begin{aligned} g_x^x(\mathbf{K}_{1,\pm}+\mathbf{q}) &= -2t_2'\,[q_x \mp \sin(k_1) q_y] \\ g_y^x(\mathbf{K}_{1,\pm}+\mathbf{q}) &= t_z' q_z, \\ g_z^x(\mathbf{K}_{1,\pm}+\mathbf{q}) &= -2t_1 q_x. \end{aligned}$$

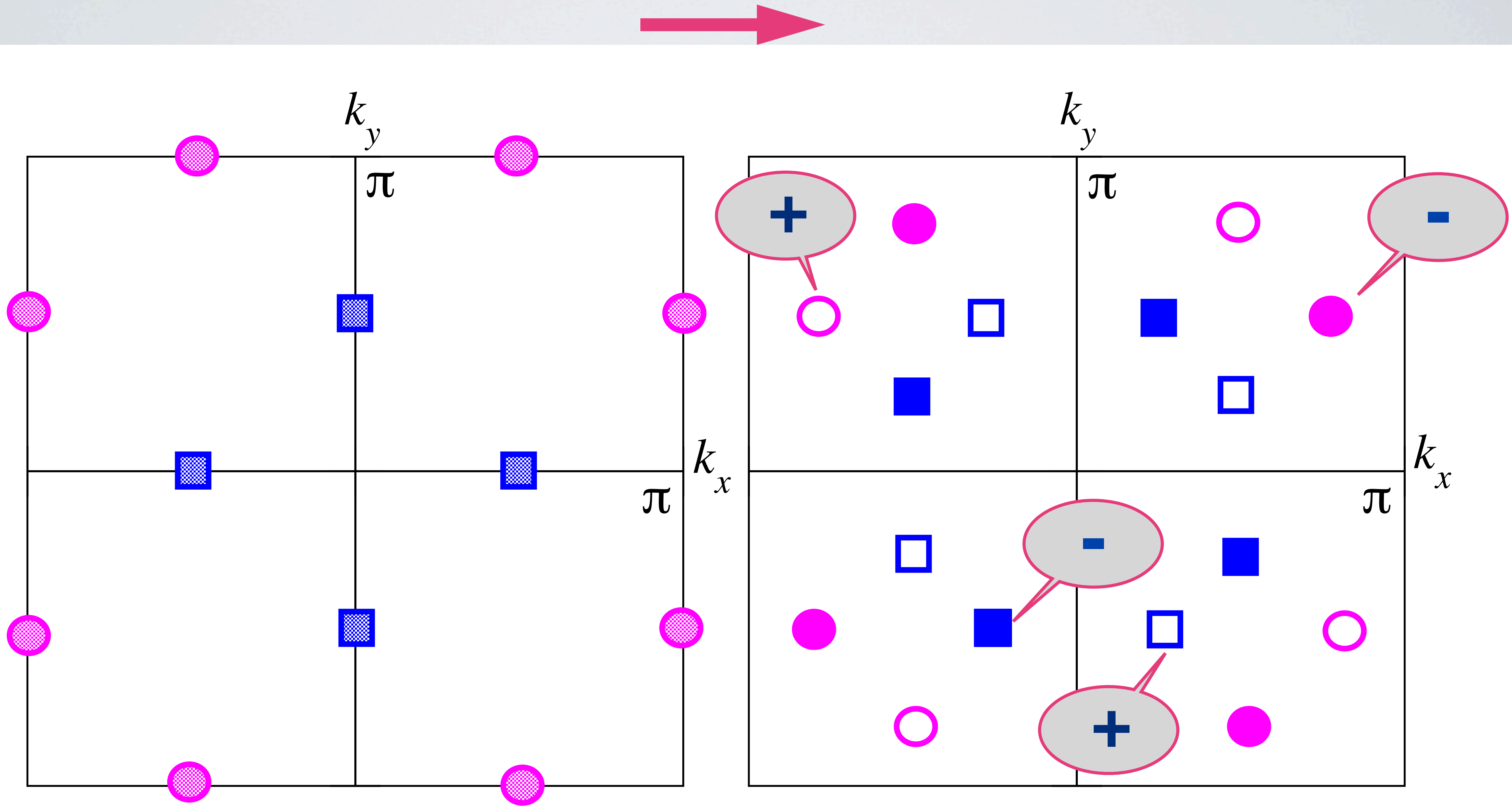
Berry curvature and monopole charge

$$\mathbf{A}(\mathbf{q}) = i\langle \Psi_-(\mathbf{q})|\nabla_{\mathbf{q}}|\Psi_-(\mathbf{q})\rangle$$

$$\rho(\mathbf{q})) = \mathrm{sg}\{J\}\delta^3(\mathbf{q})$$

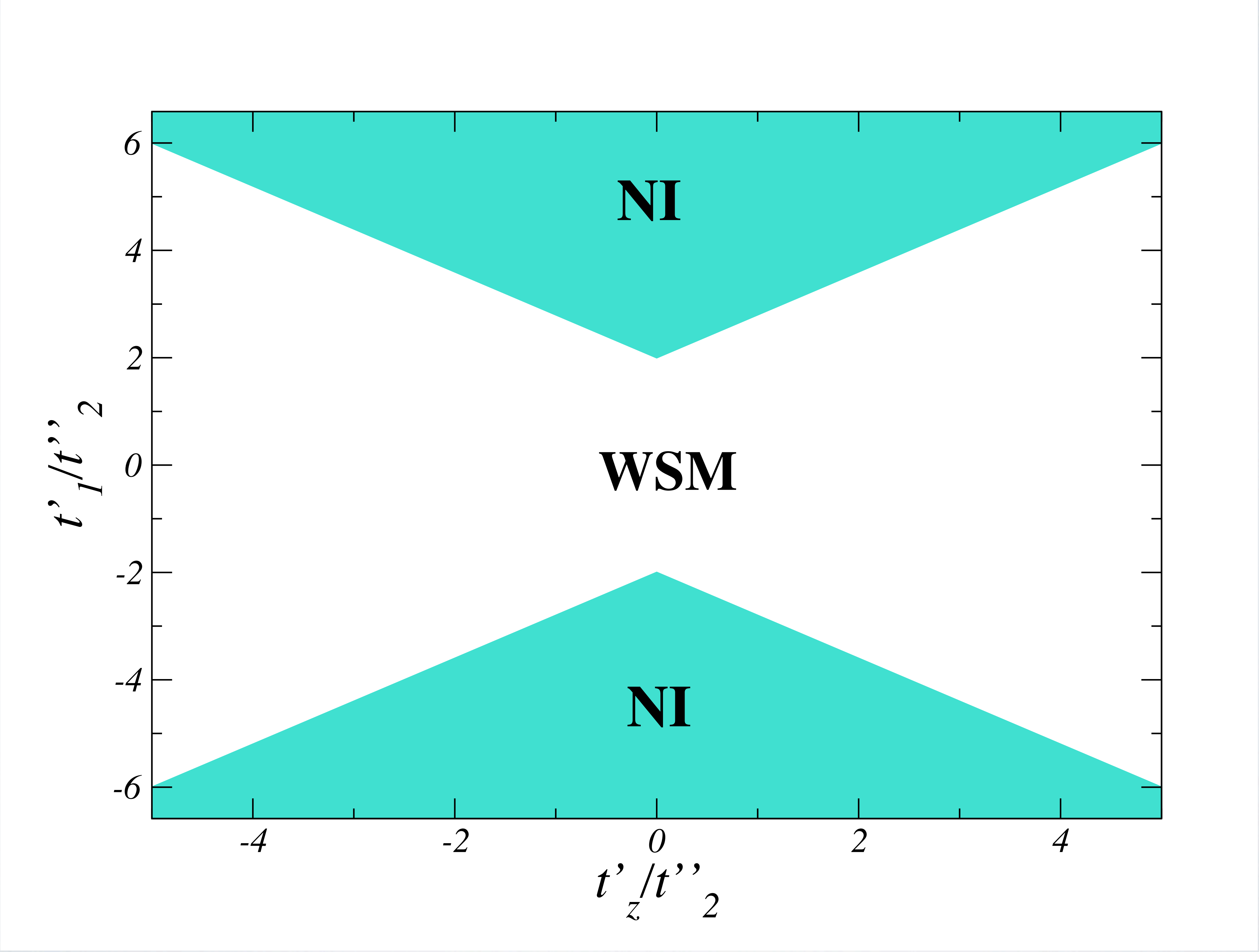
$$J = \mathrm{Det}\left[\frac{\partial(g_x^x, g_y^x, g_z^x)}{\partial(q_x, q_y, q_z)}\right]$$

NODE SPLITTING



PHASE DIAGRAM

ANALYTICAL LIMIT $t_2^A = t_2^B = 0.$



WITH IN-PLANE NNN HOPPING

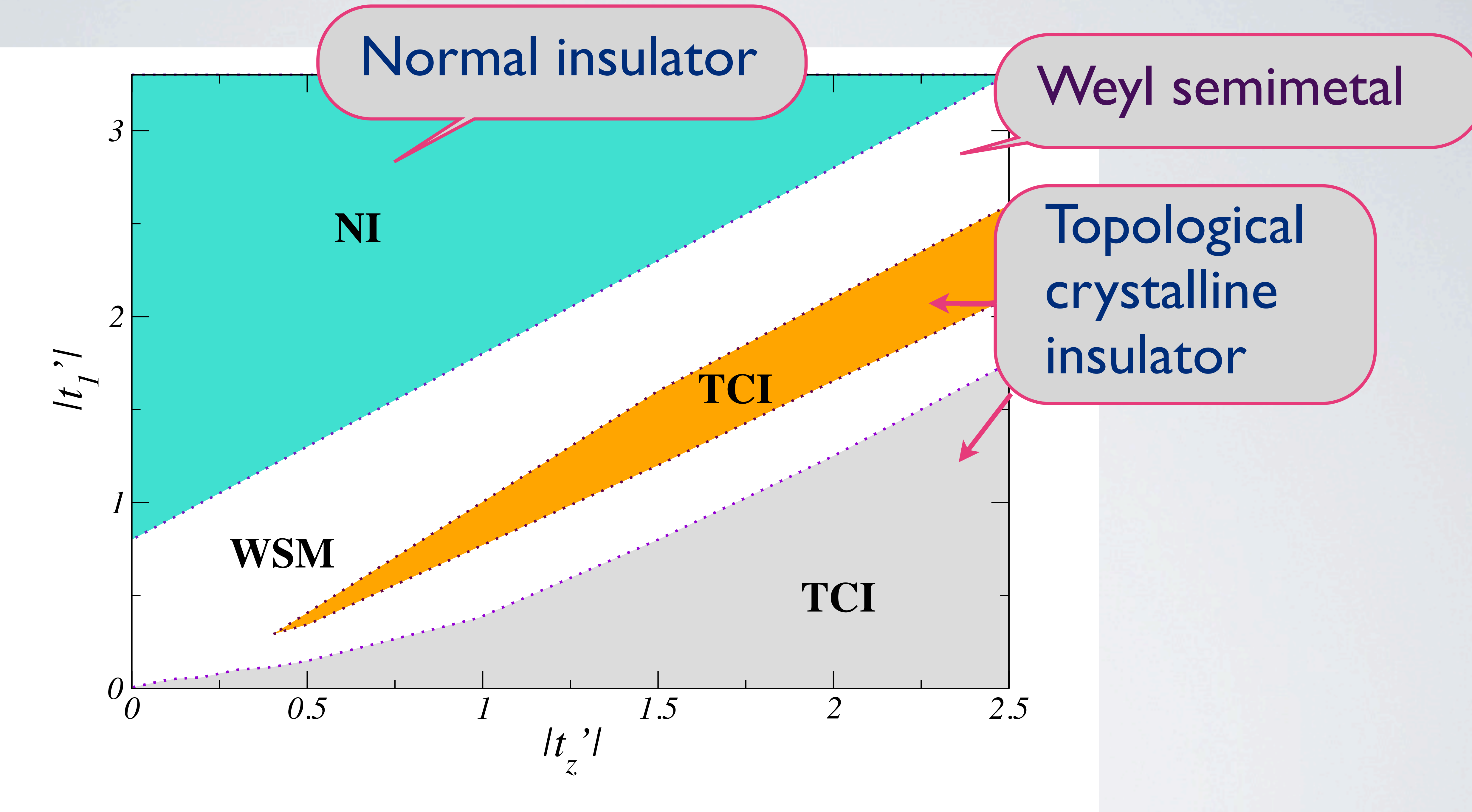


FIG. 8. Phase diagram for $t_2^A = -t_2^B = t_2 = 0.8$, $t_1^A = -t_1^B = 1$, $t_2' = 0.8$, $t_2'' = 0.1$. NI, TI and WSM denote, respectively, normal insulating phase, topological insulator and Weyl semimetal phase.

OUTLOOK

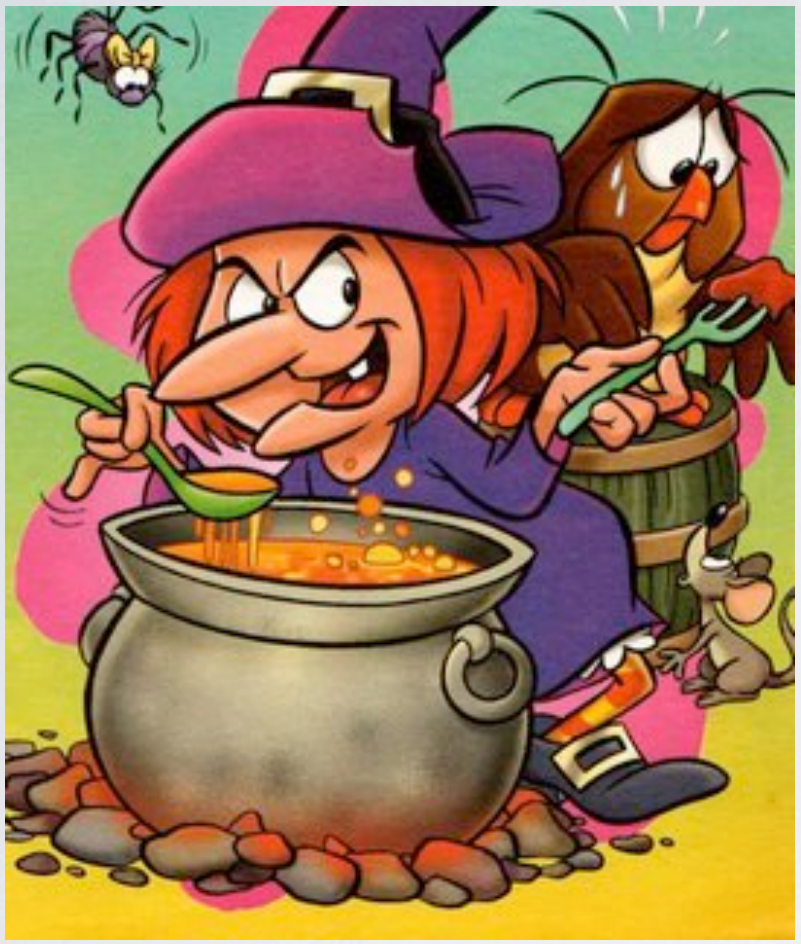
* 2 planes
* 2 orbitals

Symmetries
Time-reversal (preserved)
C4 point group (preserved)
Inversion (broken)

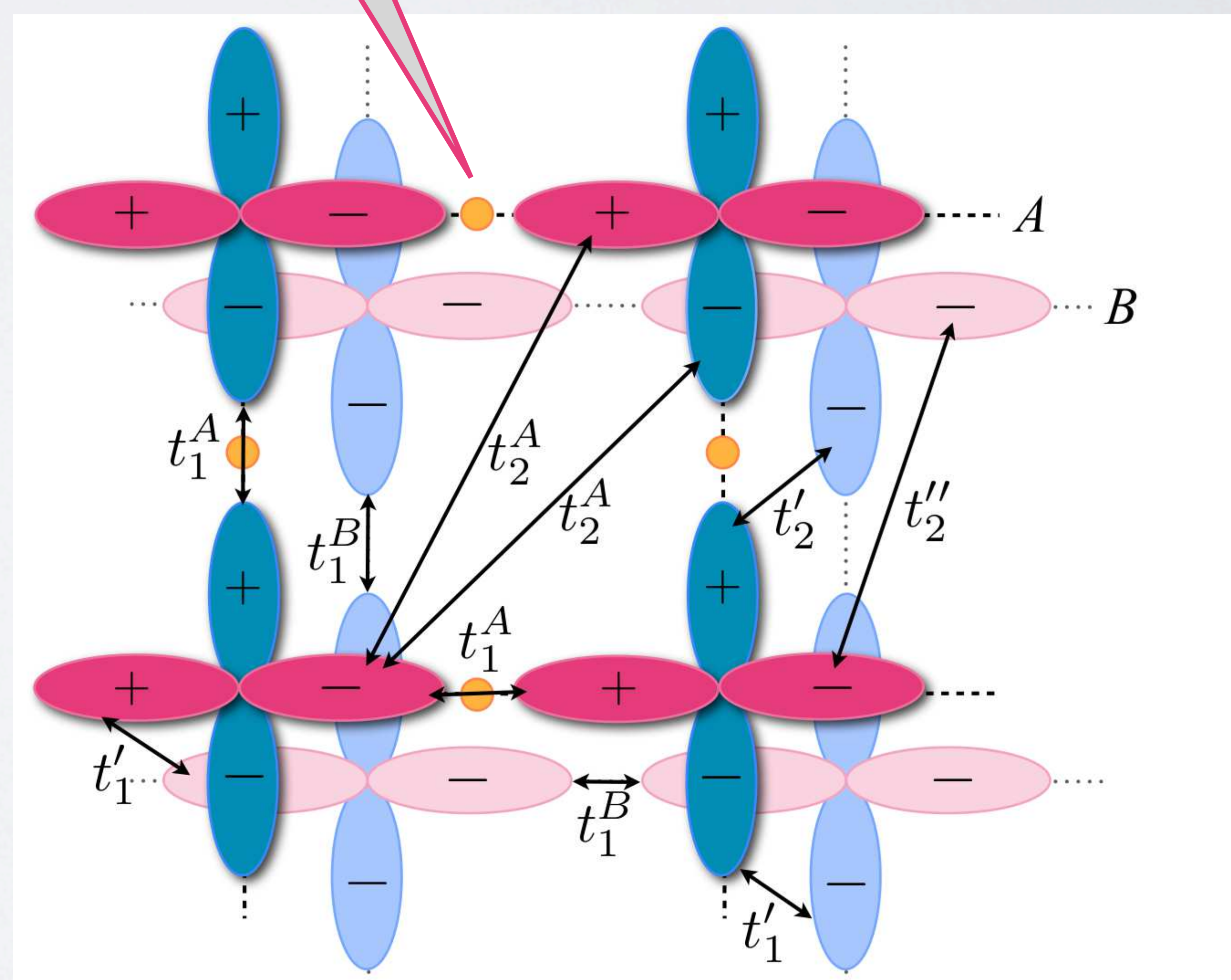
* Normal insulator
* Topological crystalline insulator
* Weyl semimetal

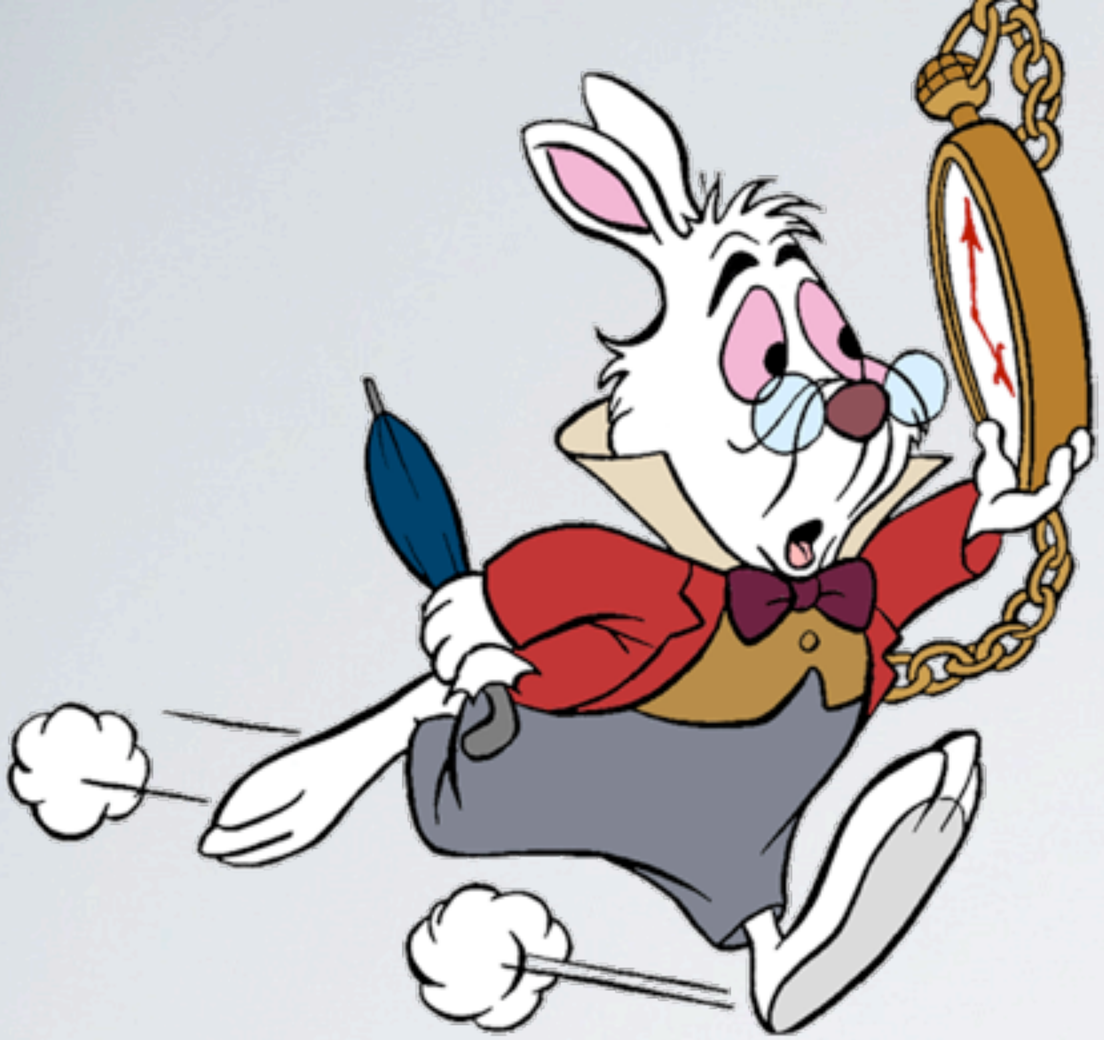
SECRET INGREDIENT

$$t_1^A = -t_1^B$$

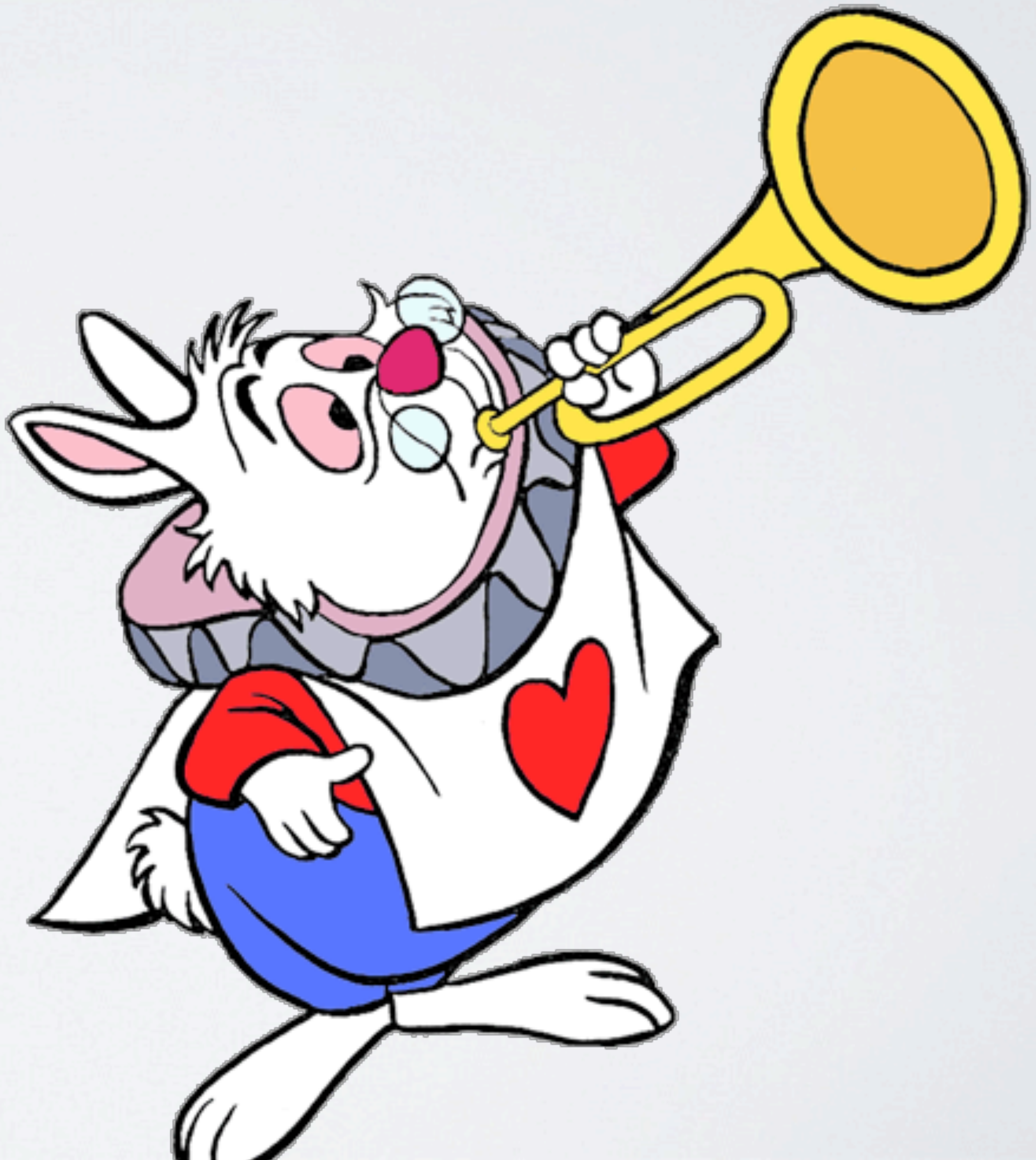


Possible mechanism:
Intermediate orbital in one of the planes





ANNOUNCEMENT



ICAS

International Center for Advanced Studies

UNSAM

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Welcome

ICAS is a center devoted to promote high-quality collaborative research in areas of basic science.

The center has a transversal structure with a few permanent groups, many associates from different institutions of Argentina and the region, short-term visitors, postdocs and PhD students.

Every year, ICAS runs several schools, conferences, seminars, workshops.

[Read more]

News & Announcements

Coming soon.

April 12th, 2016
Open Mathematics at ICAS/UNSAM
10.30-11.15: Raul Ferreira (U. Complutense Madrid, Spain)
11.30-12.15: Julio D Rossi (U. Buenos Aires, Argentina)

April 26th, 2016
Open Mathematics at ICAS/UNSAM
10.30-11.15: Daniel Galicer (U. Buenos Aires, Argentina)
11.30-12.15: Liviu Ignat (Inst. Simon Stoilov, Rumania)

May 4th, 2016
ICAS seminar
15.30: Upgrade to the CMS pixel detector, Florencia Canelli, Ben Kilminster (Zurich University, Swiss)

May 10th, 2016
Open Mathematics at ICAS/UNSAM
11.00-11.45: Leandro Vendramin (U. Buenos Aires, Argentina)
12.00-12.45: Gaston Garcia (U. La Plata, Argentina)

May 11th, 2016
ICAS seminar
11.00: Radion/Higgs phenomenology and the diphoton excess at the LHC, Anibal Medina, Université Paris Saclay, France

[See previous talks@ICAS]

Major events

November 15-18, 2016
Frontiers in Physical Sciences
ICAS- Max Planck

September 5-9, 2016
High Precision for Hard Processes at the LHC 6
Workshop in High Energy Physics
HP2.6

June 22, 2016
Inauguration Ceremony of ICAS
First meeting of National Committee

April 15, 2016
First Meeting of International Committee

June 8, 2015
Creation of ICAS
Today, the Council of UNSAM officialy created the ICAS!

Visitor info

Learn about ICAS and how to interact with us.

ICAS Conferences

Apply to organize a conference at ICAS [open Jan-Aug for next year]

ICAS Associates

Apply for ICAS Associate position
Apply for short term visit

ICAS Campus Miguelete, 25 de Mayo y Francia. C.P.: 1650. San Martín, Provincia de Buenos Aires, Argentina. Phone: +54 (11) 4006-1500. icas@unsam.edu.ar

ACTIVITIES

- Research in areas of basic sciences. Focus on: Physics, Mathematics, Chemistry.
- Organization of Schools workshops, seminars.
- Visitors programs.
- Postdocs and PhD student programs.

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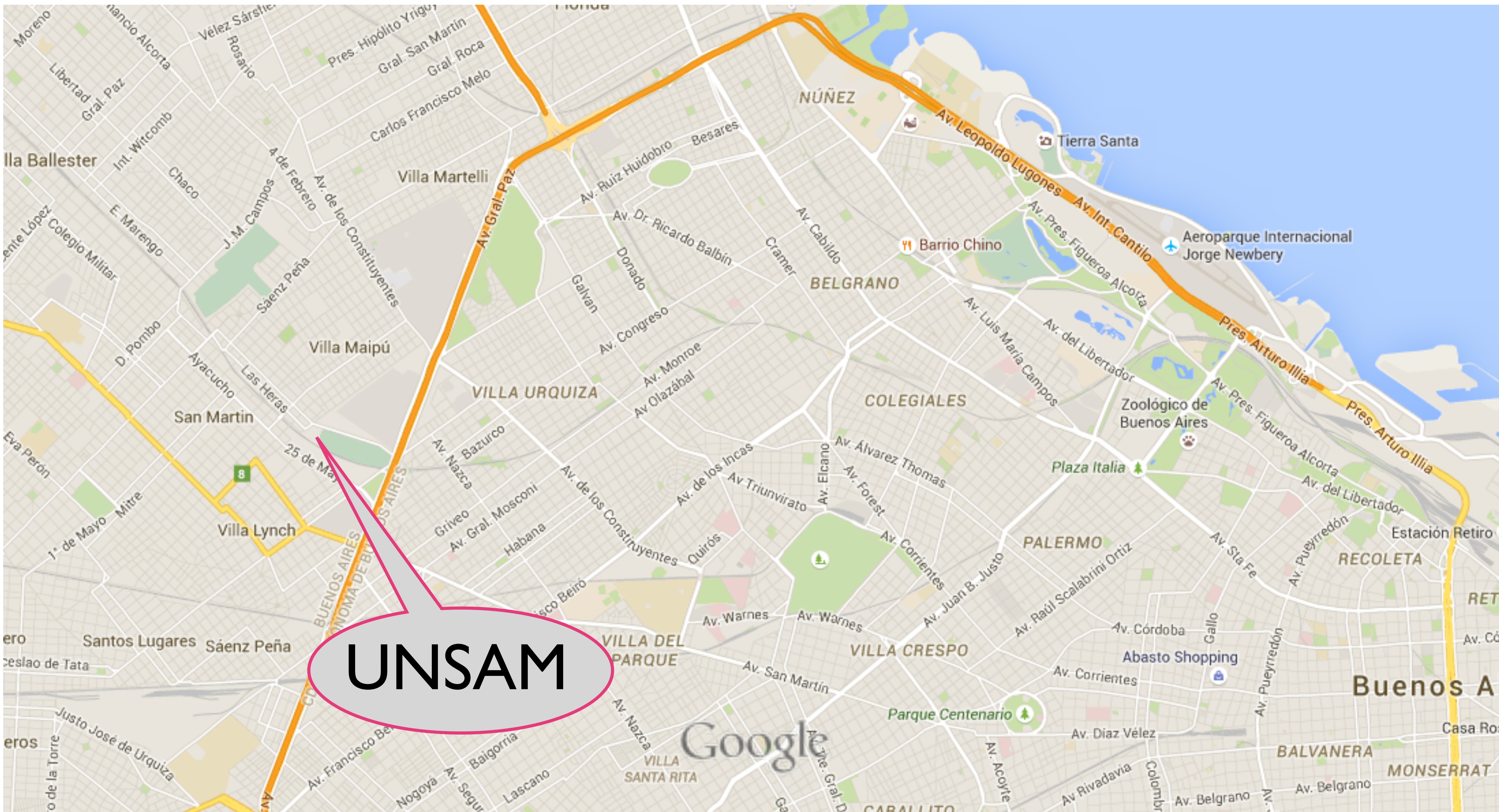

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Xul Solar, Argentina, 1937-1963