Title: Multiband superconductivity and the breaking of time reversal symmetry

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Abstract: I will discuss how spontaneous breaking of time reversal symmetry in multiband superconductors leads quite generally to the formation of small Fermi surfaces of Bogoliubov excitations, irrespective of whether inversion symmetry is absent or present in the superconducting state. In the latter case the inversion symmetry is susceptible to being dynamical broken at low temperatures by the residual interactions. A lattice model of this process will be discussed. Its final result is a reduced, but still finite Bogoliubov-Fermi surface.

Multiband superconductivity and the breaking of time-reversal symmetry

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Work with: Julia Link (TU Dresden)

J. Link, IH, PRL 125, 237004 (2020)
IH, J. Link, PRB 103, 144507 (2021)

Perimeter Institute, May 2022

Outline:

1) Bogoliubov-de Gennes Hamiltonian in absence of inversion, and the reason for Bogoliubov-Fermi surface

2) Bogoliubov-de Gennes Hamiltonian with inversion, and the analogy with classical (special) relativity

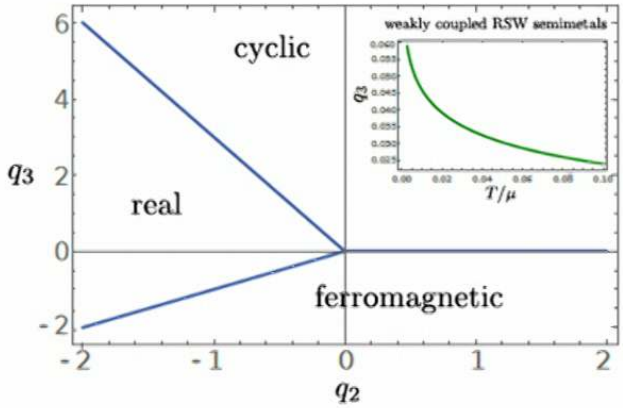
3) Dynamical breaking of inversion symmetry: lattice model of Bogoliubov-Fermi surface and its instability

Motivation: multicomponent superconductors like breaking of time-reversal symmetry

Example: pairing of S=3/2 Luttinger fermions into L=0, S=2 (d-wave) Cooper pair (Boettcher, IH, PRB 2016; Agterberg, Brydon, Timm, PRL 2017)

Ginzburg-Landau theory: $\phi_{ij} = \Delta_a M^a_{ij}$ (irr. symm. 2nd rank tensor)

$$F(\phi) = \frac{r}{2}\mathrm{tr}(\phi^\dagger\phi) + \frac{\bar{\lambda}_1}{4}[\mathrm{tr}(\phi^\dagger\phi)]^2 + \frac{\bar{\lambda}_2}{4}|\mathrm{tr}(\phi^2)|^2 + \bar{\lambda}_3\mathrm{tr}(\phi^\dagger\phi\phi^\dagger\phi)$$



Mermin, PRA 1974;
Link, Boettcher, IH, PRB 2020

Time reversal is preserved in superconducting state when all

$$\Delta_{2a} = 0$$

i.e. it is broken when

$$\Gamma \neq \Gamma^{\dagger}$$

Eigenstates of $H(\mathbf{p})$:

$$\phi_i(\mathbf{p})$$

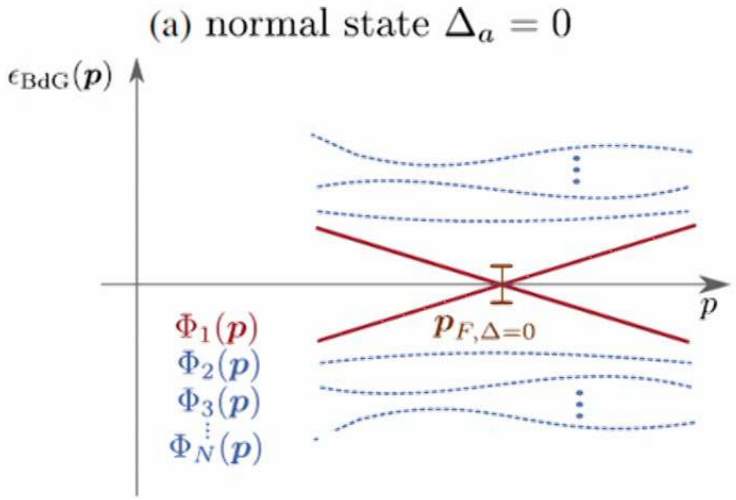
with eigenvalues $E_i(\mathbf{p})$, $i = 1, \ldots N$

Effective Hamiltonian (Link, IH, PRL 2020)

Light and heavy states: one state at each momentum

$$\phi_1(\mathbf{p})$$

is "light", the rest N-1 are "heavy": $H_{\mathrm{BdG}}(\mathbf{p}) = \begin{pmatrix} H_l(\mathbf{p}) & H_{lh}(\mathbf{p}) \\ H_{lh}^{\dagger}(\mathbf{p}) & H_h(\mathbf{p}) \end{pmatrix}$



Quasiparticle spectrum:

$$\det[H_{\mathrm{BdG}}(\mathbf{p}) - \omega] = 0$$

and the determinant

$$\det[H_{\mathrm{BdG}}(\mathbf{p}) - \omega] = \det[H_h(\mathbf{p}) - \omega] \det L_{ef}(\omega, \mathbf{p})$$

with the Schur complement (I. Schur, J. fur reine und ang. Math., 1917)

$$L_{ef}(\omega,\mathbf{p}) = H_l(\mathbf{p}) - \omega - H_{lh}(\mathbf{p})(H_h(\mathbf{p}) - \omega)^{-1} H_{lh}^{\dagger}(\mathbf{p})$$

When $|\omega| < |E_i(\mathbf{p}) - \mu| \qquad i \neq 1$ the spectrum is given by

$$\det L_{ef}(\omega, \mathbf{p}) = 0$$

Equivalent to integration over heavy modes in partition function!
(Link, IH, PRL 2020)

Bogoliubov-Fermi surface is at

$$\det H_{ef}(\mathbf{p}) = 0$$

where

$$H_{ef}(\mathbf{p}) = L_{ef}(0, \mathbf{p})$$

is the effective (2 x 2) Hamiltonian:

$$H_{ef} = \sum_{\alpha=0}^{3} f_\alpha(\mathbf{p})\sigma_\alpha$$

The zero modes are therefore at momenta that satisfy

$$\det H_{ef}(\mathbf{p}) = f_0^2(\mathbf{p}) - \sum_{i=1}^{3} f_i^2(\mathbf{p}) = 0$$

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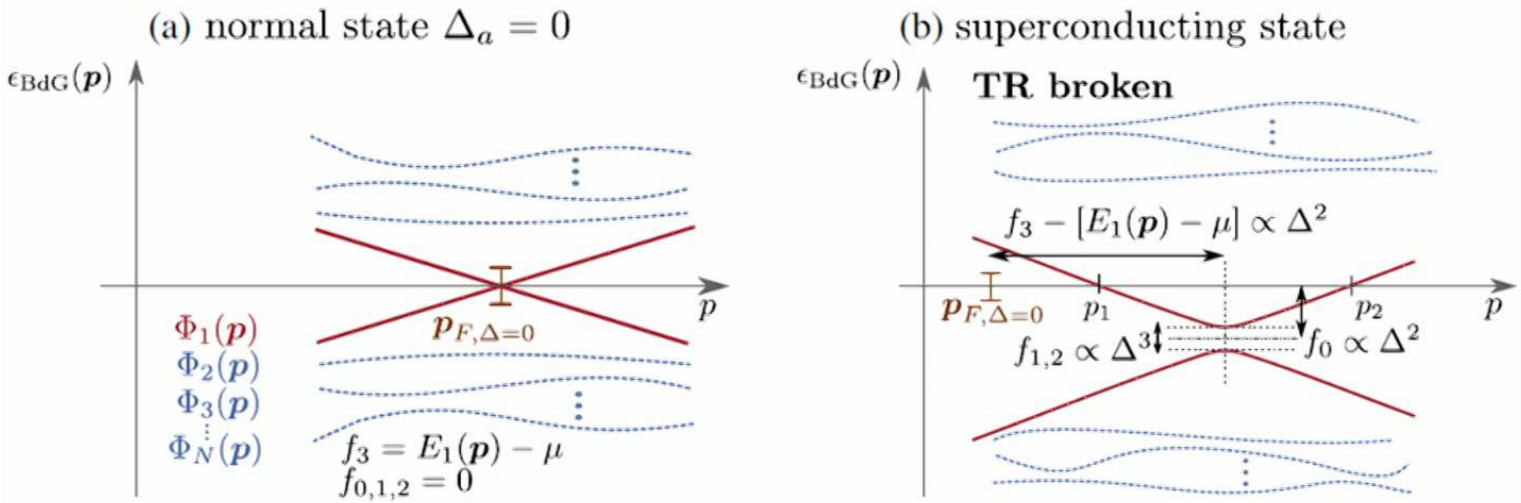
Picture: in the momentum directions where: (Link, IH, PRL 2020)

$$\mathcal{O}(\Delta) = 0$$



there are two zero modes, which yield a closed surface as the direction is varied,

i. e. a "BF surface" is formed.

Sketch of proof: rewrite (Link, IH, PRL 2020)

$$H^{(0)}_{\mathrm{BdG},N} = \begin{pmatrix} H^{(0)}_{1,1} & H^{(0)}_{1,2} & \cdots & H^{(0)}_{1,N} \\ H^{(0)\dagger}_{1,2} & H^{(0)}_{2,2} & \cdots & H^{(0)}_{2,N} \\ \vdots & \vdots & \ddots & \vdots \\ H^{(0)\dagger}_{1,N} & H^{(0)\dagger}_{2,N} & \cdots & H^{(0)}_{N,N} \end{pmatrix},$$

with two-dimensional matrices

$$H^{(0)}_{k,m} = \delta_{k,m}[E_k(\mathbf{p}) - \mu]\sigma_3 + \sum_a (\phi^\dagger_k M_a \phi_m)(\Delta_{1a}\sigma_1 - \Delta_{2a}\sigma_2).$$

By iteration:

$$\det H^{(0)}_{\mathrm{BdG},N} = \det H^{(0)}_{N,N} \det H^{(1)}_{N-1,N-1} \det H^{(2)}_{N-2,N-2} \ldots \det H^{(N-1)}_{1,1}$$

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The result:

1) When TR is preserved

$$\Delta_{2a} \equiv 0$$

and only σ_1 and σ_3 matrices participate: in effective Hamiltonian

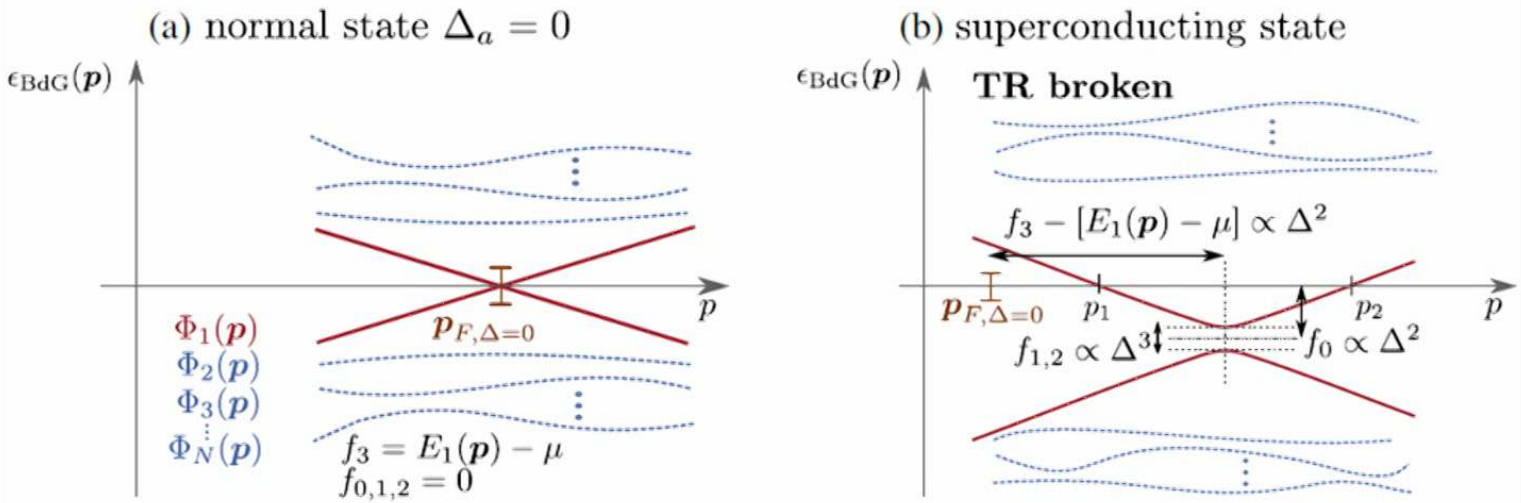
$$f_i(\mathbf{p}) \equiv 0 \qquad i = 0, 2$$

2) When TR is broken, after first iteration the Hamiltonian becomes the most general with all four coefficients finite. To leading order

$$H_{ef} = H^{(0)}_{1,1} - \sum_{k=2}^{N} H^{(0)}_{1,k} (H^{(0)}_{k,k;\Delta_a=0})^{-1} H^{(0)\dagger}_{1,k} + \mathcal{O}(\Delta^3)$$

Picture: in the momentum directions where: (Link, IH, PRL 2020)

$$\mathcal{O}(\Delta) = 0$$



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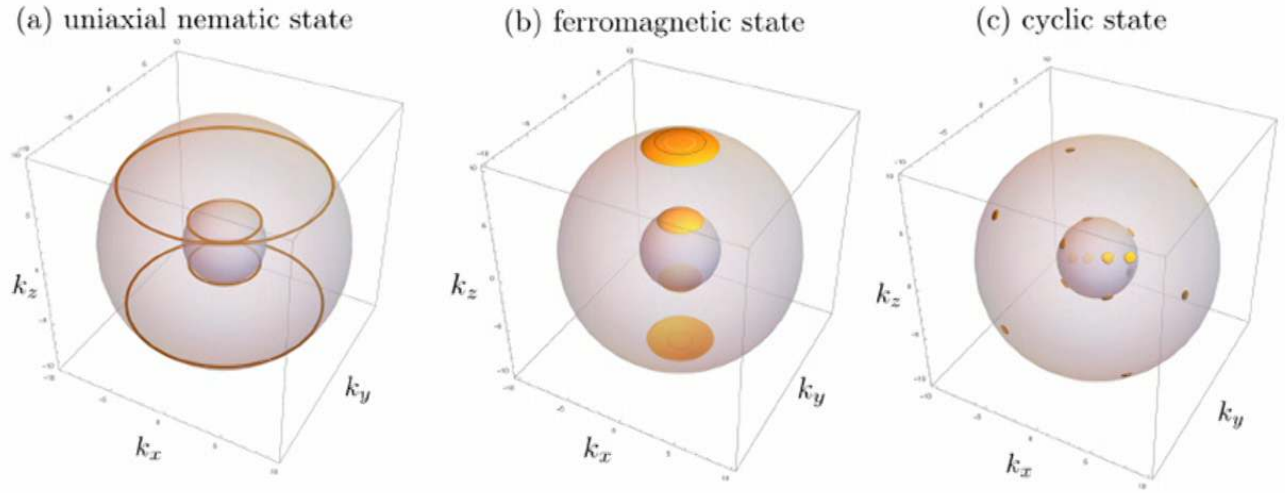
Three d-wave states in Rarita-Schwinger-Weyl system: (with two normal Fermi surfaces)



(Link, Boettcher, IH, PRB 2020)

Multicomponent superconductivity with inversion

(Agterbreg, Brydon, Timm, PRL 2017; IH, Link, PRB 2021)

Inversion symmetry:

$$P^\dagger H(\mathbf{p})P = H(-\mathbf{p})$$

$$P^\dagger \Gamma(\mathbf{p})P = \Gamma(-\mathbf{p})$$

Inversion operator is unitary

$$P^\dagger P = 1$$

and observable

$$P^\dagger = P$$

so that

$$P^2 = +1$$

and we have parity as a quantum number.

Finally, we also postulate that

$$[\mathcal{P}, \mathcal{T}] = 0$$

i.e. inversion and time reversal commute! (Otherwise massive Dirac Hamiltonian would always violate one of the two symmetries!)

BdG Hamiltonian is ($\Gamma(\mathbf{p}) = \Gamma_1(\mathbf{p}) - i\Gamma_2(\mathbf{p})$)

$$H_{\mathrm{BdG}}(\mathbf{p}) = \sigma_3 \otimes [H(\mathbf{p}) - \mu] + \sigma_1 \otimes \Gamma_1(\mathbf{p}) + \sigma_2 \otimes \Gamma_2(\mathbf{p})$$

And it anticommutes with the operator ($k = 2$)

$$\mathcal{A} = \sigma_k \otimes (\mathcal{P}\mathcal{T})$$

so its eigenstates come in pairs with energy (+E, -E).

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Most importantly

$$\mathcal{A}^2 = (\sigma_k \sigma_k^*) \otimes (\mathcal{P}^2 \mathcal{T}^2) = +1$$

and in some "real" basis: (A. Messiah, QM 1958)

$$\mathcal{A} = K$$

In this bases BdG Hamiltonian at any momentum is a imaginary (Hermitian) matrix.

Effective Hamiltonian

$$H_{ef}(\mathbf{p}) = H_l(\mathbf{p}) - H_{lh}(\mathbf{p}) H_h^{-1}(\mathbf{p}) H_{lh}^{\dagger}(\mathbf{p})$$

is therefore also imaginary Hermitian (4 x 4) matrix.

SO(4) algebra, in terms of boosts and angular momentum:

$$[J_i, J_j] = i\epsilon_{ijk} J_k,$$

$$[N_i, J_j] = i\epsilon_{ijk} N_k,$$

$$[N_i, N_j] = i\epsilon_{ijk} J_k.$$

can be factorized,

$$R_{i,\pm} = \tfrac{1}{2}(J_i \pm N_i)$$

So that

$$[R_{i,r}, R_{j,r}] = i\epsilon_{ijk} R_{k,r}$$

$$[R_{i,+}, R_{j,-}] = 0.$$

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i. e. SO(4) = SO(3) x SO(3)

The eigenvalues are then:

$$E(\mathbf{p}) = \pm\tfrac{1}{2}[|\mathbf{a}(\mathbf{p}) + \mathbf{b}(\mathbf{p})| \pm |\mathbf{a}(\mathbf{p}) - \mathbf{b}(\mathbf{p})|]$$

and this vanishes when

$$\mathbf{a}(\mathbf{p}) \cdot \mathbf{b}(\mathbf{p}) = 0$$

which determines a (BF) surface. (IH, Link, PRB 2021)

Multiplying the eigenvalues,

$$\det[H_{ef}(\mathbf{p})] = [\mathbf{a}(\mathbf{p}) \cdot \mathbf{b}(\mathbf{p})]^2$$

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The zero-energy eigenstates: (in four-vector notation)

$$\Psi = (v_0, v_1, v_2, v_3)^{\mathrm{T}}$$

so that

$$H_{ef}(\mathbf{p})\Psi(\mathbf{p}) = 0 \quad \rightarrow \quad \mathbf{a}\cdot\mathbf{v} = 0, \qquad v_0\mathbf{a} + \mathbf{b}\times\mathbf{v} = 0$$

Two (real) solutions:

a) "time-like" $\Psi_t = \dfrac{1}{\sqrt{1+\mathbf{v}^2}}(1, \mathbf{v})^{\mathrm{T}}$ $\mathbf{v} = (\mathbf{b}\times\mathbf{a})/\mathbf{b}^2$

b) ``space-like" $\Psi_s = (0, \mathbf{b}/|\mathbf{b}|)^{\mathrm{T}}$

(Orthogonal: $\Psi_t^{\dagger}\Psi_s = 0$)

Relativistic analogy: (IH, Link, PRB 2021)

Schroedinger equation: ($H_{ef} = iF$)

$$\frac{d}{dt}\Psi = F\Psi$$

Lorentz equation: ($V = V^{\mu} = \gamma(v)(c, \mathbf{v})^{\mathrm{T}}$)

$$m\frac{d}{d\tau}V = FGV$$

With G as the metric tensor $G = G_{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$

Velocity has the constant Minkowski norm:

$$V^{\mu}V_{\mu} = V^{\mathrm{T}}GV = c^2$$

Lorentz equation is not Schroedinger equation since the matrix

$$iFG$$

is not Hermitian. (SO(1,3) has no finite dimensional unitary representation.)

But: zero-modes still correspond to special velocities for which Lorentz force vanishes!

a) Ψ_t corresponds to physical four-velocity, but

b) Ψ_s has negative Minkowski norm, and is not a physical velocity

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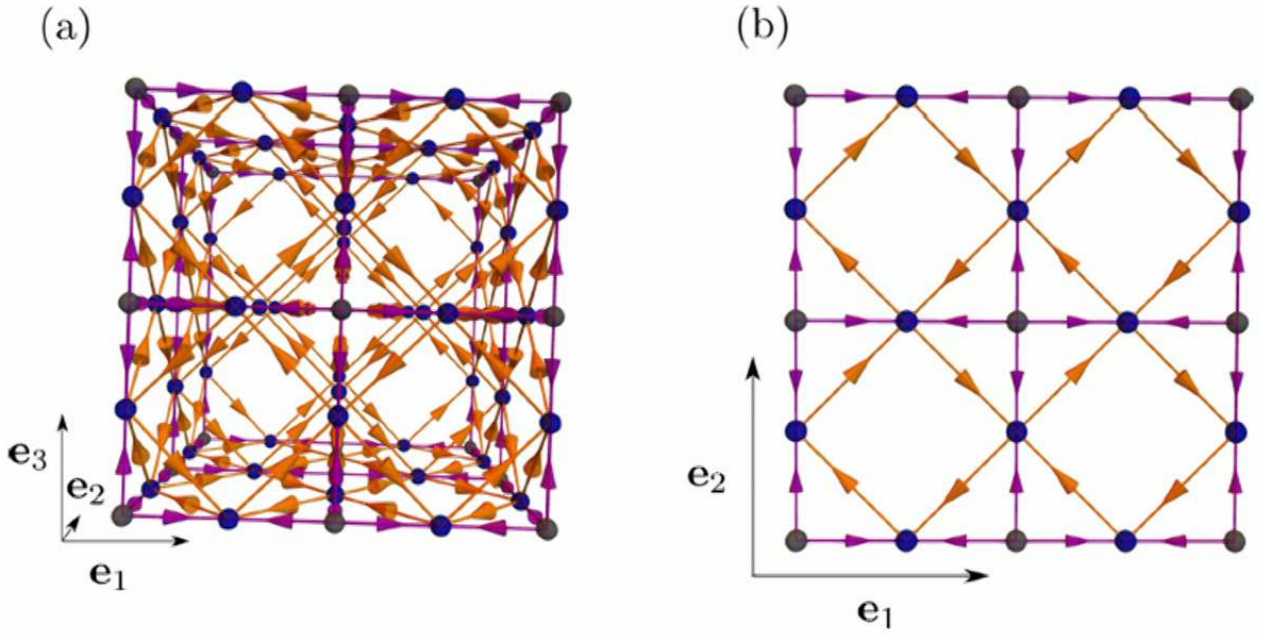
Net result of TR breaking with inversion:

Doubly degenerate surface of Weyl points

Is it stable? (Oh, Moon, PRB, 2020)

Lattice model: $H_{ef}(\mathbf{p})$, 4x4, anticommutes with an antiunitary A with A^2 = 1 (D-class condition) (IH, Link, PRB 2021)



$$H_0 = -it \sum_{\mathbf{R},k=1,2,3} c^\dagger(\mathbf{R}) c\left(\mathbf{R} \pm \frac{\mathbf{e}_k}{2}\right) + \left\{ i\chi \sum_{\mathbf{R},s=\pm 1} (s) c^\dagger\left(\mathbf{R} + \frac{\mathbf{e}_1}{2}\right) \left[c\left(\mathbf{R} + \mathbf{e}_1 + s\frac{\mathbf{e}_2}{2}\right) - c\left(\mathbf{R} + s\frac{\mathbf{e}_2}{2}\right) \right] + (1 \to 2, 2 \to 3) + (2 \to 3, 3 \to 1) \right\} + \text{H.c.},$$

The hopping Hamiltonian:

$$H_0 = \sum_{\mathbf{p}} \Psi^{\dagger}(\mathbf{p}) H_{ef}(\mathbf{p}) \Psi(\mathbf{p})$$

with the coefficients:

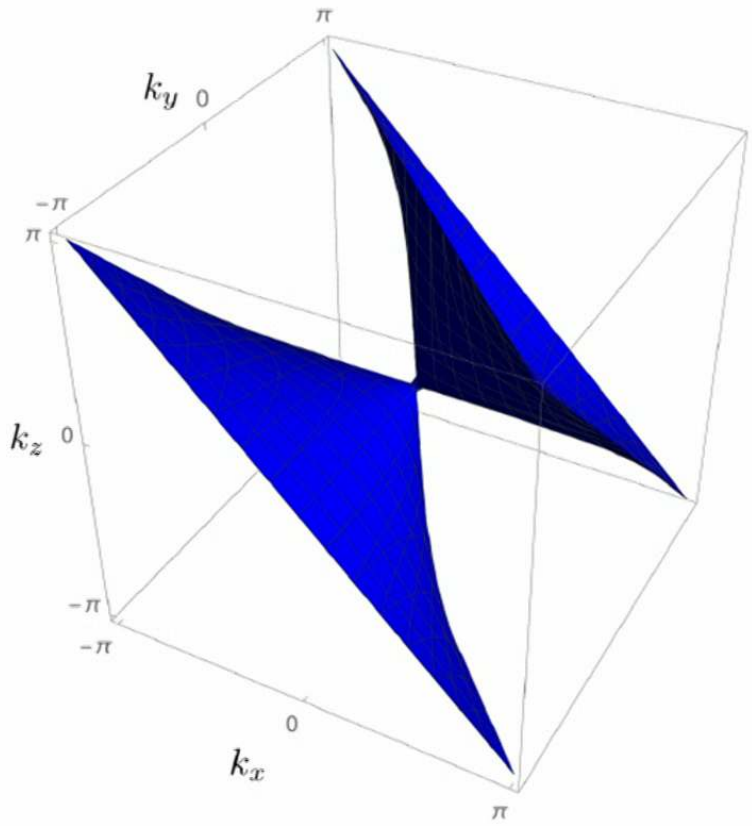
$$a_i(\mathbf{p}) = 2t \cos\left(\frac{p_i}{2}\right)$$

$$b_i(\mathbf{p}) = 4\chi \sin\left(\frac{p_j}{2}\right) \sin\left(\frac{p_k}{2}\right) \quad i \neq j,\ i \neq k,\ j \neq k$$

The surface:

$$\left[\prod_{i=1,2,3} \sin\left(\frac{p_i}{2}\right)\right] \sum_{i=1,2,3} \cot\left(\frac{p_i}{2}\right) = 0$$

In the Brillouin zone: (IH, Link, PRB 2021)



whole surface of Weil points

Nearest neighbor repulsion: (V>0)

$$H = H_0 + H_{\text{int}}$$

$$H_{\text{int}} = V \sum_{\mathbf{R},i} n(\mathbf{R}) n\left(\mathbf{R} \pm \frac{\mathbf{e}_i}{2}\right)$$

Mean-field theory:

$$H_{mf} = \sum_{\mathbf{p}} \left\{ \Psi^\dagger(\mathbf{p})[H_{ef}(\mathbf{p}) + u\mathbb{1} + vG]\Psi(\mathbf{p}) + \frac{v^2 - u^2}{2V} \right\}$$

$$u = \langle \sum \Psi^\dagger(\mathbf{p})\Psi(\mathbf{p}) \rangle$$

$$v = \langle \sum \Psi^\dagger(\mathbf{p}) G \Psi(\mathbf{p}) \rangle$$

with G as Minkowski metric. Both would violate D-class condition.

Integration over fermions yields:

$$v = \Omega e^{-1/[2V\mathcal{N}(0)]}$$

$$\mathcal{N}(\xi) = \sum_{\mathbf{p}} \delta(\xi - \xi(\mathbf{p}))\left[g_1^2(\mathbf{p}) + g_2^2(\mathbf{p})\right]$$

where

$$g_0(\mathbf{p}) = -\frac{\mathbf{a}^2(\mathbf{p})}{\mathbf{a}^2(\mathbf{p}) + \mathbf{b}^2(\mathbf{p})},$$
$$g_1(\mathbf{p}) = \frac{\mathbf{b}^2(\mathbf{p})}{\mathbf{a}^2(\mathbf{p}) + \mathbf{b}^2(\mathbf{p})}.$$

are coefficients of the projection of Minkowski's G onto zero-modes.

Critical Hamiltonian becomes

$$H_{mf,\xi} = \xi(\mathbf{p})\sigma_3 + vg_1(\mathbf{p})\sigma_1 + vg_0(\mathbf{p})$$

with

$$\xi(\mathbf{p}) = \tfrac{1}{2}[|\mathbf{a}(\mathbf{p}) + \mathbf{b}(\mathbf{p})| - |\mathbf{a}(\mathbf{p}) - \mathbf{b}(\mathbf{p})|]$$

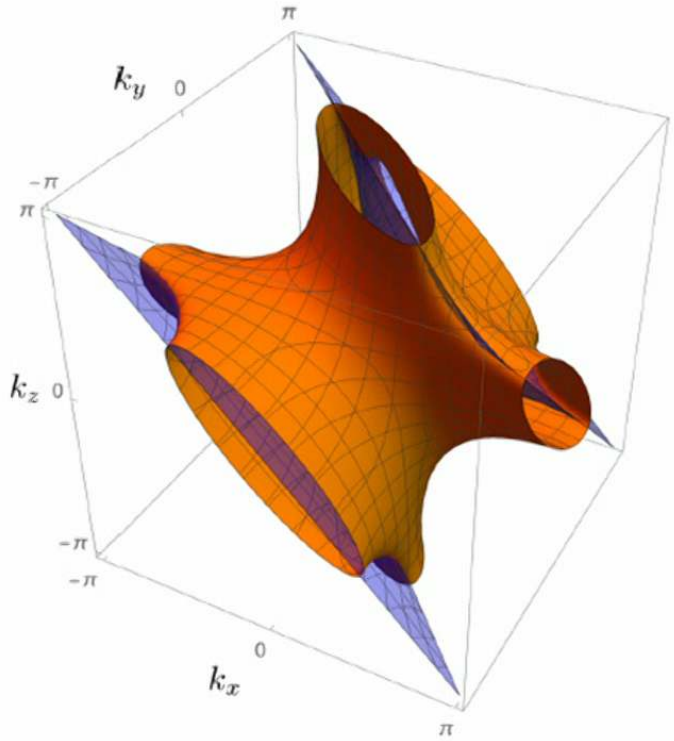
Zero-energy modes are now at

$$\xi^2(\mathbf{p}) = v^2\left[g_0^2(\mathbf{p}) - g_i^2(\mathbf{p})\right]$$

or in the lattice model, at

$$[\mathbf{a}(\mathbf{p}) \cdot \mathbf{b}(\mathbf{p})]^2 = v^2[\mathbf{a}(\mathbf{p})^2 - \mathbf{b}(\mathbf{p})^2]$$

The result: split (RHS>0) and gap (RHS<0)



new surface!

(Oh, Moon, PRB, 2020; IH, Link, PRB 2021)

Conclusions:

1) Time-reversal symmetry breaking implies BF surfaces at weak coupling, with or without inversion ; effective Hamiltonian from integration over heavy states

2) With inversion preserved, effective Hamiltonian is a generator of SO(4) in fundamental representation -> analogy with spec. relativity

3) Inversion even if present may be spontaneously broken by residual interaction, but the BF surface is only reduced (in our lattice model)