

Jackiw - Rebbi States

Solitons with fermion number 1/2

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1. Introduction

Solitons of a field theory, as discussed in a previous seminar, are wave-like solutions (that move with a constant velocity and with no dispersion) to a theory's classical equations of motion.

Back in the early 70s, understanding of solitons for scalar field theories was pretty thorough.

The first glimpse of fermionic solitons was given in a 1976 paper by Jackiw and Rebbi.

We are going to study a theory of a scalar Φ and a fermion Ψ (and possibly a non-abelian gauge field A^a_μ) with spontaneous symmetry breaking and see how this gives solitons for the fermion.

We'll expand our fermion operator in terms of Dirac eigenfunctions as

$$\Psi = a \psi_0 + \sum_{\mathbf{p}} (b_{\mathbf{p}} \psi_{\mathbf{p}^+} + d_{\mathbf{p}}^\dagger \psi_{\mathbf{p}^-}), \quad (1.1)$$

Where ψ^c indicates the charge conjugate solution, and ψ_0 is the single self-conjugate solution. These states do not necessarily represent particle annihilation and creation, but we have anticommutation relations such as

$$\{a, a^\dagger\} = 1, \quad (1.2)$$

$$\{a, a\} = \{a^\dagger, a^\dagger\} = 0.$$

We'll see that this is achieved by letting the lowest energy (soliton) state to be a degenerate doublet.

In section 2 we'll study (1+1) dimensional models and show how it would exemplify higher dimensional features. Then in section 3 we shall see how this type of state shows up in the study of topological materials, applying it to the polyacetylene molecule.

2. One dimensional models

2.1. Classical solutions

We start by studying the 1D Lagrangian

$$\mathcal{L} = \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi + \bar{\Psi} i \not{\partial} \Psi - \frac{1}{g^2} U(g\Phi) - G \bar{\Psi} V(g\Phi) \Psi \quad (2.1)$$

We use the gamma matrices $\gamma^0 = \sigma_x$, $\gamma^1 = i\sigma_z$. In this representation, the charge conjugation matrix is given by just σ_z :

$$\psi^c = \sigma_z \psi^* \quad (2.2)$$

The classical equations of motion are

$$\partial_\mu \partial^\mu \phi_c + \frac{1}{g} U'(\phi_c) + G g \bar{\psi}_c V'(\phi_c) \psi_c = 0 \quad (2.3)$$

$$(i\not{\partial} - G V(\phi_c)) \psi_c = 0 \quad (2.4)$$

We are to suppose that (2.3) has kink/antikink solutions in the absence of fermions, i.e. there's a stationary finite energy solution $\phi_c(x)$ that satisfies

$$\frac{1}{2} (\phi_c')^2 = \frac{1}{g^2} U(\phi_c), \quad (2.5)$$

$$\phi_c(+\infty) = -\phi_c(-\infty).$$

The Yukawa term is also postulated to satisfy

$$\lim_{x \rightarrow +\infty} G V(\phi_c) = - \lim_{x \rightarrow -\infty} G V(\phi_c) \equiv m > 0. \quad (2.6)$$

A nice example to show we aren't pulling things out of thin air is

$$U(\phi) = \frac{\lambda^2}{2} (1 - \phi^2)^2, \quad (2.7)$$

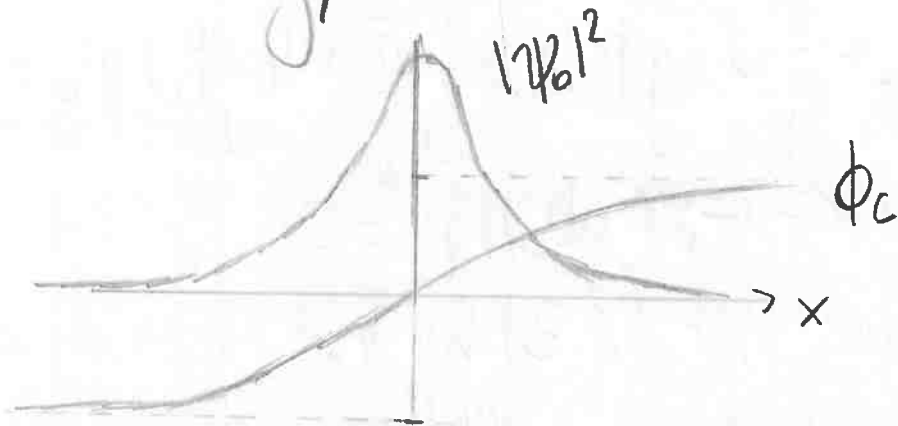
$$V(\phi) = \phi,$$

$$\phi_c = \frac{1}{g} \tanh \lambda(x - x_0), \quad m = G.$$

Note that under the conditions we've specified, the spinor has 2 single static normalizable solutions,

$$\psi_0 = N \exp \left\{ -G \int_{x_0}^x dx' V(\phi_c) \right\} s_{\pm} \quad (2.8)$$

where we are denoting $s_{+} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $s_{-} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. ψ_0 is a self-conjugate zero energy mode.



The other solutions should form a continuous spectrum of "momentum" p and energies E with $|E| \geq \sqrt{p^2 + m^2}$, labeled $\psi_{p\pm}$. Ignoring other possible bound states we must have something like

$$\int \frac{dp}{2\pi} [\psi_{p+}^{\dagger}(x) \psi_{p+}(y) + \psi_{p-}^{\dagger}(x) \psi_{p-}(y)] = \delta(x-y) - \psi_0^{\dagger}(x) \psi_0(y). \quad (2.9)$$

Let's begin to discuss quantum properties of this system.

2.2. Quantum considerations

First note that, after spontaneous symmetry breaking, the Lagrangian (2.1) describes a scalar with mass

$$\mu = \lim_{x \rightarrow +\infty} \sqrt{U''(g\phi_c)} \text{ and 2 fermions of mass}$$

$$m = \lim_{x \rightarrow +\infty} GV(g\phi_c), \text{ with respect to the vacuum.}$$

However, the existence of the stationary $\phi_c(x)$ solution indicates there should be solitons in the theory.

As such, we postulate the existence of one-soliton states of momentum P and mass M (of $O(g^{-2})$) $|P_{\pm}\rangle$. The label \pm indicates a two-fold degeneracy that is required by the zero-energy fermion solution. The state $+$ is "soliton" while $-$ is an "anti-soliton". Our goal is to work perturbatively in g .

Inspired by the ϕ^4 theory, we postulate $\langle P'_{\pm} | \Phi | P_{\pm} \rangle$ is of order g^{-1} , while other matrix elements are at least an order lower, or vanish. Sandwiching Φ 's EoM with the states we get

$$\begin{aligned} \{ (E(P') - E(P))^2 - (P' - P)^2 \} \langle P'_{\pm} | \Phi | P_{\pm} \rangle & \quad (2.10) \\ & = \frac{1}{g} \langle P'_{\pm} | U'(g\Phi) | P_{\pm} \rangle + Gg \langle P'_{\pm} | \bar{\Psi} V'(g\Phi) \Psi | P_{\pm} \rangle \end{aligned}$$

Writing $\langle P_{\pm} | \langle P_{\pm} | \Phi | P_{\pm} \rangle = \int dx e^{i(P' - P)x} f(x)$ (2.10)

To leading order, where we drop the energy difference and the first matrix element, we get

$$f'' = \frac{1}{g} V'(gf)$$

So to leading order $f = \Phi_c$. The mass is then, to this order,

$$M \approx E[\Phi_c] = \int dx \left[\frac{1}{2} (\Phi_c')^2 + \frac{1}{g^2} V(g\Phi_c) \right] = O(g^{-2}),$$

as expected.

Now we go to next order in g , and the fermions start to make a difference. We add new particles to the soliton state.

We can have an extra meson of momentum k , with a state

$$|P_{\pm}, k\rangle \text{ and energy } E(P) + w(k) = E(P) + \sqrt{\mu^2 + k^2}$$

to lowest order, and the soliton with extra fermion/anti-

$$\text{fermion } |P_{\pm}, p_{\pm}\rangle \text{ with energy } E(P) + \mathcal{E}(p) = E(P) + \sqrt{m^2 + p^2}.$$

We now show that the matrix elements

$$\begin{aligned}\langle p'_- | \Psi | p_+ \rangle &= \langle p_+ | \Psi^\dagger | p'_- \rangle^* \\ &= \int dx e^{i(p'_- - p_+)x} u_0(x), \quad (2.11a)\end{aligned}$$

$$\begin{aligned}\langle p'_\pm | \Psi | p_\pm, p_+ \rangle &= \langle p_\pm, p_+ | \Psi^\dagger | p'_\pm \rangle^* \\ &= \int dx e^{i(p'_\pm - p_\pm - p_+)x} u_p(x), \quad (2.11b)\end{aligned}$$

$$\begin{aligned}\langle p'_\pm | \Psi^\dagger | p_\pm, p_- \rangle &= \langle p_\pm, p_- | \Psi | p'_\pm \rangle^* \\ &= \int dx e^{i(p'_\pm - p_\pm - p_-)x} v_p^*(x), \quad (2.11c)\end{aligned}$$

$$\begin{aligned}\langle p'_\pm | \Phi | p_\pm, k \rangle &= \langle p_\pm, k | \Phi | p'_\pm \rangle^* \\ &= \int dx e^{i(p'_\pm - p_\pm - k)x} \frac{f_k(x)}{\sqrt{2\omega(k)}}. \quad (2.11d)\end{aligned}$$

Are of order g^0 . All other elements either vanish or are of higher order. Note that Ψ can cause transitions between $|p_\pm\rangle$. Consider the EOM for Ψ now,

$$\begin{aligned}i\gamma^0 [E(p) - E(p')] + \gamma^1 (p - p') \langle p_- | \Psi | p_+ \rangle \\ = G \langle p'_- | V(g\Phi) \Psi | p_+ \rangle\end{aligned}$$

To $O(g^0)$ the energy difference does not contribute, and

$$\begin{aligned}\langle p'_- | V(g\Phi) \Psi | p_+ \rangle &= \int \frac{dp''}{2\pi} \langle p'_- | V(g\Phi) | p''_- \rangle \langle p''_- | \Psi | p_+ \rangle \\ &= \int dx e^{i(p'_- - p_-)x} V(gf(x)) u_0(x)\end{aligned}$$

So ψ_0 satisfies the static Dirac eq

$$i\gamma^1 \psi_0' - G V(g\phi_c) \psi_0 = 0 \quad (2.12)$$

Awesome. Now for $\langle P_{\pm} | \Psi | P_{\pm}, p_{\pm} \rangle$ we analogously get to $\mathcal{O}(g_0)$

$$i\gamma^1 \psi_p' - G V(g\phi_c) \psi_p = -\mathcal{E}(p) \gamma^0 \psi_p \quad (2.13)$$

$$i\gamma^1 \psi_p^{*'} - G V(g\phi_c) \psi_p^* = \mathcal{E}(p) \gamma^0 \psi_p^*$$

$$i\gamma^1 (\sigma_z \psi_p^*)' - G V(g\phi_c) (\sigma_z \psi_p^*) = -\mathcal{E}(p) \gamma^0 (\sigma_z \psi_p^*) \quad (2.14)$$

Before we identify ψ_0, ψ_p and $\sigma_z \psi_p^*$ as the solutions $\Psi_0, \Psi_{p\pm}$, we need to normalize them. Remembering the equal time commutation relations,

$$\langle P'_{\pm} | \{ \Psi^{\dagger}(x), \Psi(y) \} | P_{\pm} \rangle = \delta(x-y) (2\pi) \delta(P-P')$$

Using the matrix elements we've defined before, and we get with completeness relations

$$\langle P'_{+} | \Psi^{\dagger}(x) \Psi(y) | P_{+} \rangle = \int dz e^{i(P'-P)z} \psi_0^{*}(x+z) \psi_0(y+z)$$

$$+ \int dz e^{i(P'-P)z} \int \frac{dp}{2\pi} \psi_p^{*}(x+z) \psi_p(y+z)$$

$$\langle P'_{-} | \Psi^{\dagger}(x) \Psi(y) | P_{-} \rangle = \int dz e^{i(P'-P)z} \int \frac{dp}{2\pi} \psi_p^{*}(x+z) \psi_p(y+z)$$

$$\langle P'_+ | \Psi(y) \Psi^\dagger(x) | P_+ \rangle = \int dz e^{i(P'_+ - P_+)z} \int \frac{dp}{2\pi} u_p^*(x+z) u_p(y+z)$$

$$\begin{aligned} \langle P'_- | \Psi(y) \Psi^\dagger(x) | P_- \rangle &= \int dz e^{i(P'_- - P_-)z} u_0^*(x+z) u_0(y+z) \\ &+ \int dz e^{i(P'_- - P_-)z} \int \frac{dp}{2\pi} u_p^*(x+z) u_p(y+z) \end{aligned}$$

So in the end, we have

$$\langle P'_\pm | \{ \Psi^\dagger(x), \Psi(y) \} | P_\pm \rangle =$$

$$\int dz e^{i(P'_\pm - P_\pm)z} \left[u_0^*(x+z) u_0(y+z) + \int \frac{dp}{2\pi} (u_p^*(x+z) u_p(y+z) + v_p^*(x+z) v_p(y+z)) \right]$$

So in order for stuff to be normalized, we should identify

$$\Psi_0 = u_0, \quad \Psi_{p+} = u_p, \quad \Psi_{p-} = v_p.$$

We have established a complete, normalized set of states!

Finally, for 2.11d, the lowest order equation of motion is

$$f_k'' + \omega(k)^2 f_k = U''(g\phi_c) f_k$$

This is almost a harmonic oscillator. The important part is that these solutions must be normalized to unity, so $f_k \sim \mathcal{O}(g^0)$

Now let's compute the fermion number of the soliton states

We must have

$$n_{\pm} = \frac{1}{2} \langle P_{\pm} | \Psi^{\dagger} \Psi - \Psi \Psi^{\dagger} | P_{\pm} \rangle$$

$$n_{\pm} = \frac{1}{2} \int dz \left\{ \pm v_0^*(z) v_0(z) \right.$$

$$\left. + \int \frac{dp}{2\pi} [v_p^*(z) v_p(z) - u_p^*(z) u_p(z)] \right\} = \pm \frac{1}{2}$$

2.3. Extensions

This calculation of the fermion number can be done with perturbative expansions using the collective position operator method. Define (PRD 11 2943 1975)

$$\hat{\Phi}(x) = \hat{\Phi}(x-X) + \phi_c(x-X)$$

$$\hat{\Psi}(x) = \hat{\Psi}(x-X) + a \psi_c(x-X)$$

with the conditions

$$\int dx \phi_c' \hat{\Phi} = 0,$$

$$\int dx \psi_0^* \hat{\Psi} = 0.$$

Postulate the existence of soliton/antisoliton states $|P_{\pm}\rangle$ and define a to be such that

$$a|P_+\rangle = |P_-\rangle$$

$$a^\dagger|P_-\rangle = |P_+\rangle, \quad \{a, a^\dagger\} = 1$$

The charge conjugation must act on a as

$$\mathcal{F} a \mathcal{F}^\dagger = a^\dagger$$

and therefore

$$\mathcal{F}|P_\pm\rangle = |P_\mp\rangle$$

From the orthogonality we've established,

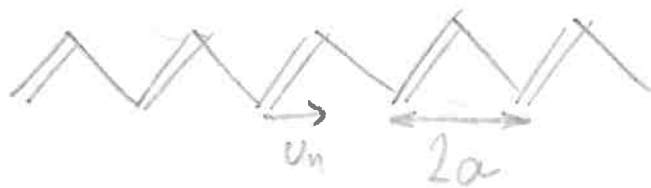
$$n_\pm = \frac{1}{2} \langle P_\pm | a^\dagger a - a a^\dagger | P_\pm \rangle$$

$$\Rightarrow n_\pm = \pm \frac{1}{2}$$

This works for any solitonic theory in any dimension of spacetime.

3. Polyacetylene

We'll now take a look at the Su-Schrieffer-Heeger model for trans-polyacetylene.



We allow the displacement of the carbon atoms from equilibrium u_n , with some spring constant K and mass M

$$H_{\text{carbon}} = \sum_n \frac{1}{2} M \dot{u}_n^2 + \frac{1}{2} K (u_n - u_{n+1})^2$$

and treat the π electrons with a tight binding model,

$$H_{\text{electrons}} = - \sum_{n,s} t_{n,n+1} (c_{n+1,s}^\dagger c_{n,s} + c_{n,s}^\dagger c_{n+1,s})$$

Where $c_{n,s}$ annihilates an electron of spin s in site n , and we approximate

$$t_{n,n+1} = t_0 - \alpha (u_{n+1} - u_n)$$

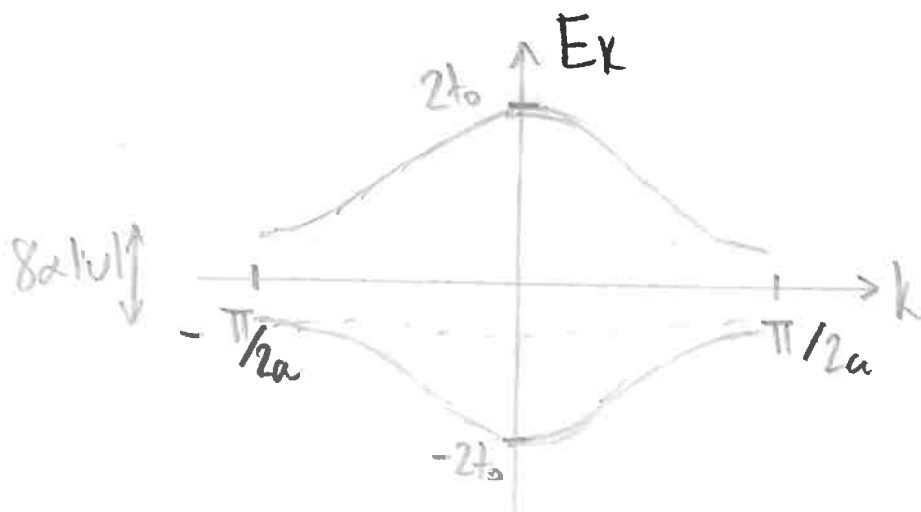
3.1. Effective u potential

We neglect the carbon kinetic energy and set $u_n = (-1)^n u$. We have

$$H_d = - \sum_{n,s} [t_0 + (-1)^n 2\alpha u] (c_{n+1,s}^\dagger c_{n,s} + c_{n,s}^\dagger c_{n+1,s}) + 2NK u^2$$

Now let's exploit the periodicity. Call $a_n = c_{2n-1}$ and $b_n = c_{2n}$. We can then write

the Hamiltonian



The system's ground state is at half-filling so we can write an effective potential for u :

$$V(u) = 2NKu^2 - 2 \sum_k [(2t_0 \cos ka)^2 + (4\alpha u \sin ka)^2]^{1/2}$$

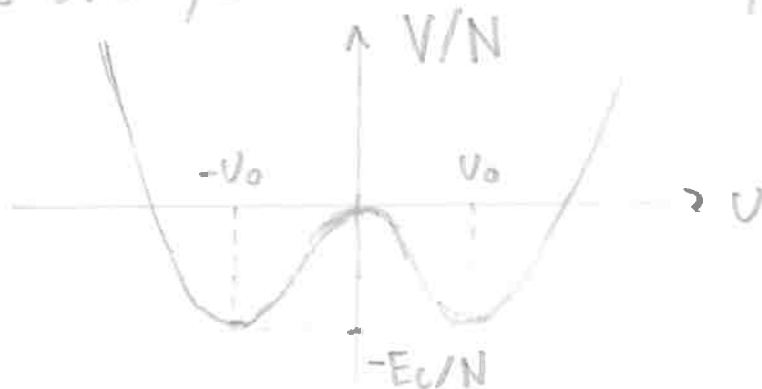
$$V(u) \approx 2NKu^2 - \frac{2L}{\pi} \int_0^{\pi/2a} dk [(2t_0 \cos ka)^2 + (4\alpha u \sin ka)^2]^{1/2}$$

$$= \frac{NKt_0^2}{2\alpha^2} z^2 - \frac{4Nt_0}{\pi} \int_0^{\pi/2} dx \sqrt{1 - (1 - z^2) \sin^2 x}$$

with $z = \frac{2\alpha u}{t_0}$. But, for small z ,

$$\int_0^{\pi/2} dx \sqrt{1 - (1 - z^2) \sin^2 x} \approx 1 + \frac{1}{2} \left(\log \frac{4}{|z|} - \frac{1}{2} \right) z^2 + O(z^4)$$

So $z=0$ is always unstable! We can plot V for typical values



$$H_d = 2NKv^2 - \sum_{n,s} \left\{ (t_0 - 2\alpha v) (b_{n+1,s}^\dagger a_{n,s} + a_{n,s}^\dagger b_{n+1,s}) + (t_0 + 2\alpha v) (a_{n,s}^\dagger b_{n-1,s} + b_{n-1,s}^\dagger a_{n,s}) \right\}$$

now we Fourier transform

$$f_k = \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} = \sqrt{\frac{2}{N}} \sum_n e^{-ik \cdot 2an} \begin{pmatrix} a_n e^{\frac{ika}{2}} \\ b_n e^{-\frac{ika}{2}} \end{pmatrix}$$

and inverting,

$$\begin{pmatrix} a_n \\ b_n \end{pmatrix} = \sqrt{\frac{2}{N}} \sum_k e^{ik \cdot 2an} \begin{pmatrix} \alpha_k e^{-\frac{ika}{2}} \\ \beta_k e^{\frac{ika}{2}} \end{pmatrix}$$

Which lets us write in momentum space

$$H_d = 2NKv^2 - \sum_{k,s} \left\{ (t_0 - 2\alpha v) (\beta_{k,s}^\dagger \alpha_{k,s} e^{ika} + \alpha_{k,s}^\dagger \beta_{k,s} e^{-ika}) + (t_0 + 2\alpha v) (\alpha_{k,s}^\dagger \beta_{k,s} e^{ika} + \beta_{k,s}^\dagger \alpha_{k,s} e^{-ika}) \right\}$$

$$H_d = 2NKv^2 - \sum_{k,s} f_{k,s}^\dagger \begin{pmatrix} 2t_0 \cos ka + 4i\alpha v \sin ka & \\ 2t_0 \cos ka - 4i\alpha v \sin ka & \end{pmatrix} f_k$$

The k-dependent part has eigenvalues

$$E_k = \pm \sqrt{(2t_0 \cos ka)^2 + (4\alpha v \sin ka)^2}, \text{ which has a band gap } 8\alpha v$$

We can then approximate

$$V(z) \approx \frac{NKt_0^2}{2\alpha^2} z^2 + \frac{2Nt_0}{\pi} \left(\frac{1}{2} + \log \frac{|z|}{4} \right) z^2 + \frac{4Nt_0}{\pi}$$

which has its true minimum at

$$\pm v_0 = \pm \frac{2t_0}{\alpha} \exp \left\{ -\frac{\pi K t_0}{4\alpha^2} \right\}$$

This indicates spontaneous symmetry breaking. A nice order parameter to use would be something like

$$\phi_n \sim (-1)^n v_n, \quad \phi_n(v_0) = m/g.$$

After some rescalings and coarse-graining, we see that the dynamics for ϕ_n can be recovered from a Lagrangian

$$\mathcal{L}_{\text{scalar}} = \frac{1}{2} \left(\frac{\partial \phi}{\partial t} \right)^2 - \frac{1}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 - U(\phi)$$

3.2. Low energy electrons

Remember the electron Hamiltonian we had,

$$H_{\text{electron}} = \sum_{k,s} \int_{k,s}^{\dagger} \begin{pmatrix} 0 & 2t_0 \cos ka + 4i\alpha v \sin ka \\ 2t_0 \cos ka - 4i\alpha v \sin ka & 0 \end{pmatrix} f_{k,s}$$

Expanding around $k = \frac{\pi}{2a} + q$,

$$H_{\text{electron}} \approx -\sum_{q,s} \int_{q,s}^{\dagger} \begin{pmatrix} 0 & -2t_0qa + 4i\alpha v \\ -2t_0qa - 4i\alpha v & 0 \end{pmatrix} \int_{q,s}$$

This is a Dirac Hamiltonian!

$$H_q = 2t_0a \sigma_x q + 4\alpha v \sigma_y$$

with $\gamma^0 = \sigma_y$, $\gamma^0 \gamma^1 = \sigma_x \Rightarrow \gamma^1 = -i\sigma_z$.

So the dynamics of the electrons can be recovered from

$$\mathcal{L}_{\text{electron}} = \bar{\Psi} (i\partial_t - G\phi) \Psi$$

with $\Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$, $\partial = \gamma^0 \frac{\partial}{\partial t} + \gamma^1 v_F \frac{\partial}{\partial x}$, $v_F = 2t_0a$.

Together with $\mathcal{L}_{\text{scalar}}$, this is exactly the Jackiw-Rebbi model!

3.3. Berry phase and topological protection

We have the two possible dimerization states for uniform ϕ :

ϕ :



$$\phi = m/G$$



$$\phi = -m/G$$

For constant Φ_0 , ignoring spin, the Hamiltonian for the electron momentum eigenstates is

$$H_k = - \begin{pmatrix} 0 & \frac{v_F}{a} \cos ka + i G \Phi_0 \sin ka \\ \frac{v_F}{a} \cos ka - i G \Phi_0 \sin ka & 0 \end{pmatrix}$$

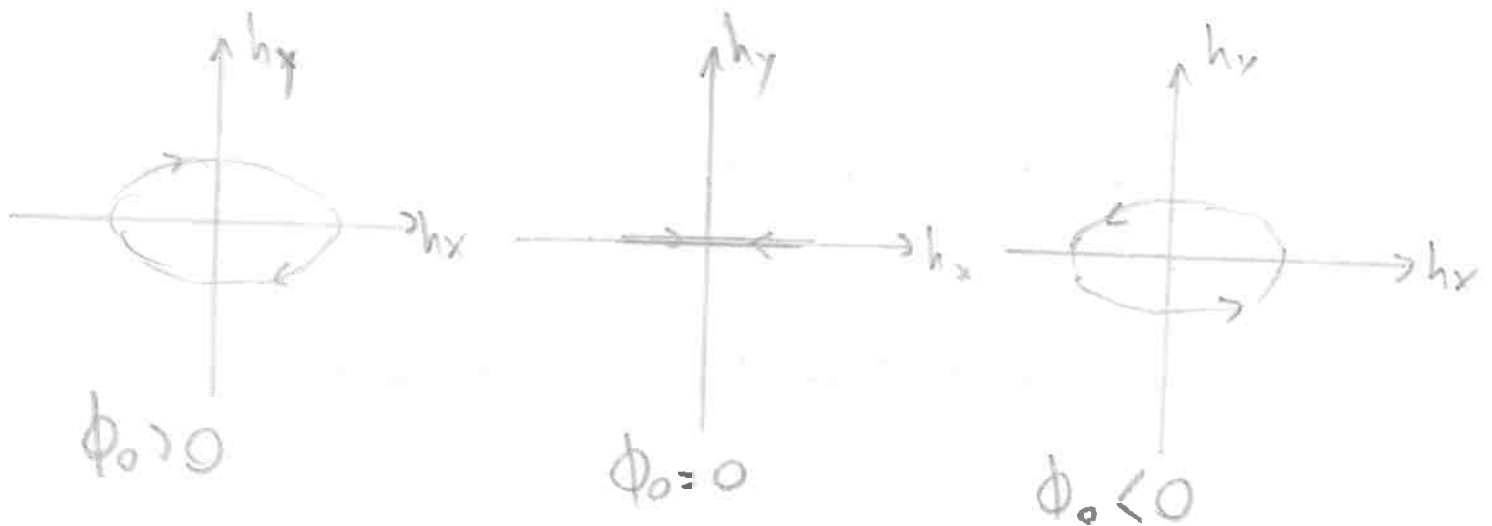
So the eigenstates are $|\Psi_{q\pm}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm e^{-i\theta_k} \end{pmatrix}$ of energy

$$\pm E_k = \pm \sqrt{\left(\frac{v_F}{a} \cos ka\right)^2 + (G \Phi_0 \sin ka)^2}, \text{ with}$$

$$\theta_k = \arctan\left(\frac{G \Phi_0 a}{v_F} \tan ka\right). \text{ If we write}$$

$$H_k = \vec{h}(k) \cdot \vec{\sigma},$$

$\vec{h}(k)$ has some nice curves



Changing the sign of Φ_0 changes the winding direction of the ellipse! There must be something topological going on.

The Berry Phase is an adiabatic invariant when discrete symmetries are to be maintained

$$\gamma = \oint \vec{A} \cdot d\vec{R}$$

$$\vec{A} = \langle u(\vec{R}) | i \nabla_{\vec{R}} | u(\vec{R}) \rangle$$

Taking $R = k$ we have

$$A = \frac{1}{2} \frac{d\theta_k}{dk} \Rightarrow \gamma = \frac{1}{2} (\theta_{\frac{\pi}{2a}} - \theta_{-\frac{\pi}{2a}})$$

In conclusion

$$\gamma = \begin{cases} \pi/2, & \phi_0 > 0 \\ 0, & \phi_0 = 0 \\ -\pi/2, & \phi_0 < 0 \end{cases}$$

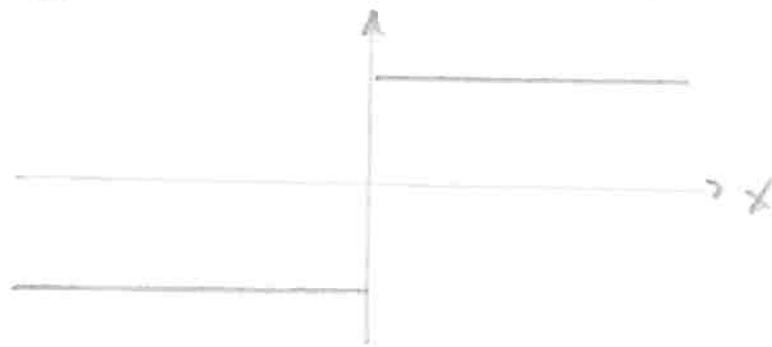
so the configurations are topologically distinct!

The transition from $m/G \leftrightarrow -m/G$ is called a topological phase transition.

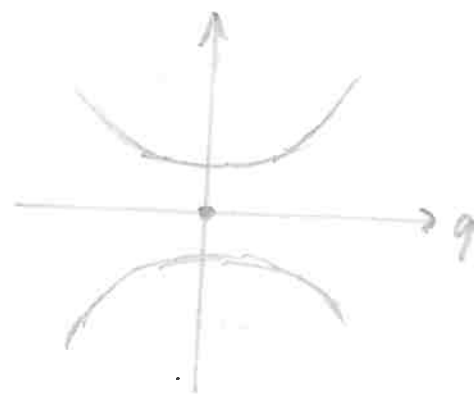
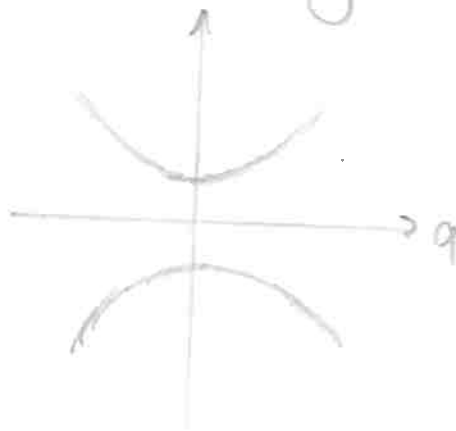
To see how Jackiw-Rebbi states show up now, consider an initial configuration with $\phi_0 = m/G$



And 2 configuration where Φ changes sign



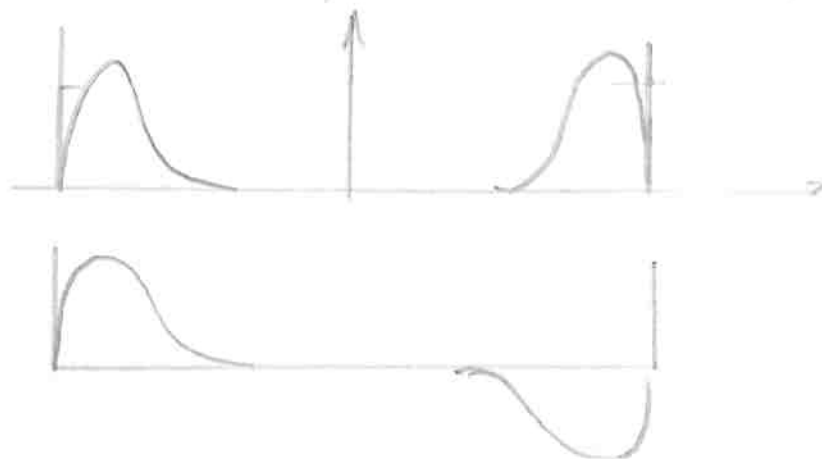
The low energy band structures are respectively



The zero energy mode has no chiral partner, so the transition between the two behaviors is protected by the chiral symmetry.

3.4. Bulk-boundary correspondence

If our object is finite in length, an expansion to $O(q^2)$ leads to boundary states with very low energy,



So even though the material has a finite band gap, electrons can hop between its edges!

This is what's called a topological insulator.

4. References

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