Note on non-Hermitian Topological Insulators

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Abstract

This note reviews basic concepts and relative techniques in $\mathcal{PT}$-symmetric Hamiltonian systems. Then we focus on recent theoretical progresses in non-Hermitian topological band theory for those systems which are not only $\mathcal{PT}$-symmetric but arbitrary form.

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Generic Discussions of $\mathcal{PT}$ Symmetry

In standard quantum theory, we learned that due to the requirement of probability conserving, the Hamiltonian operator should be Hermitian, i.e $H = H^\dagger$ where $\dagger$ denotes complex conjugation. People now realize that this axiom can be loosen and replaced by space-time reflection symmetry or $\mathcal{PT}$ symmetry. The main conclusion of quantum theory remains intact but as an expansion of Hermitian theory, this non-Hamiltonian theory also presents interesting and fancy properties.

1.1 Review of the $\mathcal{P}$ and $\mathcal{T}$ Operator

1. The parity transformation is defined as: $\mathcal{P} : \vec{x} \rightarrow -\vec{x}$ thus $\mathcal{P}^2 = 1, \mathcal{P} x \mathcal{P}^{-1} = -x$. (Definition up to a trivial phase)

2. $\mathcal{P}$: The most important consequence in non-relativistic quantum theory is that the central potential problems have selection rule.

3. The time reversal transformation is defined as: $\mathcal{T} : t \rightarrow -t$. Thus, $\mathcal{T} x \mathcal{T}^{-1} = x, \mathcal{T} p \mathcal{T}^{-1} = -p$. In short, $\mathcal{T} i \mathcal{T}^{-1} = -i$.

4. The direct consequence from the identities above is: $\mathcal{T}^2 = \phi$ and $\mathcal{T} = U \mathcal{K}$. Therefore, the TR operator cannot be represented as a normal matrix but an unitary one times the complex-conjugation operator $\mathcal{K}$. There also exists some constraints of $U$: $U = \phi U^\dagger, U^\dagger = U \phi$ thus $U = \phi U \phi$ and $\phi = \pm 1$. This is an intuitive result when we recall that $\mathcal{T}$ is anti-unitary for unitary matrix can be defined up to any phases.

5. $\mathcal{T}$: The most important consequence in TR-invariant system is the Kramers’ theorem.

6. For $\mathcal{T} \mathcal{P} \phi (x) = \mathcal{T} \phi (-x) = \phi^* (-x) = \mathcal{P} \mathcal{T} \phi (x), \mathcal{P}$ and $\mathcal{T}$ are commutable.

1.2 Real spectrum of non-Hermitian Hamiltonian

We first present a proof that if the $\mathcal{PT}$ is hold, with some constraints, the spectrum of $H$ is real. We first explore the properties of $\mathcal{PT}$ for 1-D and spinless system:

$$H \phi = E \phi$$
$$\mathcal{PT} \phi = \lambda \phi$$
$$\rightarrow \mathcal{PT} \mathcal{PT} \phi = \mathcal{PT} (\lambda \phi)$$
$$\rightarrow \mathcal{PT} \mathcal{PT} \phi = \phi = \lambda^* \mathcal{PT} \phi = \lambda^* \lambda \phi$$

Thus, $\lambda = e^{i\alpha}$ and becomes a trivial phase(by redefine the function $\phi$).

We make the assumption then: the vector $\phi$ is simultaneously an eigenstate of $H$. This is nontrivial because $\mathcal{PT}$ is not linear but antilinear. For linear operators, those commute operators have common eigenvectors. But for antilinear operator, it’s a different case because the proof of that statement involves expanding the eigen vector as a superposition of another operator’s eigen vector i.e, the operator should be block-diagonal and then the other only should be diagonalized based on the basis generated from the block-diagonalization - this where we need linear property.
Under this assumption, we have

\[ H\phi = E\phi \]
\[ \mathcal{PT}(H\phi) = E^*\mathcal{PT}\phi = E^*\phi \]
\[ H\mathcal{PT}\phi = H\phi = E\phi \] (1.2)

As the assumption implied, we have \((E - E^*)\phi\) vanishes. For nontrivial \(\phi\), we conclude that for spinless system \(E = E^*\) so \(E\) is real.

In this proof, we basically consider two assumptions:

1. Assumption 1: \(\mathcal{PT}^2 = +1\) which turns out to be correct for spinless particle.
2. Assumption 2: The vector \(\phi\) is simultaneously an eigenstate of \(H\) and \(\mathcal{PT}\).
3. Note that for \(H\) non-degeneracy case, the antilinearity does notings.

In Dirac’s bracket notation, we know that the right vector is in the dual space of left vector and because of the Hermiticity, the right vector is related to left vector. However, it can be proved that for non-Hermitian system, right vector \(|\psi^R\rangle\) have nothing to do with \(|\psi^L\rangle\) with the definition:

\[ H |\psi^R_n\rangle = E_n |\psi^R_n\rangle \]
\[ H^\dagger |\psi^L_n\rangle = E_n^* |\psi^L_n\rangle \] (1.3)

Even if they share the same eigenvalue. This make a little difficulty for us to define Chern number for there exists several different kinds of Berry curvatures.

We then recall that there exists generalization connection between right wave function and left one:

For non-degenerate and non-Hermitian \(H\), take the diagonalization of it: \(HP = PA\) where \(A = \text{diag}(\lambda_i)\) and \(P^{-1}P = I\). we have the \(n\)-th column of \(P\) as the right eigenvector corresponding to eigenvalue \(E_n\) denoted by \(|\psi^R_n\rangle\) and we have equivalently \(H^\dagger(P^{-1})^\dagger = (P^{-1})^\dagger A^*\), thus the \(n\)-th column of \((P^{-1})^\dagger\) is the left eigenvector of \(H\) corresponding to eigenvalue \(E_n^*\) denoted by \(|\psi^L_n\rangle\). Thus we conclude \(\langle\psi^L_n |\psi^R_m\rangle = \delta_{mn}\)

It naturally to ask about how to treat \(H^\dagger |\psi^R_n\rangle, H |\psi^L_n\rangle\). By using the fact that \(I = \sum_m |\psi^R_m\rangle \langle\psi^L_m|\), we have:

\[ H |\psi^L_m\rangle = \sum_n (E_n |\psi^R_n\rangle \langle\psi^L_n|) |\psi^L_m\rangle \]
\[ H^\dagger |\psi^R_m\rangle = \sum_n (E_n^* |\psi^L_n\rangle \langle\psi^R_n|) |\psi^R_m\rangle \] (1.4)

1.3 Other Perspectives in \(\mathcal{PT}\) Symmetry

Here comes a collection of hot topics in \(\mathcal{PT}\) symmetry quantum theory. Most of them can be easily google out.

1. Other symmetry: From the discussion above, \(\mathcal{P}\) is a generic class of symmetries as long as its action on the Hilbert space mimics the definition in 1.1.1.
2. Quantum measurement: It’s recently reported that the quantum

3. \( \mathcal{PT} \) symmetry breaking: is it a phase transition? Does this have
critical behavior?

**Exercise:** Find the correct \( \mathcal{P} \) and \( \mathcal{T} \) in the 0D,1D free spin-x system.

## 2 Topological Band Theory

Note that in conventional system, to keep loss and gain in balance is a nontrivial
task, and even having achieved this, the system can still be in a \( \mathcal{PT} \)
symmetry broken phase. To this end, we should develop a more generic theory without
\( \mathcal{PT} \)

### 2.1 From a 2+1D EM theory perspective

It’s natural to test the topological band theory from a pure gauge thoery because
the whole theory of Berry curvature (or quantum metric ) has been developed
in fiber bundle theory. But intuitively we can start from (2+1 D) EM thoery.
In a insulator sheet of classical electron, we have the polarization:

\[
\vec{P}(\omega) \approx \frac{Nm^{-1}}{\omega_0^2 - \omega^2 - i\omega\kappa} \vec{E}
\]

and thus, \( \epsilon = \Re + i\Im \). With the definition above, we have a functional basis in
2+1D function space \( \mathcal{W} \) generated by the wave equation of \( \vec{E} \) is \( \partial_t^2 - \nabla^2 = k^2 - \omega^2 \)
with \( \vec{k} = \vec{\beta} + i\vec{\alpha} \) where \( \vec{\beta}, \vec{\alpha} \) is real vector. To ensure the orthogonal relation, we
have to make a fake ‘left’ space \( \mathcal{W} \) which seems a good friend with
\( \mathcal{W} \):

\[
\hat{e}_{\mathcal{W}(x,t)}(\omega, \vec{k}) = e^{-\vec{\alpha} \vec{x}} e^{i(\vec{\beta} \cdot \vec{x} - \omega t)}
\]

\[
\hat{e}_{\mathcal{W}^*(x,t)}(\omega, \vec{k}) = e^{\vec{\alpha} \vec{x}} e^{i(\vec{\beta} \cdot \vec{x} - \omega t)}
\]

While the dual space of \( \mathcal{W} \) and \( \mathcal{W}^* \) is :

\[
\hat{e}_{\mathcal{W}^*(x,t)}(\omega, \vec{k})[\cdot] = \int_V d\vec{x} dt e^{-i(\vec{\beta} \cdot \vec{x} - \omega t)}[\cdot]
\]

\[
\hat{e}_{\mathcal{W}^*(x,t)}(\omega, \vec{k})[\cdot] = \int_V d\vec{x} dt e^{i(\vec{\beta} \cdot \vec{x} - \omega t)}[\cdot]
\]

It seems the ‘left’ dual space can correctly normalize the ‘right’ space : \( \hat{e}^\dagger \hat{e} = \delta \),
vice versa.

Thanks to the existence of ‘left’ space, a proper redundancy can be constructed as the ‘gauge transformation’ of the theory where

\[
\hat{e}_{\mathcal{W}(x,t)} \rightarrow \hat{e}_{\mathcal{W}(x,t)}(\omega, \vec{k}) = e^{-f(\alpha)} e^{if(\vec{\beta})} e^{-\vec{\alpha} \vec{x}} e^{i(\vec{\beta} \cdot \vec{x} - \omega t)}
\]

\[
\hat{e}_{\mathcal{W}(x,t)} \rightarrow \hat{e}_{\mathcal{W}^*(x,t)}(\omega, \vec{k}) = e^{f(\alpha)} e^{if(\vec{\beta})} e^{\vec{\alpha} \vec{x}} e^{i(\vec{\beta} \cdot \vec{x} - \omega t)}
\]

Which make the whole theory intact if there does not exist a topological defect.
Exercise: Verify the definition of basis above can safely reproduce the result of (ignore trivial $\omega$ sector):

$$(\nabla^2 - r^2)G(x, y, z) = \delta(x, y, z)$$

(In free space.)

Note that you need to use $G_R(\vec{k})$ and $G_L(\vec{k})$. When taking the inverse transformation, which dual space basis can give the proper answer? How about 2-D case?

2.2 Hint: Second Quantization Operators in Non-Hermitian Many Body System

To intuitively construct a non-Hermitian theory, we start from asking ourselves, what’s the differences between SE $i\partial_t = H$ and imaginary-time diffusion equation $\partial_t = \mathcal{L}$? That is, the solution of quantum SE, should be properly normalized according to $\langle \psi | \psi \rangle$. For a many body system, this constraint is naturally generalized to the conservation law of probability current which is the quantum version of charge continuity equation ($\partial_t \rho + \nabla \cdot j = 0$).

Beside, identical particle theory makes another constraint of the quantum system: any transformation of representation should not change the commutator of the original field operator and thus is locally unitary.

It has been learned that in non-Hermitian system, there is a violation of conservation law of probability current and in practical this can be mathematically treated by changing the boundary condition, adding source term or complex potential.

One solution of the second problem is very easy to obtain. In fundamental sense, the microscopic system is always Hermitian. The non-Hermitian Hamiltonians we encounter are always pseudo-non-Hermitian or in other words, synthetic ones. Thus, we can treat the creation and destroy operator $a^\dagger$ and $a$ as a matrix basis that represents the original system. But $a^\dagger$ no longer creates a physical quantum state of the whole system. (If it is, we need two series of them that are $a^\dagger_{L,R}, a_{L,R}$. But this seems a very tedious because the physical information are always stored in the synthetic Non Hermitian system.)
2.3 Typical Band Structure of a Dissipative Topological System

Figure 1: Some figures taken from the references.

In PRL,120,146402, H Shen, B Zhen and L Fu develop a topological band theory for non-Hermitian system. Consider a non-Hermitian Hamiltonian of a periodic system with Bloch wave eigenstate and corresponding energies $E_n(\vec{k})$, they first generalize the concepts of the gapped, fully gapped, gapless band as:

1. Separable: If $E_n(\vec{k}) \neq E_m(\vec{k})$ for all $m \neq n$ and all $\vec{k}$.
2. Isolated: if $E_n(\vec{k}) \neq E_m(\vec{k}')$ for all $m \neq n$ and all $\vec{k}, \vec{k}'$.
3. Inseparable: If at some momentum the complex-energy is degenerate with another band.

2.4 Berry curvature, Berry potential and Chern number

The corresponding band Berry curvature, Berry potential and Chern number is defined as:

1. Berry potential: $A^\alpha_{n,j} = \left\langle \psi_n^\alpha(\vec{k}) \bigg| \partial_j \psi_n^\beta(\vec{k}) \right\rangle$
2. Berry curvature: $B^\alpha_{n,i,j} = i \left\langle \partial_t \psi_n^\alpha(\vec{k}) \bigg| \partial_j \psi_n^\beta(\vec{k}) \right\rangle$
3. Chern number: $C_n^{\alpha,\beta} = \frac{1}{2\pi} \int \epsilon_{ij} B^\alpha_{n,i,j} d^2k$
Where \( \partial_i = \partial_{\xi_i} \), \( i = x, y \) for different direction, \( \alpha, \beta = R, L \) for different sector and \( n \) for different Bloch band. However, one can simply prove \( C_n^{\alpha, \beta} = C_n \). For \( R-L \) sector, one can simply take the gauge patch method to have:

\[
\tilde{A}^{RR} (\vec{k}) = A^{RR} (\vec{k}) + i \nabla_\vec{k} f (\vec{k})
\]  

(2.5)

And corresponding Chern number is:

\[
C_n^{RR} = \frac{1}{2\pi} \text{Im} \oint_{\partial P} \left( A^{RR} - \tilde{A}^{RR} \right) d\vec{l} = \frac{f (L) - f (0)}{2\pi}
\]  

(2.6)

For \( L-R \) sector, note that \( \langle \psi^L_m | \psi^R_n \rangle = \delta_{mn} \) and inspired by the Eq(1.4) we have generic transformation like:

\[
\begin{align*}
| \tilde{\psi}^R (\vec{k}) \rangle &= r (\vec{k}) e^{i f (\vec{k})} | \psi^R (\vec{k}) \rangle \\
| \tilde{\psi}^L (\vec{k}) \rangle &= \left[ r (\vec{k}) \right]^{-1} e^{i f (\vec{k})} | \psi^L (\vec{k}) \rangle
\end{align*}
\]  

(2.7)

Thus, for gauge potential:

\[
\tilde{A}^{LR} (\vec{k}) = A^{LR} (\vec{k}) + i \nabla_\vec{k} f (\vec{k}) + \nabla r (\vec{k}) r (\vec{k}) \frac{\nabla s r (\vec{k})}{r (\vec{k})}
\]

For \( \oint_{\partial P} \frac{\nabla s r (\vec{k})}{r (\vec{k})} d\vec{l} = \log \frac{r (L)}{r (0)} = 0 \), we have \( C^{LR} = C^{RR} \). With the same spirit, we have \( C^{RL} = C^{LL} \). Take the conjugate of the expression of \( C^{LR} \), one can simply obtain \( C^{LR} = C^{RL} = C^{LL} = C^{RR} \).

However, this Chern \# lost its bulk-edge correspondence as Shunyu Yao and Z. Wang have shown. They also give a very interesting proposal: to define the topological number in non-Bloch basis. Beyond the Bloch ansatz (from the inspiration of the Abelian U(1) group) \( \psi (\delta) = \exp (i k \delta) \psi (0) \), they found a generalized definition of \( \psi (\delta) = \beta^\delta \psi (0) \) which can be treated as a ‘two-side Laplace functional basis’ of original space. In this space, they thus give a non-Bloch Topological Invariant which can give a faithful bulk characterization of the bulk-edge correspondence, at least in toy model level.

If we proceed to go beyond a toy model, this ansatz may meet some difficulties: the magnetic field(ABelian gauge field) will dramatically shape the hopping matrix in a quantum level(Pierels’ substitution). In Hermitian theory, the original BZ will become a smaller magnetic BZ while we should question Yao and Wang’s theory.

Things will become even worse when we come to a non-Abelian gauge theory as I proposed in my coming paper.

To discuss those difficulties, we should first check why the Chern \# cannot characterize the edge properties.

### 2.5 Numerical Calculation of Berry Curvature and Chern Number — an Unsolved Puzzle

#### 2.5.1 Review of the Hermitian Case

The direct calculation of Chern number involves an integral of Berry curvature in the FBZ. However, the expression includes derivations of state vectors which will cause numerical obstacles. To solve this, we want to derive an expression of
Berry curvature that explicitly depends on differentiation of Hamiltonian rather than the state vectors.

To this end, we have the relation in Hermitian system that:
\[
\langle n | \partial_i (H | m) \rangle = \langle n | \partial_i (E_m | m) \rangle
\]  
(2.8)

By expanding the derivation \( \langle n | \partial_i H | m \rangle + \langle n | H \partial_i | m \rangle = 0 + E_m \langle n | H \partial_i | m \rangle \), we have a useful identity:
\[
\langle n | \partial_i m \rangle = \frac{\langle n | \partial_i H | m \rangle}{E_m - E_n}
\]  
(2.9)

Then, the berry curvature turn out to be:
\[
B_{n,ij} = i \langle \partial_i n | \partial_j n \rangle
\]
\[
= i \sum_m \langle \partial_i n | m \rangle \langle m | \partial_j n \rangle
\]
\[
= i \sum_{m \neq n} \langle \partial_i n | m \rangle \langle m | \partial_j n \rangle + i \langle \partial_i n | n \rangle \langle n | \partial_j n \rangle
\]
(2.10)

The last term can be dropped by defining the Chern number as the imaginary part of the integral. We thus have the final expression:
\[
C_n = \frac{1}{2 \pi} \int d^2 k \text{Im} \sum_{m \neq n} \frac{\langle n | \nabla H | m \rangle \times (m \leftrightarrow n) (E_m - E_n)^2}{(E_m - E_n)^2}
\]  
(2.11)

2.5.2 The non-Hermitian Case

As for non-Hermitian system, we want to verify the validity of the identity Eq(2.5). But now, the case becomes a little bit tough, e.g,
\[
\langle n^L | \partial_i (H | m^R) \rangle
\]
\[
= 0 + E_m \langle n^L | \partial_i m^R \rangle
\]
\[
= \langle n^L | \partial_i H | m^R \rangle + E_n \langle n^L | \partial_i m^R \rangle
\]  
(2.12)

Thus we have :
\[
\langle n^L | \partial_i m^R \rangle = \frac{\langle n^L | \partial_i H | m^R \rangle}{E_m - E_n}
\]  
(2.13)

Take the h.c. of it:
\[
\langle \partial_i m^R | n^L \rangle = \frac{\langle m^R | \partial_i H^\dagger | n^L \rangle}{E_m^* - E_n^*}
\]  
(2.14)

But when we try to calculate RR or LL case by inserting Eq(1.4), a simple and explicit expression cannot be obtained. Based on this, intuitively, we may find that the Chern # fails to characterize the transport properties of the system(e.g the Hall conductance). However, the transport theory has its foundation of linear response theory (e.g. the Kubo formula). A more explicit formula should have been studied or will be studied.
2.6 Edge-bulk Correspondence

From the observation above we find the edge-bulk correspondence may be broken as the topological ≠ cannot provide a full description of the transporting properties of a required theory.

3 From the Perspective of Quantum Dynamics

3.1 0D System with Synthetic 2D Parameter Space

From the gauge theory, we know that $\vec{F} \sim \vec{v} \times \vec{B}$ (the Lorentz formula) while in quantum level, it’s known from adiabatic perturbation theory that the quantum metric will cause similar behavior even for 0D system in 2D parameter space, e.g.,

$$\langle F_\mu \rangle_f = \langle F_\mu \rangle_0 + \Omega_\mu^\alpha \frac{ds_\alpha}{dt} + O \left( \left( \frac{ds_\alpha}{dt} \right)^2 \right) \quad (3.1)$$

here the generalized force $F_\mu = -\partial_\mu \dot{H}$ is along the $\mu$ direction and the quench velocity is along the $\lambda$ direction. The expectation $\langle \ldots \rangle_0$ is taken in the initial $n$th eigenstate of the Hamiltonian and $\langle \ldots \rangle_f = \langle \psi (t_f) | \ldots | \psi (t_f) \rangle$ where $| \psi (t_f) \rangle$ is the final state after an evolution due to parameter varying.

However, for a non-Hermitian theory, we even do not have adiabatic perturbation theory. Thus, this indicates a clear direction to develop such a theory and make it clear the connection of the transporting properties, topological number and quasi-adiabatic response.

3.2 2D Semi-Classical Dynamics

The dynamics equation of motion of a single band particle in a EM potential is the Bloch oscillations with a nontrivial Berry curvature:

$$\dot{k}(t) = E$$

$$\dot{r}(t) = \nabla_k E_{n,k} - E \times \Omega_n(k)$$

(3.2)

Exercise: Start from the semiclassical state $W(t) = \int d^2k \hat{w}(k)e^{i\theta(k,t)}|\psi_n,k(t)\rangle$, derive the equation. The system is a 2D sheet with an Abelian gauge potential which will shape the BZ into MBZ.

Here comes an outline for your convenience:

1. Find the dynamics of $\theta$ by Berry’s adiabatic theorem and introduce Berry term.
2. Find the transformation of Berry term and the its relation to normal Berry connection.
3. By setting $\omega(k)$ a Dirac function as a limit of Gaussian, find the state vector and transform the k-dependent wave function into real space. But A convenient way is to directly perform stationary phase approximation(That’s why the above equation is called semi-classical equation.)
Without magnetic field, the semi-classical equation of a non-Hermitian system is:

\[
\begin{align*}
\dot{k} &= E \\
\dot{x} &= \text{Re}[\nabla_k \varepsilon_k] \\
\frac{d\ln N_t}{dt} &= 2\text{Im}E(k)
\end{align*}
\]

(3.3)

It naturally to ask when there is a magnetic field, what about the semi-classical equation of motion?

References


