Discrete Symmetries in QM

We have previously analysed systems with continuous symmetries, such as rotational symmetry.

When we talk about continuous symmetries we can look at the generators of infinitesimal transformations, which form an algebra. Studying this algebra then allows us to discover unitary representations.

Frequently, however, we come upon discrete symmetries. Examples are parity, lattice translations and rotations and time-reversal. In such cases there is no notion of an infinitesimal transformation.

Let us study each of these in turn.

Parity

This can be thought of as reflection symmetry (in all dimensions) and inversion symmetry in $d=1$ and $d=3$ (but not in $d=2$)

$$\boxed{\text{Reflection means} \quad (x,y,z) \to (-x,y,z)} \qquad (1)$$

one coordinate gets reflected.

$$\boxed{\text{Inversion means} \quad (x,y,z) \to (-x,-y,-z)} \qquad (2)$$

We will consider inversions primarily. In the $\vec{x}$ basis we can write the operator that implements this as

$$\boxed{\mathbb{P} = \int d^3x \quad |-\vec{x}\rangle\langle\vec{x}|} \quad (3)$$

Inversion or Parity operator in 3D

In $d=3$ this cannot be achieved by any pure rotation.

We can represent this in the momentum basis as well

$$\mathbb{P} = \int d^3p \, d^3p' \quad |\vec{p}'\rangle \langle \vec{p}' | \mathbb{P} | \vec{p} \rangle \langle \vec{p} |$$

$$\langle \vec{p}' | \mathbb{P} | \vec{p} \rangle = \int d^3x \quad \langle \vec{p}' | -\vec{x} \rangle \langle \vec{x} | \vec{p} \rangle$$

$$= \int \frac{d^3x}{(2\pi\hbar)^3} \quad e^{+\frac{i}{\hbar}(\vec{p}'\cdot\vec{x} + i\,\vec{p}\cdot\vec{x})} \quad = \delta^3(\vec{p}+\vec{p}')$$

So $$\boxed{\mathbb{P} = \int d^3\vec{p} \quad |-\vec{p}\rangle\langle\vec{p}|} \quad (4)$$

The transformation of wave f^n's is

$$\boxed{\mathbb{P}\,\psi(x,y,z) = \psi(-x,-y,-z)} \quad (5)$$

The following two properties of $\mathbb{P}$ are evident

$$\boxed{1)\ \mathbb{P}^\dagger = \mathbb{P} \qquad 2)\ \mathbb{P}^2 = \mathbb{1} \qquad \Rightarrow \quad \mathbb{P} = \mathbb{P}^{-1}} \quad (6)$$

Let us find how operators transform.

Given some operator $\mathbb{M}$ we define the transformed operator $\mathbb{M}_{\mathbb{P}}$ by

$$\boxed{\mathbb{P}\,\mathbb{M}|\psi\rangle = \mathbb{M}_{\mathbb{P}}\,\mathbb{P}|\psi\rangle} \quad (7)$$

$$\Rightarrow \boxed{\mathbb{M}_{\mathbb{P}} = \mathbb{P}\,\mathbb{M}\,\mathbb{P}^{-1} = \mathbb{P}\mathbb{M}\mathbb{P}} \quad \text{because } \mathbb{P}^2 = \mathbb{1} \quad (8)$$

Consider the $\vec{\mathbb{X}}$ operator

$$\mathbb{P}\,\vec{\mathbb{X}}\,\mathbb{P} = \int d^3\bar{x}\, d^3\bar{x}'\, |-\bar{x}'\rangle \underbrace{\langle\bar{x}'|\,\vec{\mathbb{X}}\,|-\vec{x}\rangle}_{-\vec{x}\,\delta^3(\bar{x}+\bar{x}')} \langle\bar{x}|$$

$$= \int d^3x\, |\vec{x}\rangle(-\vec{x})\langle\bar{x}| \equiv -\vec{\mathbb{X}}$$

$$\boxed{\vec{\mathbb{X}}_{\mathbb{P}} = -\vec{\mathbb{X}}} \quad (9) \qquad \text{Similarly} \qquad \boxed{\vec{\mathbb{P}}_{\mathbb{P}} = -\vec{\mathbb{P}}} \quad (10)$$

Consider a simple problem in 1D

$$\boxed{\mathbb{H} = \frac{\mathbb{P}^2}{2M} + V(\mathbb{X})} \quad (11)$$

$$\boxed{\mathbb{H}_{\mathbb{P}} = \frac{\mathbb{P}_{\mathbb{P}}^2}{2M} + V(\mathbb{X}_{\mathbb{P}}) = \frac{\mathbb{P}^2}{2M} + V(-\mathbb{X})} \quad (12)$$

Suppose $V(x)$ is an even function. Then

$$\boxed{\mathbb{H}_{\mathbb{P}} = \mathbb{H}} \quad (13)$$

or $\quad \mathbb{P} \mathcal{H} \mathbb{P}^{-1} = \mathcal{H}$

$$\Rightarrow \quad \mathbb{P}\mathcal{H} = \mathcal{H}\mathbb{P} \quad \Rightarrow \quad \boxed{[\mathbb{P}, \mathcal{H}] = 0} \quad (14)$$

Since $\mathbb{P}$ is also a hermitian operator we can simultaneously diagonalize it and $\mathcal{H}$.

Since $\mathbb{P}^2 = \mathbb{1}$ we know that the eigenvalues of $\mathbb{P}$ can only be ± 1

$$\boxed{\begin{array}{ll} \mathbb{P}|\psi_e\rangle = |\psi_e\rangle & \text{Parity-even states} \\ \mathbb{P}|\psi_o\rangle = -|\psi_o\rangle & \text{Parity-odd states} \end{array}} \quad (15)$$

This holds in 3D as well.

How about angular momentum operators

$$\boxed{\begin{aligned} \mathbb{P}\mathbb{L}_i\mathbb{P} &= \epsilon_{ijk}\,\mathbb{P}\mathbb{x}_j\mathbb{p}_k\mathbb{P} \\ &= \epsilon_{ijk}\,\mathbb{P}\mathbb{x}_j\mathbb{P}\,\mathbb{P}\mathbb{p}_k\mathbb{P} = \mathbb{L}_i \end{aligned}} \quad (16)$$

Since spin should transform the same way as any other angular momentum we conclude

$$\boxed{\vec{\mathbb{J}}_{\mathbb{P}} = \mathbb{P}\vec{\mathbb{J}}\mathbb{P} = \vec{\mathbb{J}}} \quad (17)$$

Let us apply the parity operator to $Y_{\ell m}(\theta,\varphi)$ In spherical coordinates

$$\boxed{\vec{x} \to -\vec{x} \quad \Rightarrow \quad r \to r \qquad \theta \to \pi - \theta \qquad \varphi \to \varphi + \pi} \quad (18)$$

Since $\mathbb{P}\,\mathbb{L}_i = \mathbb{L}_i\,\mathbb{P}$ it is sufficient to look at the transformation of one member of a multiplet under parity.

We know $$\boxed{\langle \theta, \varphi \,|\, l, -l \rangle = C\,(\sin\theta)^{l}\, e^{-il\varphi}} \quad (19)$$

applying parity we get

$$\langle \theta, \varphi |\, \mathbb{P}\, | l, -l \rangle = \langle \pi - \theta, \varphi + \pi \,|\, l, -l \rangle = C\,(\sin\theta)^{l}(-1)^{l} e^{il\varphi}$$

$$\Rightarrow \quad \mathbb{P}\,|l, -l\rangle = (-1)^{l}\,|l, -l\rangle$$

$$\Rightarrow \quad \boxed{\mathbb{P}\,|l, m\rangle = (-1)^{l}\,|l, m\rangle} \quad (20)$$

Okay, how about the parity of intrinsic spin states?

There is no wavef^n to lean on. However, the fact that

$$\boxed{\mathbb{P}\,\vec{\mathbb{S}} = \vec{\mathbb{S}}\,\mathbb{P}} \quad (21)$$

means that all the m_s states for a given spin-s must have the same parity.

Every elementary particle is assigned an intrinsic parity. Later we will see that any spin-$1/2$ fermion (such as the electron, or quarks) described by the Dirac eq^n has intrinsic parity +. The corresponding antiparticle has parity −.

Spin-0 particles can be formed by combining a quark and an antiquark, for example. Depending on the wavef^{n}s of the constituents, and their intrinsic parities, the parity of the resulting particle can be + or −.

The photon is defined to have odd parity. This is consistent with its identification with the transverse components of the vector potential $\bar{A}$ which is odd under parity.

Most of the interactions conserve parity, but the weak interaction famously violates it.

Discrete translations

We have already seen examples in limited contexts before but let's make this more general. Consider 1^{st} a 1-particle Hamiltonian

$$\mathbb{H} = \frac{\vec{\mathbb{P}}^2}{2M} + V(\vec{\mathbb{X}})$$

where $V(\vec{x})$ is periodic

$$\boxed{V(\vec{x}+\bar{a}_i) = V(\vec{x})} \quad (22)$$

$\bar{a}_i$ are called the primitive lattice vectors

Now one can define Lattice translation operators

$$\boxed{\mathbb{U}_{\bar{a}_i} = e^{\frac{i}{\hbar}\bar{a}_i \cdot \vec{\mathbb{P}}}} \quad (23)$$

These are active translations because

$$\boxed{\mathbb{U}_{\bar{a}_i} \psi(\vec{x}) = \psi(\vec{x}+\bar{a}_i)} \quad (24)$$

Clearly, the $\mathbb{U}_{\bar{a}_i}$ are unitary, and they commute with each other. You can construct a translation by an arbitrary lattice vector

$$\boxed{\vec{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3} \quad (25)$$

as $$\boxed{U_{\vec{R}} = (U_{\bar{a}_1})^{n_1}(U_{\bar{a}_2})^{n_2}(U_{\bar{a}_3})^{n_3} = e^{\frac{i}{\hbar}\bar{R}\cdot\bar{p}}} \quad (26)$$

Now these U's also commute with $\mathcal{H}$ because

$$V(\vec{x}+\bar{R}) = V(\vec{x})$$

so $$\boxed{[U_{\bar{a}_i}, \mathcal{H}] = 0} \quad (27)$$

This means we can simultaneously diagonalize $\mathcal{H}$ and all 3 $U_{\bar{a}_i}$'s.

The eigenvalues of a unitary matrix are unimodular.

Say $$\boxed{\begin{aligned} U|\phi_\lambda\rangle &= \lambda|\phi_\lambda\rangle \\ \langle\phi_\lambda|U^\dagger &= \lambda^*\langle\phi_\lambda| \end{aligned}} \quad (28)$$

$$\langle\phi_\lambda|U^\dagger U|\phi_\lambda\rangle = |\lambda|^2\langle\phi_\lambda|\phi_\lambda\rangle = |\lambda|^2 \quad (29)$$

but $U^\dagger U = \mathbb{1}$ for a unitary matrix $\Rightarrow \boxed{|\lambda|^2 = 1}$

So the wavefunctions must be eigenstates such that

$$\boxed{U_{\bar{a}_i}\psi_{\alpha,\theta_1,\theta_2,\theta_3} = e^{i\theta_i}\psi_{\alpha,\theta_1,\theta_2,\theta_3}} \quad (30)$$

$$\boxed{U_{\vec{R}}\psi_{\alpha,\theta_1,\theta_2,\theta_3} = e^{i(n_1\theta_1+n_2\theta_2+n_3\theta_3)}\psi_{\alpha,\theta_1,\theta_2,\theta_3}} \quad (31)$$

$\theta_i + 2\pi$ is clearly the same as θ_i

Define a set of reciprocal lattice vectors as

$$\boxed{\vec{G}_1 = 2\pi \frac{\bar{a}_2 \times \bar{a}_3}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} \qquad \bar{G}_2 = 2\pi \frac{\bar{a}_3 \times \bar{a}_1}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)} \qquad \vec{G}_3 = 2\pi \frac{\bar{a}_1 \times \bar{a}_2}{\bar{a}_1 \cdot (\bar{a}_2 \times \bar{a}_3)}} \quad (32)$$

Now we can define the crystal momentum

$$\boxed{\bar{k} = k_1 \hat{G}_1 + k_2 \hat{G}_2 + k_3 \hat{G}_3} \quad (33)$$

$$\boxed{n_1\theta_1 + n_2\theta_2 + n_3\theta_3 = \bar{k} \cdot \vec{R} = n_1 k_1 a_1 + n_2 k_2 a_2 + n_3 k_3 a_3} \quad (34)$$

There is a 1-to-1 relation between θ_i & k_i

Note that $k_i + \frac{2\pi}{a_i}$ is the same as k_i.

So $\boxed{0 \leq k_i \leq \frac{2\pi}{a_i}}$ (35)

This region of reciprocal space is called the Brillouin Zone.

In sum, the Hamiltonian of a periodic crystal can be partially diagonalized

$$\boxed{\begin{aligned} \mathcal{H}\,\psi_{\alpha,\bar{k}} &= \varepsilon_\alpha(\bar{k})\,\psi_{\alpha,\bar{k}} \\ U_{\bar{R}}\,\psi_{\alpha,\bar{k}} &= e^{i\bar{k}\cdot\bar{R}}\,\psi_{\alpha,\bar{k}} \end{aligned}} \quad (36)$$

This is Bloch's Thm

Time Reversal

This is quite different from the other symmetries we have considered so far.

Let's first look at Classical Mechanics. The idea of time-reversal is the following. Consider some motion $\vec{x}(t)$, $\vec{p}(t)$ under a given set of forces.

You take a movie of this motion, and play it backwards to a colleague. Is the colleague able to decide whether the movie is running backwards? If not, the Hamiltonian is invariant under time-reversal.

Let's be a bit more specific. We start the system at $t=0$ in $x(0)$, $p(0)$ and let it run to t_0 with final values $x(t_0)$, $p(t_0)$.

Now consider the initial conditions

$$\boxed{x_\tau(-t_0) = x(t_0) \qquad p_\tau(-t_0) = -p(t_0)} \quad (37)$$

Let this system evolve under the same $\mathcal{H}$. If the original motion and the new one are related by

$$\boxed{x(t) = x_\tau(-t) \qquad p(t) = -p_\tau(-t)} \quad (38)$$

then the Hamiltonian is time-reversal invariant.

Mechanics without velocity-dependent forces is TRI. Take a system of particles with $\mathcal{H}(\{\bar{x}_i, \bar{p}_i\})$

$$\boxed{\frac{d\bar{x}_i}{dt} = \frac{\partial \mathcal{H}}{\partial \bar{p}_i} \qquad \frac{d\bar{p}_i}{dt} = -\frac{\partial \mathcal{H}}{\partial \bar{x}_i}} \quad (39)$$

If $\mathcal{H} = \sum_i \frac{\bar{p}_i^{\,2}}{2M_i} + V(\{\bar{x}_i\})$

then

$$\boxed{\frac{d\bar{x}_i}{dt} = \bar{p}_i \qquad \frac{d\bar{p}_i}{dt} = -\frac{\partial V}{\partial \bar{x}_i}} \quad (40)$$

Letting $\boxed{\bar{x}_{i\tau}(t) = \bar{x}_i(-t) \qquad \bar{p}_{i\tau}(t) = -\bar{p}_i(-t)}$ (41)

we see that, letting $\boxed{t' = -t}$ (42)

$$\frac{d\bar{x}_i}{dt} = \frac{d(\bar{x}_{i\tau}(-t))}{dt} = -\frac{d\bar{x}_{i\tau}(-t)}{d(-t)} = -\frac{d\bar{x}_{i\tau}(t')}{dt'} = \bar{p}_i(t)$$
$$= -\bar{p}_{i\tau}(t')$$

$$\Rightarrow \boxed{\frac{d\bar{x}_{i\tau}(t')}{dt'} = \bar{p}_{i\tau}(t')} \quad (43)$$

Similarly

$$\boxed{\frac{d\bar{p}_i(t)}{dt} = \frac{d\bar{p}_{i\tau}(t')}{dt'} = -\frac{\partial V}{\partial \bar{x}_{i\tau}}} \quad (44)$$

So Hamilton's eq^{n}s are unchanged as long as velocity-dependent forces are not present.

Now let's go to QM. The fundamental point is that time-reversal for a real-space wavef^n has to involve complex conjugation. It could involve more, but the complex conjugation is essential.

$$\boxed{\mathbb{T} = \text{time-reversal operation}} \quad (45)$$

$$\boxed{\mathbb{T}\,\psi(\bar{x},t) = \psi^*(x,-t)} \quad \text{Simplest case}$$

(46)

The easiest way to see this is on an eigenstate of $\mathcal{H}$

$$\boxed{\begin{aligned} &\mathcal{H}\,\psi_\alpha(\bar{x},t) = i\hbar\,\partial_t \psi_\alpha(\bar{x},t) = \varepsilon_\alpha\,\psi_\alpha(\bar{x},t) \\ \Rightarrow\ &\psi_\alpha(\bar{x},t) = e^{-i\varepsilon_\alpha t/\hbar}\,\psi_\alpha(\bar{x},0) \end{aligned}} \quad (47)$$

All the t-dependence is in the prefactor. $t \to -t$ is achieved by complex conjugation.

Another way to see it is that time-reversal is motion-reversal $\bar{p}_T = -\bar{p}$. Take a plane wave

$$\boxed{\frac{e^{\frac{i}{\hbar}\,\bar{p}\cdot\vec{x}}}{(2\pi\hbar)^{3/2}}} \quad (48)$$

$\bar{p} \to -\bar{p}$ is achieved by complex conjugation

Finally, consider the probability current

$$\boxed{\vec{J}_p(\vec{x},t) = -\frac{i\hbar}{2M}\left\{\psi^* \vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right\}} \quad (49)$$

under $\psi \to \psi^*$ this changes sign, as it should under time-reversal.

Now consider kets. For eigenkets of $\vec{x}$ we can demand.

$$\boxed{\mathbb{T}\,|\vec{x}\rangle = |\vec{x}\rangle} \quad (50)$$

The analog of $x_T = x$ in classical mechanics

This is consistent with our earlier demand to complex conjugate the wave f^n.

$$\boxed{\begin{aligned} \mathbb{T}\,|\psi\rangle &= \mathbb{T}\int d\vec{x}\;\langle\vec{x}|\psi\rangle\;|\vec{x}\rangle \\ &= \int d\vec{x}\;(\langle\vec{x}|\psi\rangle)^*\;|\vec{x}\rangle \end{aligned}} \quad (51)$$

So $\mathbb{T}$ complex conjugates all the numbers!

$$\boxed{\mathbb{T}\left(\alpha|\psi\rangle + \beta|\phi\rangle\right) = \alpha^*\left(\mathbb{T}|\psi\rangle\right) + \beta^*\left(\mathbb{T}|\phi\rangle\right)} \quad (52)$$

such an operator is called antilinear.

How does $\mathbb{T}$ act on a momentum eigenstate?

$$\boxed{\begin{aligned} \mathbb{T}\,|\vec{p}\rangle &= \mathbb{T}\int d\vec{x}\;e^{i\vec{p}\cdot\vec{x}/\hbar}\;|\vec{x}\rangle \\ &= \int d\vec{x}\;e^{-i\vec{p}\cdot\vec{x}/\hbar}\;|\vec{x}\rangle = |-\vec{p}\rangle \end{aligned}} \quad (53)$$

which makes sense.

Since $\mathbb{T}$ is not a linear operator, we cannot use many of the features we normally use for linear operators. For example $\mathbb{T}$ does not have an adjoint.

To proceed further in general let us define

$$\boxed{\mathbb{T}|\phi\rangle = |\phi_\tau\rangle \qquad \mathbb{T}|\psi\rangle = |\psi_\tau\rangle} \quad (54)$$

What is the relation between $\langle\phi|\psi\rangle$ and $\langle\phi_\tau|\psi_\tau\rangle$? Since $\mathbb{T}$ is antilinear, the only possibility is

$$\boxed{\langle\phi_\tau|\psi_\tau\rangle = \langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*} \quad (55)$$

Suppose we start with some orthonormal basis $|j\rangle$ in our Hilbert space.

Define $\boxed{\mathbb{T}|j\rangle = |j_\tau\rangle}$ (56)

Now since $\boxed{\langle j|k\rangle = \delta_{jk}}$ (57) we see that

$$\boxed{\langle j_\tau|k_\tau\rangle = \langle k|j\rangle = \delta_{jk}} \quad (58)$$

So $|j_\tau\rangle$ is another orthonormal basis set. It must be related to $|j\rangle$ by a unitary transformation

$$\boxed{|j_\tau\rangle = \sum_k U_{kj}\,|k\rangle} \quad (59)$$

$$\Rightarrow \quad \boxed{\mathbb{T}\,|j\rangle = |j_\tau\rangle = \sum_k U_{kj}\,|k\rangle} \quad (60)$$

Consider

$$\boxed{\mathbb{T} \sum_j \psi_j |j\rangle = \sum_j \psi_j^* |j_\tau\rangle = \sum_{jk} U_{kj} \psi_j^* |k\rangle} \quad (61)$$

We also have the following important physical principle: If we reverse time twice it should be the same as "doing nothing".

In QM multiplying by a global phase counts as "doing nothing"

So $\boxed{\mathbb{T}^2 |\psi\rangle = e^{i\varphi} |\psi\rangle}$ (62)

$$\Rightarrow \quad \boxed{\begin{aligned} \mathbb{T} \sum_{jk} U_{kj} \psi_j^* |k\rangle &= \sum_{jk} U_{kj}^* \psi_j \mathbb{T} |k\rangle \\ &= \sum_{jk\ell} U^*_{kj} \psi_j U_{\ell k} |\ell\rangle = \sum_{\ell k j} U_{\ell k} U^*_{kj} \psi_j |\ell\rangle \end{aligned}} \quad (63)$$

This must be $e^{i\varphi} \sum_\ell \psi_\ell |\ell\rangle$

$$\Rightarrow \quad \boxed{U_{\ell k} U^*_{kj} = e^{i\varphi} \delta_{\ell j}} \quad (64)$$

or writing them as matrices

$$\boxed{\mathbb{U}\,\mathbb{U}^* = e^{i\varphi}\,\mathbb{1}} \quad (65)$$

Now recall $\mathbb{U}^{-1} = \mathbb{U}^\dagger$ because $\mathbb{U}$ is unitary

$\Rightarrow$ multiply by $U^\dagger$ from the left

$$\boxed{U^* = e^{i\varphi} U^\dagger} \quad (66)$$

Take a complex conjugate

$$\boxed{U = e^{-i\varphi} U^T = e^{-i\varphi}\left(e^{-i\varphi} U^T\right)^T = e^{-2i\varphi} U} \quad (67)$$

which shows that $e^{-2i\varphi} = 1 \Rightarrow \boxed{e^{i\varphi} = \pm 1}$ (68)

So we have the possibilities

$$\boxed{\mathbb{T}^2 = \mathbb{1} \qquad \text{or} \qquad \mathbb{T}^2 = -\mathbb{1}} \quad (69)$$

Both possibilities are realized in QM.

The states of a scalar particle (spin 0) satisfy $\mathbb{T}^2 = \mathbb{1}$. In fact, the usual Schrödinger eqn we write is for a scalar particle. For such a particle $\mathbb{T}$ is simply complex conjugation. For a spin-1/2 particle the correct realization has $\mathbb{T}^2 = -\mathbb{1}$.

A commonly used notation is $\hat{K}$ for complex conjugation. So one writes

$$\boxed{\mathbb{T} = U \hat{K}} \quad (70)$$

We now need to understand how operators transform under $\mathbb{T}$.

Consider some operator $\mathbb{M}$ acting on $|\psi\rangle$

$$\boxed{|\psi\rangle = \sum_j \psi_j |j\rangle \qquad \mathbb{M}|\psi\rangle = \sum_{ij} |i\rangle\langle i|\mathbb{M}|j\rangle \psi_j} \quad (71)$$

$$\boxed{\begin{aligned} \mathbb{T}\,\mathbb{M}|\psi\rangle &= \mathbb{T} \sum_{ij} M_{ij} \psi_j |i\rangle = \sum_{ij} M_{ij}^* \psi_j^* |i_\tau\rangle \\ &= \sum_{ijk} |k\rangle U_{ki} M_{ij}^* \psi_j^* \end{aligned}} \quad (72)$$

We would like to write this as a transformed operator acting on $\mathbb{T}|\psi\rangle$.

By convention we write this as

$$\boxed{\mathbb{T}\,\mathbb{M}|\psi\rangle = \left(\mathbb{T}\,\mathbb{M}\,\mathbb{T}^{-1}\right)\mathbb{T}|\psi\rangle = \mathbb{M}_\tau |\psi_\tau\rangle} \quad (73)$$

We want to compare (72) and (73) to find $\mathbb{M}_\tau$.

$$\boxed{\begin{aligned} \mathbb{M}_\tau|\psi_\tau\rangle &= \mathbb{M}_\tau \sum_{ij} \psi_j^* U_{ij} |i\rangle \\ &= \sum_{ij} \psi_j^* U_{ij} |k\rangle (\mathbb{M}_\tau)_{ki} \end{aligned}} \quad (74)$$

Comparing the two eq^{n}s we see

$$\boxed{U_{ki} M_{ij}^* = (\mathbb{M}_\tau)_{ki} U_{ij}} \quad (75)$$

or as matrices $\boxed{\mathbb{U}\,\mathbb{M}^* = \mathbb{M}_\tau \mathbb{U}}$ (76)

Multiply from the right by $\mathbb{U}^{-1} = \mathbb{U}^{\dagger}$

$$\Rightarrow \quad \boxed{\mathbb{M}_{\tau} = \mathbb{U}\, \mathbb{M}^{*}\, \mathbb{U}^{\dagger}} \quad (77)$$

Let's check to see that this gives sensible answers for spin-0 particles (Schrödinger eq^{n})

$\boxed{\mathbb{U} = \mathbb{1} \text{ in the } x \text{ basis}}$ (78) So in the x-basis

$$\boxed{\mathbb{M}_{\tau} = \mathbb{M}^{*}} \quad (79)$$

The matrix elements of $\mathbb{X}$ and $\mathbb{P}$ in this basis are

$$\langle x_1 | \mathbb{X} | x_2 \rangle = x_1\, \delta(x_1 - x_2)$$

$$\langle x_1 | \mathbb{P} | x_2 \rangle = i\hbar \frac{\partial}{\partial x_2} \delta(x_1 - x_2)$$

$\mathbb{X}_{\tau}$ will have the matrix elements of $\mathbb{X}$ complex conjugated. Since this is real

$$\boxed{\mathbb{X}_{\tau} = \mathbb{X}} \quad (80)$$

Since the matrix elements of $\mathbb{P}$ are imaginary in this basis

$$\boxed{\mathbb{P}_{\tau} = -\mathbb{P}} \quad (81)$$

This holds in any dimension $\boxed{\vec{\mathbb{X}}_{\tau} = \vec{\mathbb{X}}, \quad \vec{\mathbb{P}}_{\tau} = -\vec{\mathbb{P}}}$ (82)

Since $\vec{\mathbb{L}} = \vec{\mathbb{X}} \times \vec{\mathbb{P}}$ $\boxed{\vec{\mathbb{L}}_\tau = -\vec{\mathbb{L}}}$ (83)

First let's consider an orbital angular momentum in the $l=1$ representation In the l,m basis

$$\boxed{\mathbb{L}_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \qquad \mathbb{L}_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad \mathbb{L}_y = \frac{-i\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}}$$ (84)

$\mathbb{L}_x$ and $\mathbb{L}_z$ are real while $\mathbb{L}_y$ is imaginary.

Recall the general relation $\mathbb{M}_\tau = \mathbb{U}\,\mathbb{M}^*\,\mathbb{U}^\dagger$ (85)

We want $\boxed{(\mathbb{L}_x)_\tau = -\mathbb{L}_x \quad (\mathbb{L}_y)_\tau = -\mathbb{L}_y \quad (\mathbb{L}_z)_\tau = -\mathbb{L}_z}$

Now $\boxed{\mathbb{L}_y^* = -\mathbb{L}_y}$ (86), so we can assume that $\mathbb{U}$ and $\mathbb{U}^\dagger$ commute with $\mathbb{L}_y$. However, since $\mathbb{L}_x^* = \mathbb{L}_x$ and $\mathbb{L}_z^* = \mathbb{L}_z$ we need $\mathbb{U}$ to be nontrivial. That is, $\mathbb{U}$ cannot be the unit matrix.

We realize that a rotation of π around the y-axis will change the signs of $\mathbb{L}_x$ & $\mathbb{L}_y$

So let's try (87)

$$\boxed{\mathbb{U} = e^{-\frac{i\pi}{\hbar}\mathbb{L}_y} = \mathbb{1} - i\sin\pi\,\frac{\mathbb{L}_y}{\hbar} + (\cos\pi - 1)\left(\frac{\mathbb{L}_y}{\hbar}\right)^2}$$

$$\left(\frac{\mathbb{L}_y}{\hbar}\right)^2 = \frac{1}{2}\begin{bmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix} \qquad \cos\pi - 1 = -2$$

$$\boxed{\mathbb{U} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}} \quad (88)$$

Note that $\boxed{\mathbb{U}^T = \mathbb{U} = \mathbb{U}^\dagger}$ (89) which implies, according to (67), (68) that

$$\boxed{\mathbb{I}^2 = \mathbb{1}} \quad (90)$$

Check $\mathbb{U}\frac{\mathbb{L}_z}{\hbar}\mathbb{U}^\dagger = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$

$$= \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = -\frac{\mathbb{L}_z}{\hbar}$$

Similarly you can check that $\mathbb{U}\mathbb{L}_x\mathbb{U}^\dagger = -\mathbb{L}_x$

Now let's talk about spin-½

In the basis diagonalizing $\mathbb{J}_z$ we know

$$\boxed{\begin{gathered} \mathbb{J}_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \mathbb{J}_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ \mathbb{J}_z = \frac{\hbar}{2}\sigma_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{gathered}} \quad (91)$$

Note again that

$$\boxed{\mathbb{J}_x^* = \mathbb{J}_x \qquad \mathbb{J}_y^* = -\mathbb{J}_y \qquad \mathbb{J}_z^* = \mathbb{J}_z} \quad (92)$$

Again we can take the (2x2) matrix $\mathbb{U}$ to commute with $\mathbb{J}_y$ since the complex conjugate already does the job.

Once again we can take

$$\boxed{\mathbb{U} = e^{\frac{i\pi}{\hbar}\mathbb{J}_y} = e^{\frac{i\pi}{2}\sigma_y}} \quad (93)$$

Now
$$\boxed{e^{i\psi\sigma_y} = \cos\psi\, \mathbb{1} + i\sin\psi\, \sigma_y} \quad (94)$$

So
$$\boxed{\mathbb{U} = i\sigma_y = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}} \quad (95)$$

Note that $\boxed{\mathbb{U}^T = -\mathbb{U}}$ (96) which means, according to (67), (68)

$$\boxed{\mathbb{T}^2 = -\mathbb{1}} \quad (97)$$

In general, integer spin problems have $\mathbb{T}^2 = +\mathbb{1}$ while half-odd-integer spins have $\mathbb{T}^2 = -\mathbb{1}$

Let us be explicit about the transformation for electronic wavefunctions. Say we have a state $|\psi\rangle$. The wave f^n has two components

$$\boxed{\langle \vec{x}, \uparrow | \psi \rangle = \psi_\uparrow(\vec{x}) \qquad \langle \vec{x}, \downarrow | \psi \rangle = \psi_\downarrow(\vec{x})} \quad (98)$$

Normally we combine them into a "spinor"

$$\boxed{\underset{\sim}{\Psi}(\bar{x}) = \begin{pmatrix} \psi_\uparrow(\bar{x}) \\ \psi_\downarrow(\bar{x}) \end{pmatrix}} \quad (99)$$

The time-reversal operation complex conjugates this and then multiplies by $\mathbb{U}$ (100)

$$\boxed{\mathbb{T}\begin{bmatrix} \psi_\uparrow(\bar{x}) \\ \psi_\downarrow(\bar{x}) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \hat{K} \begin{bmatrix} \psi_\uparrow(\bar{x}) \\ \psi_\downarrow(\bar{x}) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \psi_\uparrow^* \\ \psi_\downarrow^* \end{bmatrix} = \begin{bmatrix} \psi_\downarrow^*(\bar{x}) \\ -\psi_\uparrow^*(\bar{x}) \end{bmatrix}}$$

$$\boxed{\mathbb{T}^2 \begin{bmatrix} \psi_\uparrow(\bar{x}) \\ \psi_\downarrow(\bar{x}) \end{bmatrix} = \mathbb{T}\begin{bmatrix} \psi_\downarrow^*(\bar{x}) \\ -\psi_\uparrow^*(\bar{x}) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \psi_\downarrow(\bar{x}) \\ -\psi_\uparrow(\bar{x}) \end{bmatrix} = - \begin{bmatrix} \psi_\uparrow(\bar{x}) \\ \psi_\downarrow(\bar{x}) \end{bmatrix}}$$

(101)

At this point let us make an important distinction between linear operators and anti-linear operators.

Suppose one has a linear operator $\mathbb{M}$, which when applied twice "does nothing".

$$\boxed{\mathbb{M}^2 = e^{i\varphi}\,\mathbb{1}} \quad (102)$$

because in QM multiplying by a global phase = doing nothing

Define $\boxed{\mathbb{M} = e^{\frac{i\varphi}{2}}\,\mathbb{M}' \Rightarrow \mathbb{M}'^2 = \mathbb{1}}$ (103). So for a linear operator $\mathbb{M}^2 = \mathbb{1}$ is the same as $\mathbb{M}^2 = -\mathbb{1}$.

Let's try this for an anti-linear operator $\mathbb{A}$

Suppose $\boxed{\mathbb{A}^2 = -\mathbb{1}}$ (104)

Let's define $\boxed{\mathbb{A} = e^{i\varphi}\,\mathbb{A}'}$ (105)

$$\boxed{\mathbb{A}^2 = e^{i\varphi}\,\mathbb{A}'\,e^{i\varphi}\,\mathbb{A}' = e^{i\varphi}\,e^{-i\varphi}\,\mathbb{A}'\,\mathbb{A}' = \mathbb{A}'^2 = -\mathbb{1}} \quad (106)$$

$\mathbb{A}'$ complex conjugates $e^{i\varphi}$

So for an anti-linear operator $\mathbb{A}^2 = \mathbb{1}$ and $\mathbb{A}^2 = -\mathbb{1}$ are totally different.

The two commonly applied anti-linear operations are time-reversal and charge-conjugation. We will encounter charge conjugation when we study the Dirac eq^n.

Let's go back to $\mathbb{T}$. An important consequence of $\mathbb{T}^2 = -\mathbb{1}$ is Kramers' degeneracy.

Suppose we have a Hamiltonian that is time-reversal invariant. From (77) this means

$$\boxed{\mathbb{H}_\tau = \mathbb{U}\,\mathbb{H}^*\,\mathbb{U}^\dagger = \mathbb{U}\,\mathbb{H}^T\,\mathbb{U}^\dagger = \mathbb{H}} \quad (107)$$

Suppose we find an eigenstate of $\mathbb{H}$

$$\boxed{\mathbb{H}\,|\alpha\rangle = \varepsilon_\alpha\,|\alpha\rangle} \quad (108)$$

Now consider $\boxed{\mathbb{T}\,|\alpha\rangle = |\alpha_\tau\rangle}$ (109)

Claim 1: $\boxed{\mathbb{H}\,|\alpha_\tau\rangle = \varepsilon_\alpha\,|\alpha_\tau\rangle}$ (110)

This is easy to check (111)

$$\boxed{\mathbb{T}\,\mathbb{H}\,|\alpha\rangle = \mathbb{T}\,\mathbb{H}\,\mathbb{T}^{-1}\,\mathbb{T}\,|\alpha\rangle = \mathbb{H}_\tau\,|\alpha_\tau\rangle = \mathbb{H}\,|\alpha_\tau\rangle}$$

On the other hand $\boxed{\mathbb{T}\left(\mathbb{H}\,|\alpha\rangle\right) = \varepsilon_\alpha\,\mathbb{T}\,|\alpha\rangle = \varepsilon_\alpha\,|\alpha_\tau\rangle}$ because ε_α is real. (112)

So either $|\alpha_\tau\rangle$ is the same state as $|\alpha\rangle$ or it is a different state degenerate with $|\alpha\rangle$.

Claim 2: $\boxed{\langle\alpha|\alpha_\tau\rangle = 0}$ (113) So $|\alpha\rangle$ is orthogonal to $|\alpha_\tau\rangle$

To show this we go back to (55)

$$\langle \phi | \psi \rangle = \langle \psi_\tau | \phi_\tau \rangle$$

So $$\boxed{\langle \alpha | \alpha_\tau \rangle = \langle (\alpha_\tau)_\tau | \alpha_\tau \rangle} \quad (114)$$

(115)

Now $$\boxed{|\alpha_\tau\rangle = \mathbb{T} |\alpha\rangle \Rightarrow |(\alpha_\tau)_\tau\rangle = \mathbb{T}^2 |\alpha\rangle}$$

$$\boxed{\text{For} \quad \mathbb{T}^2 = -\mathbb{1} \qquad |(\alpha_\tau)_\tau\rangle = -|\alpha\rangle} \quad (116)$$

$$\Rightarrow \boxed{\langle \alpha | \alpha_\tau \rangle = -\langle \alpha | \alpha_\tau \rangle} \quad (117)$$

The only possibility is $\langle \alpha | \alpha_\tau \rangle = 0$

So in systems with $\mathbb{T}^2 = -\mathbb{1}$ and time-reversal invariant $\mathcal{H}$ the states come in pairs called Kramers doublets.

The fact that this degeneracy does not require any spatial symmetries is the reason for the robustness $\cap$ topological insulators.

Let us consider some example Hamiltonians. 1st let's look at a 2D system in an external $\bar{B}$ field.

$$\boxed{\mathcal{H} = \frac{\left[p_x - qA_x(x,y)\right]^2 + \left[p_y - qA_y(x,y)\right]^2}{2M}} \quad (118)$$

Since $\mathbb{T} p_i \mathbb{T}^{-1} = -p_i \qquad \mathbb{T} x_i \mathbb{T}^{-1} = x_i$ (119)

$$\boxed{\mathcal{H}_\tau = \mathbb{T}\mathcal{H}\mathbb{T}^{-1} = \frac{[-p_x - qA_x(x,y)]^2 + [-p_y - qA_y(x,y)]^2}{2M}}$$

So $\boxed{\mathcal{H}_\tau \neq \mathcal{H}}$ (120) and the system is not TRI.

Now consider another 2D system, subject to an $\bar{E}$ field $\perp$ to the 2D plane.
In the frame of the moving electron, the $\bar{E}$ field is a linear combination of $\bar{E}$ and $\bar{B}$ fields so there is a spin-orbit coupling.

$$\boxed{\mathcal{H} = \frac{\vec{p}^{\,2}}{2M} + \lambda_{so}\, \bar{E}\cdot\bar{p}\times\vec{\sigma}} \quad (121)$$

This is Rashba spin-orbit coupling.

$\vec{\sigma}$ = Pauli matrices acting on the spin of the electron.

The Hamiltonian must be hermitian. (122)

$$\boxed{(\epsilon_{ijk} E_i p_j \sigma_k)^\dagger = \epsilon_{ijk} E_i \sigma_k^\dagger p_j^\dagger = \epsilon_{ijk} E_i \sigma_k p_j}$$

Since $\vec{\sigma}$ and $\bar{p}$ commute this operator is hermitian and λ_{so} is real.

$$\boxed{\mathbb{T}\mathcal{H}\mathbb{T}^{-1} = \frac{(\vec{p}_\tau)^2}{2M} + \underbrace{\lambda_{so}^*}_{=\lambda_{so}}\, \bar{E}\cdot(\bar{p}_\tau \times \vec{\sigma}_\tau)} \quad (123)$$

$\bar{p}_\tau = -\bar{p} \qquad \vec{\sigma}_\tau = -\vec{\sigma} \Rightarrow \boxed{\mathcal{H}_\tau = \mathcal{H}}$ (124)

This Hamiltonian is TRI. Let us find its eigenstates. Since it has no potential the Hamiltonian is translation invariant and can be partially diagonalized by Fourier transformation.

Let. $$\boxed{\underset{\sim}{\Psi}_{\bar{k}}(\bar{x}) = \frac{e^{i\bar{k}\cdot\vec{x}}}{2\pi}\begin{bmatrix} u_\uparrow(\bar{k}) \\ u_\downarrow(\bar{k}) \end{bmatrix}} \quad (125)$$

$$\vec{\mathbb{P}}\,\underset{\sim}{\Psi}_{\bar{k}}(\bar{x}) = \hbar\bar{k}\,\underset{\sim}{\Psi}_{\bar{k}}(\bar{x})$$

So $\mathcal{H}\,\underset{\sim}{\Psi}_{k}(\bar{x}) = \varepsilon_{\bar{k}}\,\underset{\sim}{\Psi}_{\bar{k}}(\bar{x})$ leads to

$$\boxed{\left\{\frac{\hbar^2\bar{k}^2}{2M}\mathbb{1} + \hbar\lambda_{so}\,\bar{E}\cdot(\bar{k}\times\vec{\sigma})\right\}\begin{bmatrix} u_\uparrow(\bar{k}) \\ u_\downarrow(\bar{k}) \end{bmatrix} = \varepsilon_{\bar{k}}\begin{bmatrix} u_\uparrow(\bar{k}) \\ u_\downarrow(\bar{k}) \end{bmatrix}} \quad (126)$$

Since $\bar{E} = E_0\,\hat{e}_z$

$$\bar{E}\cdot(\bar{k}\times\vec{\sigma}) = E_0\left(k_x\sigma_y - k_y\sigma_x\right)$$

Let $\boxed{k_x = k\cos\varphi \qquad k_y = k\sin\varphi}$ (127)

$$\boxed{\bar{E}\cdot(\bar{k}\times\vec{\sigma}) = E_0 k\begin{bmatrix} 0 & -k_y - ik_x \\ -k_y + ik_x & 0 \end{bmatrix} = -iE_0 k\begin{bmatrix} 0 & e^{-i\varphi} \\ -e^{i\varphi} & 0 \end{bmatrix}} \quad (128)$$

Consider the eigenvalues and eigenstates of

$$\begin{bmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{bmatrix}$$

Characteristic eq^n $\quad \lambda^2 - 1 = 0 \quad \lambda = \pm 1$

For $+1$ we want

$$\begin{bmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{bmatrix} \begin{bmatrix} u_{+\uparrow} \\ u_{+\downarrow} \end{bmatrix} = \begin{bmatrix} u_{+\uparrow} \\ u_{+\downarrow} \end{bmatrix}$$

$\Rightarrow$

$$-iu_{+\downarrow} e^{-i\varphi} = u_{+\uparrow} \qquad u_{+\downarrow} = u_{+\uparrow}\, i e^{i\varphi}$$

Normalize

$$\boxed{\underset{\sim}{u}_+ = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ ie^{i\varphi} \end{bmatrix}} \tag{129}$$

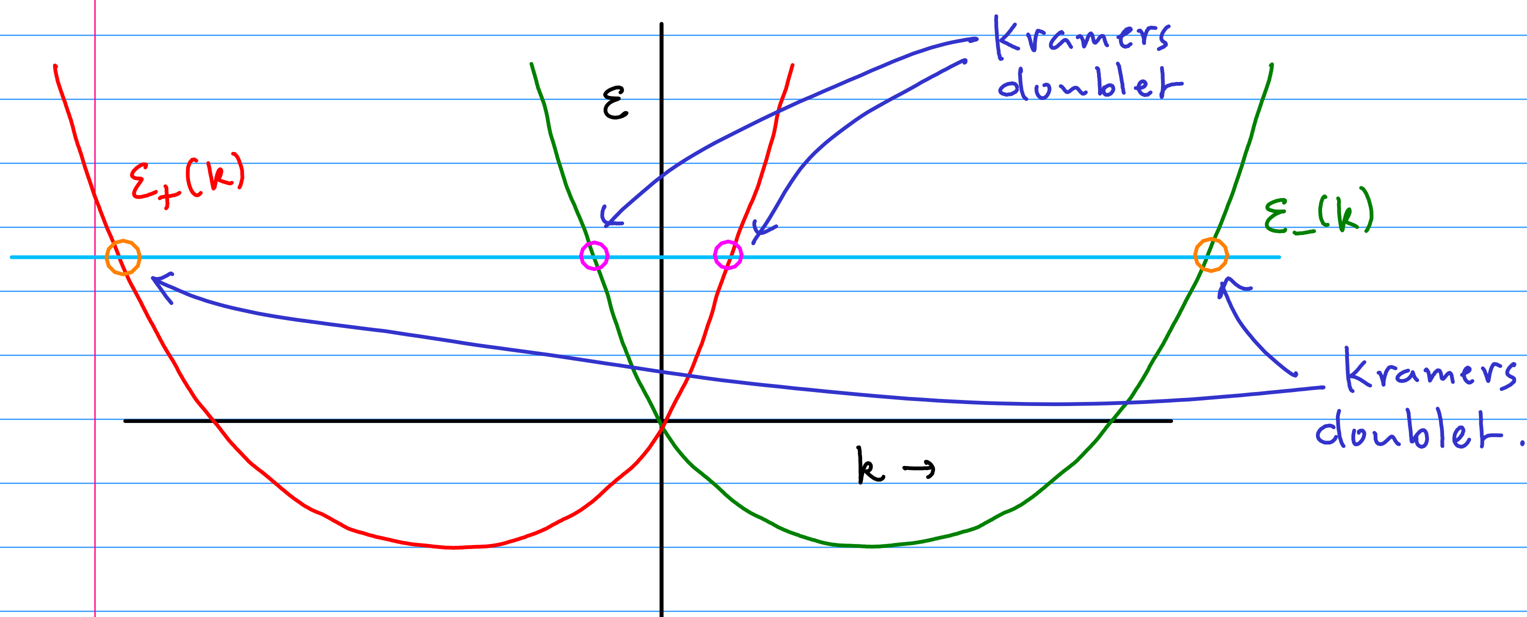
Similarly

$$\boxed{\underset{\sim}{u}_- = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -ie^{i\varphi} \end{bmatrix}}$$

So

$$\boxed{\varepsilon_\pm(\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2M} \pm \hbar k \lambda_{SO} E_0} \tag{130}$$

Here is a section on a line in $\bar{k}$ through 0.



At any given energy there are two sets of Kramers doublets.