Theoretical Physics

Advanced Quantum Mechanics

PHY-MWPT1

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1.1.1 Reminder: Symmetries in Classical Physics

One defines the Lagrangian $\mathcal{L}(q_i, \dot{q}_i)$ of generalized coordinates q_i and generalized velocities $\dot{q}_i$. Consider a displacement $q_i \to q_i + \delta q_i$ for a fixed i. If the Lagrangian does not change, i.e.

$$\mathcal{L}(q_i, \dot{q}_i) = \mathcal{L}(q_i + \delta q_i, \dot{q}_i) \,,$$

then one finds

$$\frac{\partial \mathcal{L}}{\partial q_i} = 0 \,.$$

Example: Free particle Lagrangian $\mathcal{L} = m/2 \cdot (\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$.

- **Canonical Momentum:**
$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$$

- **Lagrange Equation:**
$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i}$$

  Using the symmetry this is
$$0 = \frac{\mathrm{d}p_i}{\mathrm{d}t} \,.$$

  The canonical momentum p_i is a conserved quantity if the Lagrangian is invariant under translation $q_i \to q_i + \delta q_i$.

Similarly, in the Hamiltonian formalism of classical mechanics, with $\mathcal{H}(q_i, p_i)$, one finds

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = 0 \text{ whenever } \frac{\partial \mathcal{H}}{\partial q_i} = 0 \,.$$

The Hamilton equations of motion are

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial \mathcal{H}}{\partial q_i} \text{ and } \frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial p_i} \,.$$

If $\mathcal{H}$ is independent of q_i, then p_i is a conserved quantity.

1.1.2 Symmetries in Quantum Mechanics

In Quantum Mechanics operations like translation or rotation are described by a unitary operator $\hat{S}$:

$$\hat{S}^\dagger \hat{S} = \hat{S}\hat{S}^\dagger = \mathbb{1} \,, \text{ that is } \hat{S}^{-1} = \hat{S}^\dagger \text{ where } (\psi, \hat{A}\varphi) = (\hat{A}^\dagger \psi, \varphi) \,.$$

- **Translation operator:**
$$\hat{T}_{\underline{a}} = e^{-\boldsymbol{i}\, \underline{a} \cdot \underline{\hat{p}}/\hbar}$$

- **Rotation operator:**

$$\hat{D}(\underline{\varphi}) = e^{-\boldsymbol{i}\,\underline{\varphi}\cdot\underline{\hat{l}}/\hbar}$$

Symmetry operations that differ infinitesimally from the identity transformation can be written as

$$\hat{S} = \mathbb{1} - \frac{\boldsymbol{i}\,\varepsilon}{\hbar}\,\hat{G}$$

where $\hat{G}$ is a Hermitian operator called the generator of the symmetry operator $\hat{S}$.
An operator is Hermitian if $\hat{G} = \hat{G}^\dagger$.
Properties of Hermitian operators:

- real eigenvalues
- eigenvectors to different eigenvalues are orthogonal to each other.

$g \in \mathbb{R}$ is called an eigenvalue of $\hat{G}$ with the eigenstate $|g\rangle$ if

$$\hat{G}|g\rangle = g|g\rangle\,.$$

For a discrete spectrum g_i: $\langle g_n|g_m\rangle = \delta_{n,m}$.
For a continuous spectrum: $\langle g|g'\rangle = \delta(g-g')$.

Physical observables like position and momentum are associated with hermitian operators, which have a *complete* eigensystem.

$$\sum_n |g_n\rangle\langle g_n| = \mathbb{1} \qquad\qquad |\varphi\rangle = \sum_n c_n|g_n\rangle$$
$$\int \mathrm{d}g\;|g\rangle\langle g| = \mathbb{1} \qquad\qquad |\varphi\rangle = \int \mathrm{d}g\;c(g)\,|g\rangle$$

where the expansion coefficients are given by

$$c_n = \langle g_n|\varphi\rangle \text{ and } c(g) = \langle g|\varphi\rangle\,,\ \text{respectively.}$$

When $\hat{H}$ is invariant under the symmetry $\hat{S}$, the transformed operator satisfies

$$\hat{S}^\dagger\hat{H}\hat{S} = \hat{H} \text{ or } \hat{H}\hat{S} = \hat{S}\hat{H} \Leftrightarrow \hat{H}\hat{S} - \hat{S}\hat{H} \equiv [\hat{H}\,,\,\hat{S}] = 0\,.$$

This is equivalent to $[\hat{G}\,,\,\hat{H}] = 0$, when $\hat{G}$ is the generator of $\hat{S}$.
Due to the Heisenberg equation of motion for an operator in the Heisenberg picture $\hat{F}_\mathrm{H}(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{F}_\mathrm{H}(t) = \frac{\boldsymbol{i}}{\hbar}\,[\hat{H}\,,\,\hat{F}_\mathrm{H}(t)] + \frac{\partial\hat{F}_\mathrm{H}(t)}{\partial t} \Rightarrow \frac{\mathrm{d}\hat{G}}{\mathrm{d}t} = 0\,.$$

(The subscript in $\hat{G}_\mathrm{H}$ is now implicit.)

Example: Translation operator: $\hat{T}_{\underline{a}} = e^{-\boldsymbol{i}\,\underline{a}\cdot\underline{\hat{p}}/\hbar} \Rightarrow \hat{G} = \underline{\hat{p}}$ and $\dfrac{\mathrm{d}\underline{\hat{p}}}{\mathrm{d}t} = 0$ in case of translation symmetry.

$\hat{G}$ is a constant of motion. For example, if $\hat{H}$ is invariant under translation, then momentum $\hat{p}$ is

constant of motion. In the case of invariance under rotation, angular momentum $\hat{l}$ is a constant of motion.

It is instructive to look at eigenstates $|g\rangle$ of $\hat{G}$ when $[\hat{H}\,,\,\hat{G}]=0$.
(In the Schrödinger picture the state kets are time dependent, given by the Schrödinger equation.)
The time evolution of $|g\rangle$ can be obtained by using the time evolution operator $\hat{U}(t,t_0)$ according to:

$$|g;t_0,t\rangle=\hat{U}(t,t_0)|g,t_0\rangle\ .$$

At the starting time $|g;t_0,t_0\rangle=|g,t_0\rangle$ is an eigenstate $\hat{G}|g,t_0\rangle=g|g,t_0\rangle$.
Reminder: The time evolution operator satisfies the differential equation:

$$\boldsymbol{i}\hbar\,\frac{\partial\hat{U}(t,t_0)}{\partial t}=\hat{H}\,\hat{U}(t,t_0)\text{ with initial condition }\hat{U}(t_0,t_0)=\mathbb{1}\ .$$

If the Hamiltonian does not depend explicitly on time then

$$\hat{U}(t,t_0)=e^{-\frac{\boldsymbol{i}}{\hbar}\,\hat{H}(t-t_0)}\Rightarrow[\hat{G}\,,\,\hat{U}(t,t_0)]=0\text{ if }[\hat{G}\,,\,\hat{H}]=0\ .$$

If $\hat{G}|g,t_0\rangle=g|g,t_0\rangle$ then $|g;t_0,t\rangle$ is an eigenket of $\hat{G}$ with the same eigenvalue (if $[\hat{H}\,,\,\hat{G}]=0$):

$$\hat{G}\left(\hat{U}(t,t_0)|g,t_0\rangle\right)=\hat{U}(t,t_0)\hat{G}|g,t_0\rangle=\hat{U}(t,t_0)g|g,t_0\rangle=g\left(\hat{U}(t,t_0)|g,t_0\rangle\right)\ .$$

Example: $|p,t_0\rangle$ is eigenstate of $\hat{p}$ at time t_0, it will be an eigenstate at all times if the system is translationally invariant with $[\hat{H}\,,\,\hat{p}]$.

One can transform between the pictures (where $\hat{G}_{\mathrm{S}}$ is a time-independent Schrödinger operator)

$$\hat{G}_{\mathrm{H}}(t)=\hat{U}^{\dagger}(t,t_0)\hat{G}_{\mathrm{S}}\hat{U}(t,t_0)\text{ and }|g;t_0,t\rangle_{\mathrm{S}}=\hat{U}(t,t_0)|g,t_0\rangle_{\mathrm{H}}\ .$$

1.1.3 Degeneracies

In classical mechanics, degeneracies occur for example in the context of closed orbits in the Kepler problem (many solutions rotated around the focal point).

In Quantum Mechanics, we consider a symmetry operator $\hat{S}$ (unitary and commutes with the Hamiltonian) with $[\hat{H}\,,\,\hat{S}]=0$.
Consider every eigenket $|n\rangle$ with $\hat{H}|n\rangle=E_n|n\rangle$. Then $\hat{S}|n\rangle$ is also an eigenket with the same eigenvalue E_n because

$$\hat{H}\left(\hat{S}|n\rangle\right)=\left(\hat{H}\hat{S}\right)|n\rangle=\hat{S}\hat{H}|n\rangle=E_n\left(\hat{S}|n\rangle\right)\ .$$

Suppose now that $|n\rangle$ and $\hat{S}|n\rangle$ represent different states, then this states have the same energy and are hence degenerate.
Consider $\hat{S}$ characterized by a continuous parameter, e.g. a rotation

$$\hat{D}(\underline{\varphi})=e^{-\boldsymbol{i}\,\underline{\varphi}\cdot\hat{\underline{l}}/\hbar}\ .$$

Assume now $[\hat{D}(\underline{\varphi})\,,\,\hat{H}] = 0 \Longrightarrow [\hat{\underline{l}}\,,\,\hat{H}] = 0$ and $[\hat{\underline{l}}^{\,2}\,,\,\hat{H}] = 0$. (The implication can be shown using the commutator rule $[\hat{A}\hat{B}\,,\,\hat{C}] = \hat{A}[\hat{B}\,,\,\hat{C}] + [\hat{A}\,,\,\hat{C}]\hat{B}$.)
Consider simultaneous eigenkets of $\hat{H}, \hat{\underline{l}}^{\,2}$, and $\hat{l}_z$, denote them by $|n; l, m\rangle$:

$$\hat{\underline{l}}^{\,2}|n; l, m\rangle = \hbar^2 l(l+1)|n; l, m\rangle$$
$$\hat{l}_z|n; l, m\rangle = \hbar m|n; l, m\rangle \ .$$

$\Rightarrow$ all states $\hat{D}(\underline{\varphi})|n; l, m\rangle$ have the same energy.
In general, $\hat{D}(\underline{\varphi})|n; l, m\rangle$ is a linear combination of the $2l{+}1$ independent states $|n; l, m'\rangle$ $(-l \leq m' \leq l)$ which is independent of E_n:

$$\hat{D}(\underline{\varphi})|n; l, m\rangle = \sum_{m'} |n; l, m'\rangle \hat{D}^{(l)}_{m',m}(\underline{\varphi}) \text{ with } \hat{D}^{(l)}_{m',m}(\underline{\varphi}) = \langle l, m'|\hat{D}(\underline{\varphi})|l, m\rangle \ .$$

[The total angular momentum is not changed under rotation. $\hat{D}(\underline{\varphi})$ has a block form: $l = 0$ scalar, $l = 1$ vector,...].
By changing $\underline{\varphi}$ continuously, we obtain different linear combinations of $|n, l, m'\rangle$. If all states with $\hat{D}(\underline{\varphi})|n; l, m\rangle$ have the same energy, then all the $|n; l, m'\rangle$ have the same energy $\Rightarrow E_n$ is $(2l + 1)$-fold degenerate.
Alternative argument: The $|n; l, m\rangle$ can be constructed by successive application of $\hat{l}_\pm = \hat{l}_x \pm \boldsymbol{i}\hat{l}_y$, which commute with $\hat{H}$ as well.
Application: Atomic electron moving in rotationally invariant potential $V(\underline{r}) = V(|\underline{r}|) \Rightarrow$ expect a $(2l + 1)$-fold degeneracy of atomic energy levels.
In the presence of an external electric or magnetic field, the rotational symmetry is broken and the degeneracy is lifted (Stark and Zeemann effect).
E_n of hydrogen atom ($l = 0, 1, ..., n$) is n^2 degenerate (higher than expected because of a dynamic SO4 symmetry).

1.2 Discrete Symmetries, Parity, or Space Inversion

1.2.1 Parity

There are three important discrete symmetry operations: parity, lattice translations, and time-reversal.
When applying the parity operator to the coordinate system, then a right-handed coordinate system is changed into a left-handed one.

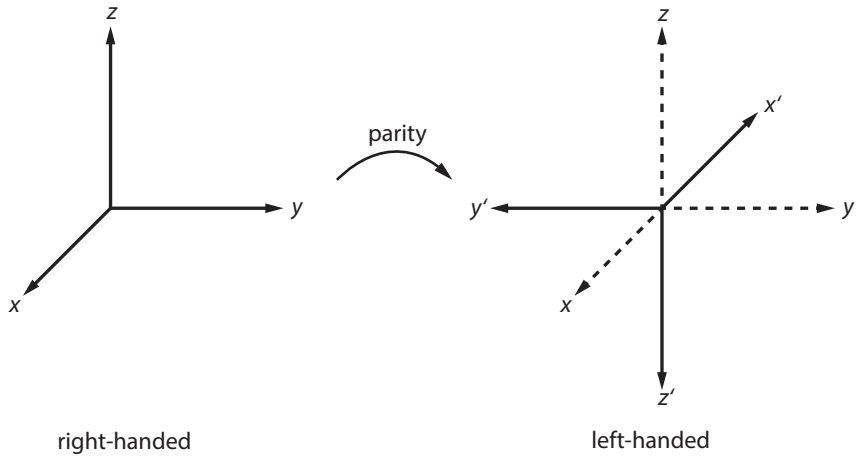

Figure 1.1: A parity operator transforms a right-handed to a left-handed coordinate system.

However, here we consider transformation of state kets and operators rather than transformations of the coordinate system.
Given a ket $|\alpha\rangle$, we consider a space-inverted state obtained by applying the unitary *parity operator* $\hat{\Pi}$ as follows: $|\alpha\rangle \mapsto \hat{\Pi}|\alpha\rangle$. We require the position operator $\hat{\underline{x}}$ taken with respect to $\hat{\Pi}|\alpha\rangle$ to have opposite sign

$$\left(\langle\alpha|\hat{\Pi}^\dagger\right)\hat{\underline{x}}\left(\hat{\Pi}|\alpha\rangle\right) \stackrel{!}{=} -\langle\alpha|\hat{\underline{x}}|\alpha\rangle\ .$$

If this is true for all possible kets $|\alpha\rangle$, then due to the associative character of operator multiplication, this is achieved if

$$\hat{\Pi}^\dagger\hat{\underline{x}}\hat{\Pi} = -\hat{\underline{x}} \text{ or } \hat{\underline{x}}\hat{\Pi} = -\hat{\Pi}\hat{\underline{x}}\ .$$

Hence, $\hat{\underline{x}}$ and $\hat{\Pi}$ must anti-commute with each other:

$$\hat{\underline{x}}\hat{\Pi} + \hat{\Pi}\hat{\underline{x}} = 0\,,\ \text{anti-commutator notation: } \{\hat{\underline{x}}\,,\,\hat{\Pi}\} = 0\ .$$

Eigenkets of the position operator must transform in the following way, we claim that

$$\hat{\Pi}|\underline{x}'\rangle = e^{i\delta}|-\underline{x}'\rangle\ . \tag{1.1}$$

This is true because $\hat{\underline{x}}\hat{\Pi}|\underline{x}'\rangle = -\hat{\Pi}\hat{\underline{x}}|\underline{x}'\rangle = -\underline{x}'\hat{\Pi}|\underline{x}'\rangle$. $\Rightarrow \hat{\Pi}|\underline{x}'\rangle$ is again eigenket of the position operator $\hat{\underline{x}}$ with eigenvalue $-\underline{x}'$. $\Rightarrow$ Up to a phase factor $e^{i\delta}$ it must be equal to $|-\underline{x}'\rangle$.
It is customary to choose $e^{i\delta} = 1$. Using this conversion in Eq. (1.1) we find $\hat{\Pi}^2|\underline{x}'\rangle = |\underline{x}'\rangle$, and hence $\hat{\Pi}^2 = \mathbb{1}$ with eigenvalues $\lambda^2 = 1 \Rightarrow \lambda = \pm 1$. Using $\hat{\Pi}^\dagger\hat{\Pi} = \mathbb{1} \Rightarrow \hat{\Pi} = \hat{\Pi}^\dagger$.
$\hat{\Pi}$ is both unitary and Hermitian, and has eigenvalues ± 1.
(For a unitary operator one can show $\hat{S}^\dagger\hat{S} = \mathbb{1} \Rightarrow \lambda^*\lambda = 1 \Rightarrow \lambda = e^{i\alpha}$.)

How does the momentum operator transform under parity?
$\hat{\underline{p}}$ is related to $m\,\dfrac{\mathrm{d}\hat{\underline{x}}}{\mathrm{d}t}$, so we expect it to be odd under parity. More rigorous: $\hat{\underline{p}}$ is the generator of translation. A translation followed by parity is equivalent to parity followed by a translation in the opposite direction.

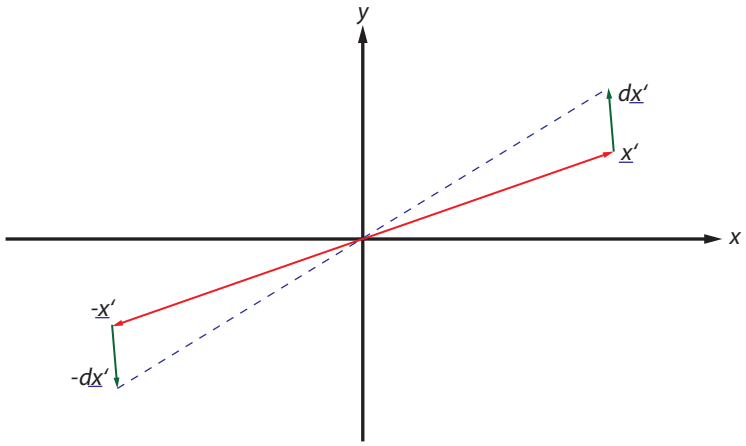

Figure 1.2: Visualization of the different order of applying a translation and parity operator.

Let $\hat{\mathrm{T}}(\mathrm{d}\underline{x}')$ denote a translation operator by $\mathrm{d}\underline{x}'$.

$$\hat{\Pi}\hat{\mathrm{T}}(\mathrm{d}\underline{x}') = \hat{\mathrm{T}}(-\mathrm{d}\underline{x}')\hat{\Pi}$$
$$\hat{\Pi}\left[\mathbb{1} - \frac{\boldsymbol{i}\hat{\underline{p}}\cdot\mathrm{d}\underline{x}'}{\hbar}\right] = \left[\mathbb{1} + \frac{\boldsymbol{i}\hat{\underline{p}}\cdot\mathrm{d}\underline{x}'}{\hbar}\right]\hat{\Pi}$$
$$\hat{\Pi}\left[\mathbb{1} - \frac{\boldsymbol{i}\hat{\underline{p}}\cdot\mathrm{d}\underline{x}'}{\hbar}\right]\hat{\Pi}^\dagger = \mathbb{1} + \frac{\boldsymbol{i}\hat{\underline{p}}\cdot\mathrm{d}\underline{x}'}{\hbar}$$
$$\mathbb{1} = \hat{\Pi}\hat{\Pi}^\dagger \Rightarrow \hat{\Pi}^\dagger\hat{\underline{p}}\hat{\Pi} = -\hat{\underline{p}} \text{ or } \{\hat{\Pi}\,,\,\hat{\underline{p}}\} = 0$$

Angular momentum $\hat{\underline{l}} = \hat{\underline{x}} \times \hat{\underline{p}} \Rightarrow$ we have $[\hat{\Pi}\,,\,\hat{\underline{l}}] = 0$.
More generally angular momentum $\hat{\underline{J}}$ is the generator of rotations and has the same properties as 3×3 orthogonal matrices in $\mathbb{R}^3$.

$$\underline{\underline{\mathbb{R}}}^{(\text{parity})} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = -\mathbb{1}$$
$$\underline{\underline{\mathbb{R}}}^{(\text{parity})}\underline{\underline{\mathbb{R}}}(\underline{\varphi}) = \underline{\underline{\mathbb{R}}}(\underline{\varphi})\underline{\underline{\mathbb{R}}}^{(\text{parity})}$$

$\Rightarrow$ Rotations and parity commute.
We postulate the same for rotation operators: $\hat{\Pi}\hat{D}(\underline{\varphi}) = \hat{D}(\underline{\varphi})\hat{\Pi}$.
Consider a infinitesimal rotation $\hat{D}(\underline{\varepsilon}) = \mathbb{1} - \dfrac{\boldsymbol{i}}{\hbar}\,\underline{\varepsilon}\cdot\hat{\underline{J}}$ with the rotation axis unit vector $\underline{n}$ and the rotation angle ε: $\underline{\varepsilon} = \varepsilon\,\underline{n}$.
From this follows

$$[\hat{\Pi}\,,\,\hat{\underline{J}}] = 0 \text{ or } \hat{\Pi}^\dagger\hat{\underline{J}}\hat{\Pi} = \hat{\underline{J}}\,.$$

We know $[\hat{J}_i\,,\,\hat{J}_j] = \boldsymbol{i}\hbar\varepsilon_{ijk}\hat{J}_k \Rightarrow [\hat{\underline{J}}^{\,2}\,,\,\hat{J}_z] = 0$.
$\Rightarrow \hat{\underline{J}}^{\,2}$ and $\hat{J}_z$ have a common set of eigenfunctions/kets $|j,m\rangle$:

$$\hat{\underline{J}}^{\,2}|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle \text{ and } \hat{J}_z|j,m\rangle = \hbar m|j,m\rangle$$

where $-j \leq m \leq j$ and m increases in integer fashion from $-j$ to j. j can take on either integer or half integer values.
Example:

$$|0,0\rangle$$
$$|1/2,-1/2\rangle\ ,\ \ |1/2,1/2\rangle$$
$$|1,-1\rangle\ ,\ \ |1,0\rangle\ ,\ \ |1,1\rangle$$
$$|3/2,-3/2\rangle\ ,\ \ |3/2,-1/2\rangle\ ,\ \ |3/2,1/2\rangle\ ,\ \ |3/2,3/2\rangle$$

Consider eigenfunctions $\langle\theta,\varphi|j,m\rangle = Y_l^m(\theta,\varphi)$.
$Y_l^m(\theta,\varphi)$ are solutions to the eigenvalue equation $\hat{\underline{l}}^2 Y_l^m(\theta,\varphi) = \hbar^2 l(l+1)Y_l^m(\theta,\varphi)$,
$\hat{l}_z Y_l^m(\theta,\varphi) = \hbar m Y_l^m(\theta,\varphi)$, and $Y_l^m(\theta,\varphi) = f(\theta)\, e^{\boldsymbol{i}m\varphi}$.
The uniqueness of the wave function requires

$$e^{\boldsymbol{i}m\varphi} = e^{\boldsymbol{i}m(\varphi+2\pi)} \Rightarrow 2\pi m = n2\pi$$

$\Rightarrow$ In wave function only values $m \in \mathbb{N}_0$ are allowed.
$\Rightarrow$ $Y_l^m(\theta,\varphi)$ are only single-valued if m is integer.
$\Rightarrow$ Orbital angular momentum related wave functions can only take integer values of l.

- "internal angular momentum" operator $\hat{\underline{s}}$ (realizes the $\mathbb{N}+1/2$ representations of the rotation group) $\Rightarrow [\hat{\underline{s}}\,,\hat{\Pi}] = 0$
- $\hat{\underline{J}} = \hat{\underline{l}} + \hat{\underline{s}}$

Under rotations $\hat{\underline{x}}, \hat{\underline{p}}$, and $\hat{\underline{J}}$ transform in the same way, hence they are all vectors. However, $\hat{\underline{x}}$ and $\hat{\underline{p}}$ are odd under parity, and $\hat{\underline{J}}$ is even: $\hat{\Pi}^\dagger \hat{\underline{x}} \hat{\Pi} = -\hat{\underline{x}}$ but $\hat{\Pi}\hat{\underline{J}}\hat{\Pi} = \hat{\underline{J}}$.
For this reason $\hat{\underline{x}}$ and $\hat{\underline{p}}$ are called polar vectors (Schubvektoren) and $\hat{\underline{J}}$ is an axial vector.
$\hat{\underline{x}} \cdot \hat{\underline{p}}$ is a scalar (invariant under rotations) and even under parity.
$\hat{\underline{s}} \cdot \hat{\underline{x}}$ is odd under parity and called a pseudo-scalar:

$$\hat{\Pi}^{-1}\hat{\underline{s}} \cdot \hat{\underline{x}}\hat{\Pi} = -\hat{\underline{s}} \cdot \hat{\underline{x}}\ .$$

1.2.1.1 Wave Functions under Parity

Let $\psi_\alpha(\underline{x}')$ be the wave function of a spinless particle whose state ket is $|\alpha\rangle$:

$$\psi_\alpha(\underline{x}') = \langle \underline{x}'|\alpha\rangle\ .$$

The wave function of the space inverted ket $\hat{\Pi}|\alpha\rangle$ is

$$\langle \underline{x}'|\hat{\Pi}|\alpha\rangle = (\langle \underline{x}'|\hat{\Pi})|\alpha\rangle = \langle -\underline{x}'|\alpha\rangle = \psi_\alpha(-\underline{x}')\ .$$

Assume now that $|\alpha\rangle$ is eigenket of parity with $\hat{\Pi}|\alpha\rangle = \pm|\alpha\rangle$. Then the corresponding wave function is

$$\langle \underline{x}'|(\hat{\Pi}|\alpha\rangle) = \pm\langle \underline{x}'|\alpha\rangle = \pm\psi_\alpha(\underline{x}')\ .$$

For parity eigenstates: $\psi_\alpha(-\underline{x}') = \pm\psi_\alpha(\underline{x}')$ where the $+$ is for even and $-$ for odd parity.
We note that not all wave functions have definite parity, even if $[\hat{\Pi}\,,\hat{H}] = 0$. One example are

momentum eigenkets $|\underline{p}\rangle$. Since $[\hat{\Pi}\,,\,\hat{\underline{l}}] = 0$, eigenkets of orbital angular momentum are expected to be eigenkets of parity as well.
Wave functions in a rotationally invariant potential have the following form:

$$\langle \underline{x}'|n;l,m\rangle = R_n(r)\, Y_l^m(\theta,\varphi)\ .$$

We want to find the parity of Y_l^m.
In spherical coordinates, the transformation $\underline{x}' \mapsto -\underline{x}'$ corresponds to

$$r \mapsto r\ ,\quad \theta \mapsto \pi - \theta \text{ and } \varphi \mapsto \varphi + \pi \Rightarrow \cos\theta \mapsto -\cos\theta\ ,\ \ \sin\theta \mapsto \sin\theta \text{ and } e^{\boldsymbol{i}m\varphi} \mapsto (-1)^m e^{\boldsymbol{i}m\varphi}\ .$$

We have

$$Y_l^m = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\ P_l^{|m|}(\cos\theta)\, e^{\boldsymbol{i}m\varphi}$$

where the Legendre polynomials are given by

$$P_l^{|m|}(\cos\theta) = \frac{(-1)^{m+l}(l+|m|)!}{2^l l!(l-|m|)!}\ (\sin\theta)^{-|m|}\ \left(\frac{\mathrm{d}}{\mathrm{d}\cos\theta}\right)^{l-|m|} (\sin\theta)^{2l}$$

$\Rightarrow e^{\boldsymbol{i}m\varphi} \mapsto (-1)^m e^{\boldsymbol{i}m\varphi}$ and $P_l^m \mapsto (-1)^{l-|m|} P_l^m$:

$$\boxed{Y_l^m \mapsto (-1)^l Y_l^m \text{ and } \hat{\Pi}|n;l,m\rangle = (-1)^l |n;l,m\rangle}$$

When $[\hat{H}\,,\,\hat{\Pi}] = 0$, and $|n\rangle$ is a non degenerated eigenket of $\hat{H}$ with eigenvalue E_n, then $|n\rangle$ is also a parity eigenket.
Consider the 1d harmonic oscillator as an example. The ground state $|0\rangle$ has a Gaussian wave function, and has even parity for this reason. (This is a consequence of the Sturm–Liouville theory: 0 nodes for ground state.)
The first excited state $|1\rangle = \hat{a}^\dagger|0\rangle$ has odd parity ($\hat{a}^\dagger \sim \hat{x} + \boldsymbol{i}\hat{p} \Rightarrow$odd).
Using $\hat{\Pi} = \hat{\Pi}^\dagger = \hat{\Pi}^{-1}$ we find $\hat{\Pi}\hat{a}^\dagger|0\rangle = \hat{\Pi}^{-1}\hat{a}^\dagger|0\rangle = \hat{\Pi}^{-1}\hat{a}^\dagger\hat{\Pi}\hat{\Pi}^{-1}|0\rangle = -\hat{a}^\dagger|0\rangle$. In general, the parity of harmonic oscillator eigenstates $|n\rangle$ is $(-1)^n$.
For the non-relativistic hydrogen atom, 2p ($n=2, l=1$) and 2s ($n=2, l=0$) are degenerate and parity eigenstates each.
However, the linear combination $c_p|2p\rangle + c_s|2s\rangle$ is obviously not a parity eigenket. As a further example, the free particle Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$ is invariant under parity, but momentum eigenstates $|\underline{p}'\rangle$ and $|-\underline{p}'\rangle$ are not: $\hat{\Pi}|\underline{p}'\rangle = |-\underline{p}'\rangle$. However, since they are degenerate, parity eigenstates can be formed: $1/\sqrt{2}\ (|\underline{p}'\rangle \pm |-\underline{p}'\rangle)$. In terms of wave functions, $e^{\boldsymbol{i}\underline{p}'\cdot\underline{x}/\hbar}$ does not have a definite parity, but $\cos(\underline{p}'\cdot\underline{x}/\hbar)$ and $\sin(\underline{p}'\cdot\underline{x}/\hbar)$ do.

1.2.1.2 Symmetrical Double-Well Potential

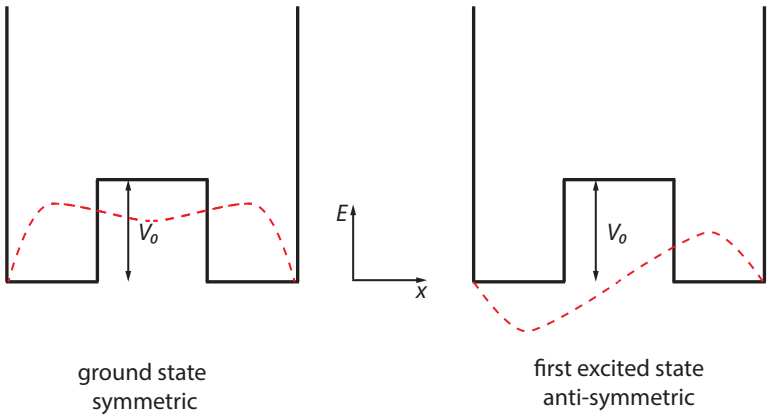

Figure 1.3: Symmetric (S) and assymetric (A) state, where $E_A > E_S$ and for $V_0 \to \infty$: $E_A - E_S \to 0$

We can from states $|R\rangle$ and $|L\rangle$, which are localized in the right and left potential well, respectively.

$$|R\rangle = \frac{1}{\sqrt{2}} \left(|S\rangle + |A\rangle\right) \text{ and } |L\rangle = \frac{1}{\sqrt{2}} \left(|S\rangle - |A\rangle\right) .$$

$|R\rangle$ and $|L\rangle$ are neither eigenstates of the Hamiltonian nor parity eigenstates.

$$\hat{\Pi}|L\rangle = \frac{1}{\sqrt{2}} \left(\hat{\Pi}|S\rangle - \hat{\Pi}|A\rangle\right) = \frac{1}{\sqrt{2}} \left(|S\rangle + |A\rangle\right) = |R\rangle .$$

Instead, they are typical examples of non-stationary states. The time evolution of the state $|R\rangle$ is given by

$$|R; t_0 = 0, t\rangle = \frac{1}{\sqrt{2}} \left(e^{-\frac{i}{\hbar} E_S t}|S\rangle + e^{-\frac{i}{\hbar} E_A t}|A\rangle\right) = \frac{1}{\sqrt{2}} e^{-\frac{i}{\hbar} E_S t} \left(|S\rangle + e^{-\frac{i}{\hbar} (E_A - E_S) t}|A\rangle\right) .$$

While the system is represented by $|R\rangle$ at $t = 0$, at time

$$t = \frac{T}{2} = \frac{2\pi\hbar}{2(E_A - E_S)} \text{ where } \frac{1}{\hbar} (E_A - E_S) t = \pi$$

the system is found in pure $|L\rangle$. At $t = T$, we are back in pure $|R\rangle$, and so on. We observe an oscillation between $|R\rangle$ and $|L\rangle$ with angular frequency

$$\omega = \frac{E_A - E_S}{\hbar} .$$

An example demonstrating the importance of the symmetry is the Amonia molecule.

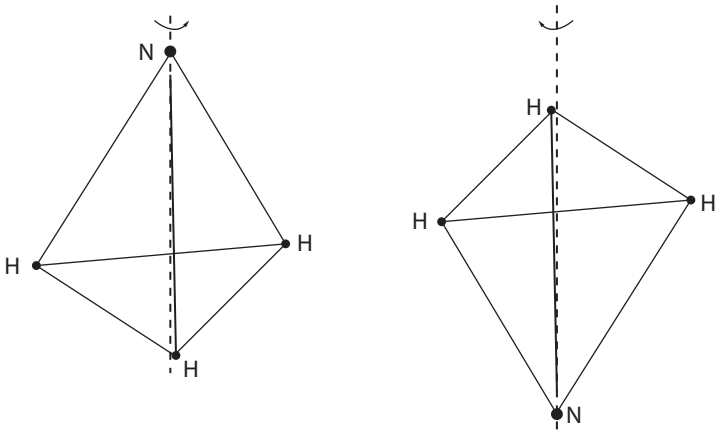

Figure 1.4: The Amonia molecule rotates arround the dashed axis. Due to the rotation both orientations can be distinguished by the direction of the angular momentum.

Up and down for the Nitrogen are analogous to $|L\rangle$ and $|R\rangle$ in the double-well.
The energy and parity eigenstates are superpositions and the energy difference corresponding to an oscillation frequency of 24000MHz, a wavelength of about 1cm (microwave).

There are naturally occurring organic molecules, such as amino acids or sugars, which are of R-type or L-type only.
For such molecules with a definite handedness, in many cases, the oscillation time is infinite for practical purposes (10^4-10^6 years).
Examples are chiral amino acids (L-versions: rotate the orientations of linear polarized light to the left) and sugars (R-versions) in biochemistry.
The origin of symmetry breaking is unclear, since the synthesis in the laboratory yields equal amounts of L- and R-types.

1.2.1.3 Parity Selection Rule

We consider parity eigenstates $|\alpha\rangle$ and $|\beta\rangle$ with eigenvalues $\lambda_\alpha, \lambda_\beta \in \{\pm 1\}$: $\hat{\Pi}|\alpha\rangle = \lambda_\alpha|\alpha\rangle$ and $\hat{\Pi}|\beta\rangle = \lambda_\beta|\beta\rangle$. We now show that $\langle\beta|\underline{\hat{x}}|\alpha\rangle = 0$ unless $\lambda_\alpha = -\lambda_\beta$.

$$\langle\beta|\underline{\hat{x}}|\alpha\rangle = \langle\beta|\hat{\Pi}^{-1}\underbrace{\hat{\Pi}\underline{\hat{x}}\hat{\Pi}^{-1}}_{-\underline{\hat{x}}}\hat{\Pi}|\alpha\rangle = -\langle\beta|\hat{\Pi}^\dagger\underline{\hat{x}}\hat{\Pi}|\alpha\rangle = -\lambda_\alpha\lambda_\beta\langle\beta|\underline{\hat{x}}|\alpha\rangle$$

which is only possible if either $-\lambda_\alpha\lambda_\beta = 1$ or $\langle\beta|\underline{\hat{x}}|\alpha\rangle = 0$.
This selection rule is important for transitions between atomic states.
The vector potential operator of incoming light with frequency ω is given by

$$\underline{\hat{A}}(\underline{x}, t) = \underline{A}_0\, e^{\boldsymbol{i}\,\underline{k}\cdot\underline{\hat{x}} - \boldsymbol{i}\omega t}\ .$$

Since the wavelength of light is much larger then the Bohr radius, we can expand a plane wave:

$$e^{\boldsymbol{i}\underline{k}\cdot\underline{\hat{x}}} \approx 1 + \boldsymbol{i}\ \underbrace{\underline{k}\cdot\underline{\hat{x}}}_{\text{dipole}} - \frac{1}{2}\underbrace{(\underline{k}\cdot\underline{\hat{x}})^2}_{\text{quadrupol}}\ ,$$

(we consider only the stronger dipole transitions) and for the application of Fermis golden rule (transition probability from initial state I to final state F; only when energy difference is equal to photon energy)

$$\Lambda_{IF} \approx \frac{2\pi}{\hbar} \, |\langle F|\hat{H}_1|I\rangle|^2 \, \delta(E_F - E_I - \hbar\omega)$$

we need to compute matrix elements of the position operator $\underline{\hat{x}}$ between different atomic states. Together with our result for the parity of angular momentum eigenstates, $\hat{\Pi}|n;l,m\rangle = (-1)^l|n;l,m\rangle$ we can immediately conclude that optical dipole transitions are only possible between states with different angular momentum.

1.2.1.4 Parity Non-Conservation

During β-decay, a neutron is transformed into a proton by emission of an electron ("beta ray") and a neutrino, or conversely a proton is transformed into a neutron by emission of a positron and a neutrino.
The basic Hamiltonian for this so-called weak interaction is not invariant under parity. Observables like the angular distribution of emitted β-rays depends on pseudo-scalars like $\langle\underline{\hat{s}}\rangle \cdot \underline{\hat{p}}$, where $\langle\underline{\hat{s}}\rangle$ is the expectation value of the nuclear spin. In the experiment by Wu, Ambler, et al. [Phys. Rev. **105**, 1413 (1957)] it was demonstrated that the emission of β-rays occurs preferentially in the direction opposite to the orientation of the nuclear spin.

1.2.2 Lattice Translations as a Discrete Symmetry

We consider a periodic potential in one dimension, with $V(x+a) = V(x)$.

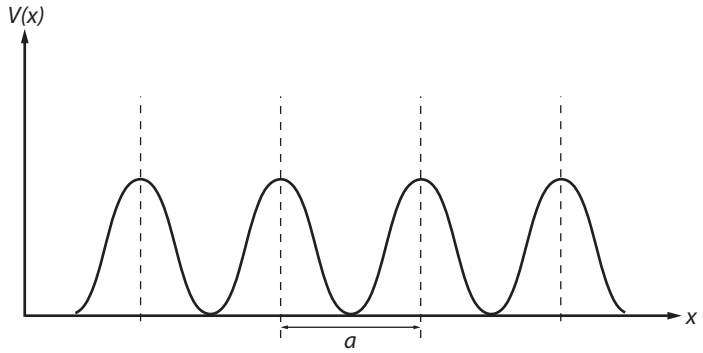

Figure 1.5: Periodic lattice potential

Such a potential may describe the motion of an electron in a chain of regularly spaced ions. In general the Hamiltonian is not invariant under a translation by an arbitrary amount l as described by the translation operator $\hat{T}_l$ which transforms the position operator according to

$$\hat{T}_l^\dagger \hat{x} \hat{T}_l = \hat{x} + l \,, \text{ and } \hat{T}_l|x'\rangle = |x' + l\rangle \,.$$

Only when l coincides with the lattice spacing a, one finds

$$\hat{T}_a^\dagger V(\hat{x}) \hat{T}_a = V(\hat{x} + a) = V(\hat{x}) \,.$$

Since the kinetic energy contained in the Hamiltonian is invariant under arbitrary displacements, the entire Hamiltonian satisfies

$$\hat{T}_a^\dagger \hat{H} \hat{T}_a = \hat{H}, \text{ and since } \hat{T}_a \text{ is unitary, also } [\hat{H}\,,\,\hat{T}_a]\,.$$

$\hat{H}$ and $\hat{T}_a$ can be simultaneously diagonalized for this reason.
First, we study a periodic potential with infinitely high boundaries.

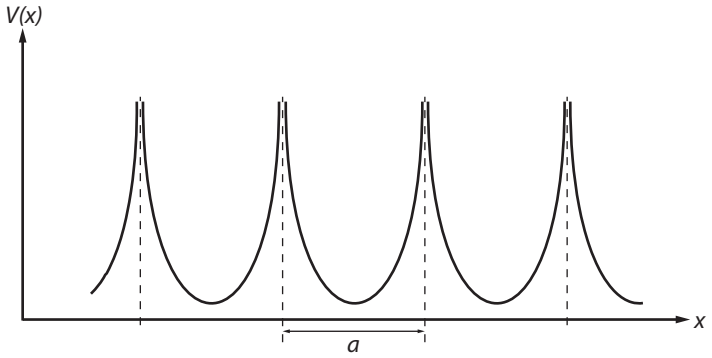

Figure 1.6: Periodic lattice potential with infinite boundaries

A particle located at lattice site n is a ground state of the Hamiltonian. We denote this state by $|n\rangle$, $\hat{H}|n\rangle = E_0|n\rangle$. The wave function $\langle x'|n\rangle$ is finite only on the n-th lattice site. $|n\rangle$ is not an eigenstate of $\hat{T}_a$:

$$\hat{T}_a|n\rangle = |n+1\rangle\,.$$

This is possible because of the degeneracy.
Consider the state

$$\begin{aligned} |\theta\rangle &\equiv \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle \text{ with } \theta \in [-\pi,\pi] \\ \hat{T}_a|\theta\rangle &= \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = \sum_{n'=-\infty}^{\infty} e^{i(n'-1)\,\theta}|n'\rangle \\ &= e^{-i\theta}\,|\theta\rangle\,. \end{aligned}$$

$\Rightarrow |\theta\rangle$ is eigenstate of $\hat{T}_a$ with eigenvalue $e^{-i\theta}$ with $|e^{-i\theta}| = 1$.
In the limit of infinitely high barriers, the energy is independent of θ. Now we consider the more realistic case of potential barriers with finite height. Then, the wave functions $\langle x'|n\rangle$ also have tails extending to neighboring sites.

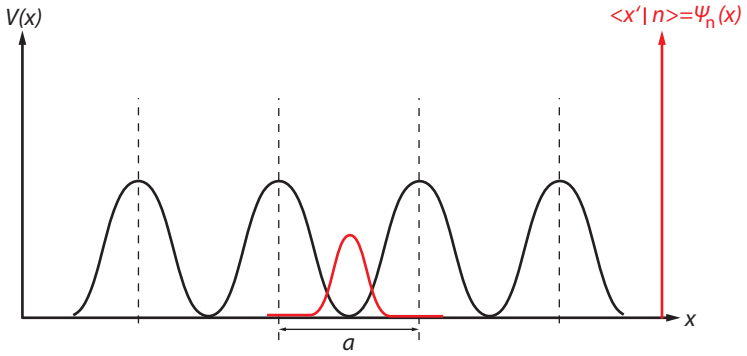

Figure 1.7: Periodic finite lattice potential and wave function on lattice site n

The diagonal matrix elements $\langle n|\hat{H}|n\rangle = E_0$ are all equal because of translational invariance. We assume that the only non-diagonal elements of importance are the one connecting immediate ("neutral") neighbors.

$$\langle n'|\vec{H}|n\rangle \neq 0 \text{ only if } n' = n \text{ or } n' = n \pm 1 \ .$$

This assumption is known as "tight-binding" approximation. More specifically $\langle n\pm 1|\hat{H}|n\rangle = -\Delta$ independent of n due to translational invariance. We thus obtain

$$\hat{H}|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle$$

valid to the extend that $\langle n'|n\rangle = \delta_{n,n'}$. We now again form the linear combination $|\theta\rangle$:

$$|\theta\rangle = \sum_n e^{in\theta}|n\rangle \text{ with } \hat{T}_a|\theta\rangle = e^{-i\theta}|\theta\rangle \ .$$

Applying the tight-binding Hamiltonian yields

$$\begin{aligned}
\hat{H}|\theta\rangle = \hat{H}\sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle &= E_0\sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle - \Delta\sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle - \Delta\sum_{n=-\infty}^{\infty} e^{in\theta}|n-1\rangle \\
&= E_0\sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle - \Delta\sum_{n=-\infty}^{\infty} e^{in\theta}e^{-i\theta}|n\rangle - \Delta\sum_{n=-\infty}^{\infty} e^{in\theta}e^{i\theta}|n\rangle \\
&= (E_0 - 2\Delta\cos\theta)\sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle = (E_0 - 2\Delta\cos\theta)|\theta\rangle \ .
\end{aligned}$$

The eigenstates depend on the parameter θ. The degeneracy is lifted, and we have a contineous spectrum of eigenvalues between $E_0 - 2\Delta$ and $E_0 + 2\Delta$.

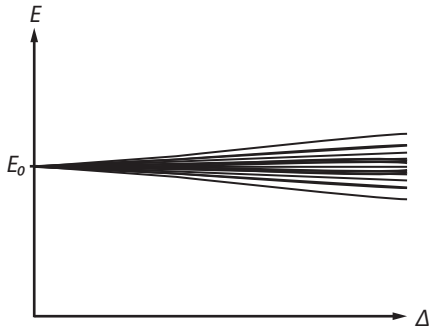

Figure 1.8: Energy spectrum

(In the homework the SSH-model, the simplest model of an topological insulator, is discussed. It has a diatomic unit cell (A, B labeled with n) and two different hopping strengths. The idea is to express the wave function as $\psi_n = (\psi_{nA}, \psi_{nB})$ separate.)

Physical significance of θ: Consider the wave function $\langle x'|\theta\rangle$. For the translated state $\hat{T}_a|\theta\rangle$, we find $\langle x'|\hat{T}_a|\theta\rangle = \langle x' - a|\theta\rangle$ by using $\langle x'|\hat{T}_a = \langle x'|\hat{T}^\dagger_{-a} = (\hat{T}_{-a}|x'\rangle)^\dagger = (|x' - a\rangle)^\dagger$ because $\hat{T}^\dagger_a = \hat{T}^{-1}_a = \hat{T}_{-a}$.
On the other hand, we know $\hat{T}_a|\theta\rangle = e^{-i\theta}|\theta\rangle$, such that

$$\langle x' - a|\theta\rangle = \langle x'|\theta\rangle\, e^{-i\theta} \ .$$

We find a solution by making the ansatz:

$$\langle x'|\theta\rangle = e^{ikx'}\, u_k(x') \text{ with } \theta = ka \text{ and } u_k(x') = u_k(x' \pm a) \ .$$

We varify by substitution that this ansatz indeed satisfies the condition

$$\langle x' - a|\theta\rangle = e^{ik(x'-a)} u_k(x' - a) = e^{ikx'} u_k(x') e^{-ika} = \langle x'|\theta\rangle e^{-ika} \ .$$

For wave functions in a periodic potential we thus find the condition known as **Bloch theorem**: *The wave function of the eigenket $|\theta\rangle$ can be written as a plane wave times a periodic function with periodicity of the lattice.*
Since we only used that $|\theta\rangle$ is an eigenket of $\hat{T}_a$ with eigenvalue $e^{-i\theta}$, the theorem even holds, when the tight-binding approximation breaks down.
We can now reinterpret our earlier result $|\theta\rangle = \sum_n e^{in\theta}|n\rangle$.

$$\langle x'|\theta\rangle = \sum_n e^{in\theta}\langle x'|n\rangle = e^{ikx'} \underbrace{\sum_n e^{-ik(x'-na)}\langle x'|n\rangle}_{u_k(x')} \text{ with } \theta = ka$$

As θ varies from $-\pi$ to π, the wave vector varies from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$.
The energy eigenvalue E depends on k as follows:

$$E(k) = E_0 - 2\Delta\cos(ka) \ .$$

This is independent of the detailed shape of the lattice potential, as long as the tight-binding approximations stays valid.

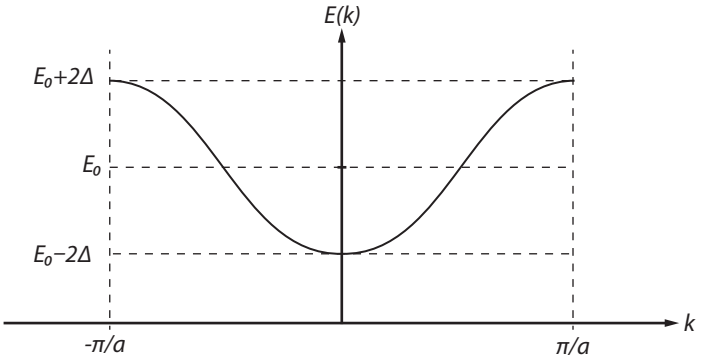

Figure 1.9: Dispersion relation $E(k)$

The range of allowed k values that yield linear independent wave functions is called Brillouin zone: $(-\frac{\pi}{a}, \frac{\pi}{a}]$.

(The velocity $v = \partial_k E(k)/\hbar = \partial_k \omega$ of electrons moving through the lattice. $p = \hbar k$ and $\dot{p} = eE \Rightarrow$ velocity can decrease when the momentum increases after passing $k = \pi/a$. In a clean atomic crystal a dc B-field can lead to an ac current. A Ohmic current-voltage dependence is only due to impurities.)
So far we considered only one electron in a periodic potential. In the case of many electrons, the Pauli exclusion principle must be satisfied: each state can only be occupied by one electron.

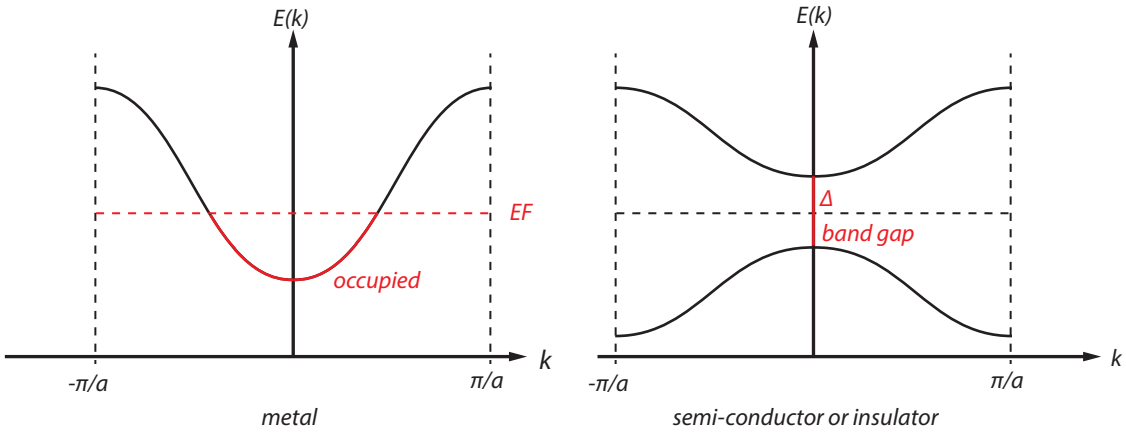

Figure 1.10: Band structure of a metal and a semi-conductor

The Fermi energy is referring to the energy difference between the highest and lowest occupied single-particle states in a quantum system of non-interacting fermions at absolute zero temperature.
If the band gap in the second case is $\Delta \sim k_B T$ it is a semi-conductor and for $\Delta \gg k_B T$ an insulator.
Electrons fill up the low energy states of the band, and the main quantitative features of metal, semi-conductors, and insulators can be explained.

1.2.3 The Time-Reversal Discrete Symmetry

This topic sounds initially difficult, because "time-reversal" is a misnomers, some what reminiscent of science fiction. What is meant here is a "reversal of motion".
We consider the trajectory of a particle subject to a given force-field. At time $t = 0$, we let the particle stop and reverse its motion, $\underline{p}|_{t=0^+} = -\underline{p}_{t=0^-}$. The particle runs backwards along the same trajectory.

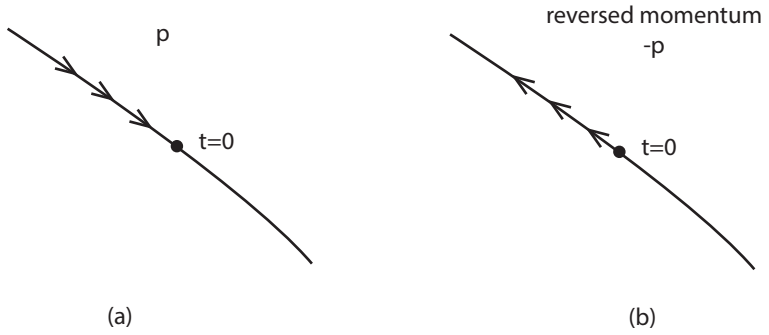

Figure 1.11: Reversing of motion to check time-reversal symmetry

If we run video recordings of trajectories (a) and (b), it looks as if the video of (b) was the video of (a) played backwards. This is the definition of time-reversal symmetry in classical mechanics. A system in classical mechanics is called time-reversal invariant if motion-reversal looks the same as playing video (a) backwards.
More formally, if $\underline{x}(t)$ is a solution of Newton's equation $m\ddot{x} = -\nabla V(x)$, then $x(-t)$ is a solution as well:

$$t' = -t \Rightarrow \frac{\mathrm{d}}{\mathrm{d}t'} = -\frac{\mathrm{d}}{\mathrm{d}t} \Rightarrow \frac{\mathrm{d}^2}{\mathrm{d}t'^2} = \frac{\mathrm{d}^2}{\mathrm{d}t^2} \ .$$

In the presence of a magnetic field, one can tell the difference between "motion reversal" and "playing the video backwards".

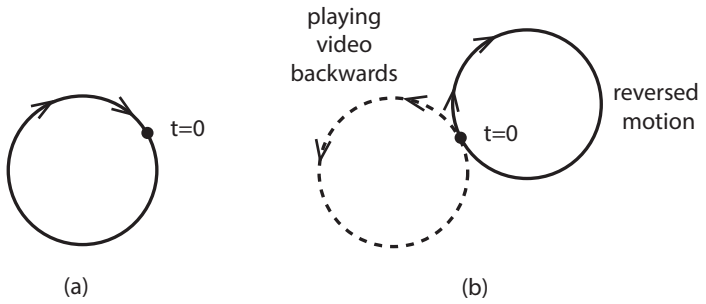

Figure 1.12: Electron in a constant magnetic field as an example of non-time-reversal-invariant system

This is since the Lorentz force $q\underline{v} \times \underline{B} = q\dot{\underline{x}} \times \underline{B}$ contains the first time derivative $\Rightarrow x(-t)$ is not a solution to the equation of motion.

We now consider the Schrödinger equation

$$\boldsymbol{i}\hbar\,\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\,\nabla^2 + V(\underline{x})\right)\psi\ . \qquad (*)$$

When we have a solution $\psi(\underline{x},t)$, then $\psi(\underline{x},-t)$ is clearly not a solution due to the appearance of the first time derivative.
The complex conjugate of (*) is

$$-\boldsymbol{i}\hbar\,\frac{\partial\psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m}\,\nabla^2 + V(\underline{x})\right)\psi^*\ .$$

However, $\psi^*(\underline{x},-t)$ is a solution as one sees by complex conjugation.
This can be seen explicitly when considering an energy eigenstate

$$\psi(\underline{x},t) = u_n(\underline{x})\,e^{-\boldsymbol{i}\,\frac{E_n}{\hbar}\,t}\ ,\ \psi^*(\underline{x},-t) = u_n^*(\underline{x})\,e^{-\boldsymbol{i}\,\frac{E_n}{\hbar}\,t}$$

substituted into the Schrödinger equation. We thus conjecture that time-reversal is related to complex conjugation.

1.2.3.1 Digression on Symmetry Operations

Consider a symmetry operation $|\alpha\rangle \mapsto |\widetilde{\alpha}\rangle\ ,\ \ |\beta\rangle \mapsto |\widetilde{\beta}\rangle$. So far, we required that the inner product stays unchanged

$$\langle\widetilde{\beta}|\widetilde{\alpha}\rangle = \langle\beta|\alpha\rangle\ .$$

This was natural because the symmetry operations considered so far were unitary:

$$|\widetilde{\beta}\rangle = \hat{U}|\beta\rangle\ ,\ \langle\widetilde{\beta}| = \langle\beta|\hat{U}^\dagger = \langle\beta|\hat{U}^{-1} \Longrightarrow \langle\widetilde{\beta}|\widetilde{\alpha}\rangle = \langle\beta|\underbrace{\hat{U}^\dagger\hat{U}}_{\mathbb{1}}|\alpha\rangle = \langle\beta|\alpha\rangle$$

For time-reversal this condition is too restrictive, and we impose the weaker requirement that

$$|\langle\widetilde{\beta}|\widetilde{\alpha}\rangle| = |\langle\beta|\alpha\rangle|\ .$$

This is obviously satisfied if $\langle\widetilde{\beta}|\widetilde{\alpha}\rangle = \langle\beta|\alpha\rangle$, but $\langle\widetilde{\beta}|\widetilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle$ works equally well.

The transformation $|\alpha\rangle \mapsto |\widetilde{\alpha}\rangle = \hat{\theta}|\alpha\rangle\ \ ,\ \ |\beta\rangle \mapsto |\widetilde{\beta}\rangle = \hat{\theta}|\beta\rangle$ is said to be **anti-unitary** if

$$\langle\widetilde{\beta}|\widetilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* \qquad \text{(I)}$$

$$\hat{\theta}\,(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^*\hat{\theta}|\alpha\rangle + c_2^*\hat{\theta}|\beta\rangle \qquad \text{(II)}$$

The second condition (II) defines an anti-linear operator. We now claim that an anti-unitary operator can be written as $\hat{\theta} = \hat{U}\hat{K}$, with a unitary operator $\hat{U}$, and with $\hat{K}$ denoting the complex conjugation operator. $\hat{K}$ takes the complex conjugate of any coefficient multiplying a ket, e.g.

$$\hat{K}c|\alpha\rangle = c^*\hat{K}|\alpha\rangle\ .$$

If $|\alpha\rangle$ is expended in terms of base kets $|a'\rangle$, then

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle$$
$$\hat{K}|\alpha\rangle = \sum_{a'} \langle a'|\alpha\rangle^* \hat{K}|a'\rangle = \sum_{a'} \langle a'|\alpha\rangle^* |a'\rangle \ .$$

Important is that the base kets are not changed under the action of $\hat{K}$. This is due to the fact that the explicit representation of the base ket $|a'\rangle$ corresponds to $(0, ..., 0, 1, 0, ..., 0)$ which is not changes by $\hat{K}$ (no proof given here).

One can ask whether the $\hat{s}_y$-eigenkets for spin $\frac{1}{2}$ are changed by $\hat{K}$. When the $\hat{s}_y$-eigenkets are used as space-kets, they stay unchanged. If the $\hat{s}_z$-eigenkets are used however, then

$$\hat{K}\ \left(\frac{1}{\sqrt{2}}\ |+\rangle \pm \frac{\boldsymbol{i}}{\sqrt{2}}\ |-\rangle\right) = \frac{1}{\sqrt{2}}\ |+\rangle \mp \frac{\boldsymbol{i}}{\sqrt{2}}\ |-\rangle \ .$$

Thus, the effect of $\hat{K}$ changes with bases, and the form of $\hat{U}$ also depends on the particular representation.

Let us check the anti-linearity for $\hat{\theta} = \hat{U}\hat{K}$.

$$\begin{aligned}\hat{\theta}\ (c_1|\alpha\rangle + c_2|\beta\rangle) &= \hat{U}\hat{K}\ (c_1|\alpha\rangle + c_2|\beta\rangle) \\ &= c_1^*\hat{U}\hat{K}|\alpha\rangle + c_2^*\hat{U}\hat{K}|\beta\rangle \\ &= c_1^*\hat{\theta}|\alpha\rangle + c_2^*\hat{\theta}|\beta\rangle\end{aligned}$$

Before checking condition (I), we state that it is safer to work with the action of $\hat{\theta}$ on kets only, and to not consider the action of $\hat{\theta}$ on bras or the Hermitian adjoint $\hat{\theta}^\dagger$.
We find

$$\begin{aligned}|\widetilde{\alpha}\rangle = \hat{\theta}|\alpha\rangle &= \sum_{a'} \langle a'|\alpha\rangle^* \hat{U}|a'\rangle \\ &= \sum_{a'} \langle \alpha|a'\rangle\ \hat{U}|a'\rangle\end{aligned}$$

similarly for

$$\begin{aligned}|\widetilde{\beta}\rangle &= \sum_{a'} \langle \beta|a'\rangle\ \hat{U}|a'\rangle \\ \langle\widetilde{\beta}| &= \sum_{a'} \langle a'|\beta\rangle\langle a'|\ \hat{U}^\dagger \\ \Rightarrow \langle\widetilde{\beta}|\widetilde{\alpha}\rangle &= \sum_{a'}\sum_{a''} \langle a''|\beta\rangle\ \underbrace{\langle a''|\underbrace{\hat{U}^\dagger\hat{U}}_{\mathbb{1}}|a'\rangle}_{\delta_{a',a''}}\langle\alpha|a'\rangle \\ &= \sum_{a'} \langle\alpha|a'\rangle\langle a'|\beta\rangle = \langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* \ .\end{aligned}$$

1.2.3.2 Time-Reversal Operator

In the following, we denote the time-reversal operator by $\hat{T}$, and $|\widetilde{\alpha}\rangle = \hat{T}|\alpha\rangle$ is the time-reversed (or better motion-reversed) state.
If $|\alpha\rangle = |\underline{p}'\rangle$ is a momentum eigenstate, then we expect $\hat{T}|\underline{p}'\rangle = |-\underline{p}'\rangle$. Similarly, we expect angular momentum $\hat{J}$ to be reversed under time-reversal.
We now establish a fundamental property of $\hat{T}$ by studying the time evolution of the motion reversed state. For a infinitesimal δt we have

$$|\alpha; t_0 = 0, t = \delta t\rangle = \left[1 - \frac{\boldsymbol{i}\hat{H}}{\hbar}\,\delta t\right]|\alpha\rangle \text{ with initial state } |\alpha\rangle = |\alpha; t_0 = 0, t = 0\rangle$$

as the time evolution of $|\alpha\rangle$. The time evolution of the time-reversed state is given by

$$\left[1 - \frac{\boldsymbol{i}\hat{H}}{\hbar}\,\delta t\right]\hat{T}\,|\alpha\rangle\ .$$

According to our classical considerations, if motion obeys symmetry under time reversal, then $\hat{T}|\alpha; t_0 = 0, t = \delta t\rangle$ is the same state as the above.

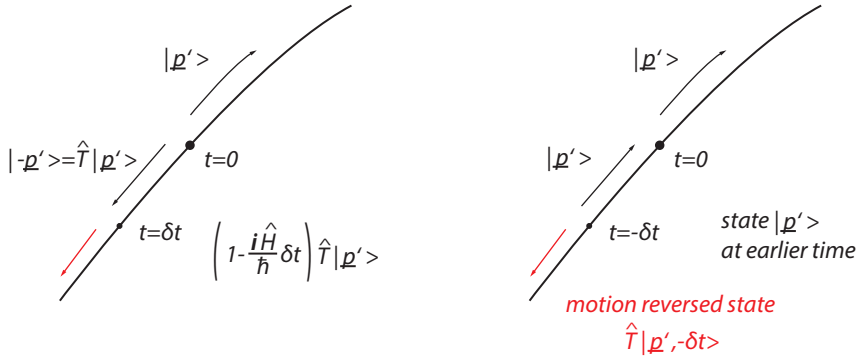

Figure 1.13: Illustration of the condition for time reversal symmetry

Considering a state at an earlier time and motion reversing is the same as propagating the motion reversed state forward in time. Mathematically, we obtain

$$\hat{T}\left(1 - \frac{\boldsymbol{i}\hat{H}}{\hbar}\,(-\delta t)\right)|\alpha\rangle = \left(1 - \frac{\boldsymbol{i}\hat{H}}{\hbar}\,\delta t\right)\hat{T}\,|\alpha\rangle$$

If this relation is true for every ket $|\alpha\rangle$, it must be an operator identity

$$\boxed{-\boldsymbol{i}\hat{H}\hat{T} = \hat{T}\boldsymbol{i}\hat{H}}$$

If $\hat{T}$ was unitary, it was also linear and we could cancel the factors $\boldsymbol{i}$ in the above equation, and would find that $-\hat{H}\hat{T} = \hat{H}\hat{T}$.
Consider now an energy eigenstate $\hat{n}$ with eigenvalues E_n. Then, the time reversed state $\hat{T}|n\rangle$ satisfies

$$\hat{H}\hat{T}|n\rangle = -\hat{T}\hat{H}|n\rangle = (-E_n)\hat{T}|n\rangle\ ,$$

i.e. an eigenstate with eigenvalue $-E_n$. This is not possible even in the elementary case of a free particle: the energy spectrum $\frac{\hbar^2 k^2}{2m}$ is positive semidefinite and thus not contain negative eigenvalues.

We also see this contradiction when looking at the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$. Under time reversal, we expect $\underline{p} \mapsto -\underline{p}$, but $\underline{p}^2$ should not change sign $\Rightarrow$ we are not allowed to cancel factors of $\boldsymbol{i}$ in $-\boldsymbol{i}\hat{H}\hat{T} = \hat{T}\boldsymbol{i}\hat{H}$, and that $\hat{T}$ should better be anti-unitary.
Then, $-\boldsymbol{i}\hat{H}\hat{T} = \hat{T}\boldsymbol{i}\hat{H} = -\boldsymbol{i}\hat{T}\hat{H}$ and

$$\boxed{\hat{H}\hat{T} = \hat{T}\hat{H}} \; .$$

The Hamiltonian is $\hat{T}$-invariant if $[\hat{T}\,,\,\hat{H}] = 0$.

We now consider a general operator $\hat{O}$, and prove that the identity

$$\boxed{\langle\beta|\hat{O}|\alpha\rangle = \langle\tilde{\alpha}|\hat{T}\hat{O}^\dagger\hat{T}^{-1}|\tilde{\beta}\rangle}$$

follows from the anti-linear property of $\hat{T}$.

Proof: We define $|\gamma\rangle \equiv \hat{O}^\dagger|\beta\rangle$, the corresponding bra is $\langle\gamma| = \langle\beta|\hat{O}$. Then using $|\tilde{\gamma}\rangle = \hat{T}|\gamma\rangle$ yields

$$\langle\beta|\hat{O}|\alpha\rangle = \langle\gamma|\alpha\rangle = \langle\tilde{\alpha}|\tilde{\gamma}\rangle = \langle\tilde{\alpha}|\hat{T}\hat{O}^\dagger|\beta\rangle\langle\tilde{\alpha}|\hat{T}\hat{O}^\dagger\hat{T}^{-1}(\hat{T}|\beta\rangle) = \langle\tilde{\alpha}|\hat{T}\hat{O}^\dagger\hat{T}^{-1}|\tilde{\beta}\rangle \; . \; \square$$

For a Hermitian observable $\hat{A}$, we find that

$$\langle\beta|\hat{A}|\alpha\rangle = \langle\tilde{\alpha}|\hat{T}\hat{A}\hat{T}^{-1}|\tilde{\beta}\rangle \; . \qquad (*)$$

We define an observable to be even or odd under time-reversal according to whether the upper or lower sign in the following equation applies:

$$\hat{T}\hat{A}\hat{T}^{-1} = \pm\hat{A}$$

Taking this equation together with the rule (*) for matrix elements, we find the following restriction on matrix elements

$$\langle\beta|\hat{A}|\alpha\rangle = \pm\langle\tilde{\beta}|\hat{A}|\tilde{\alpha}\rangle^* \; .$$

For expectation values with $|\beta\rangle \equiv |\alpha\rangle$, we find

$$\langle\alpha|\hat{A}|\alpha\rangle = \pm\langle\tilde{\alpha}|\hat{A}|\tilde{\alpha}\rangle \; .$$

Example: Expectation value of $\hat{\underline{p}}$. We will reasonably assume that the expectation value of $\hat{\underline{p}}$ taken with respect to the time-reversed state will have the opposite sign as compared to the original state:

$$\langle\alpha|\hat{\underline{p}}|\alpha\rangle = -\langle\tilde{\alpha}|\hat{\underline{p}}|\tilde{\alpha}\rangle \; .$$

$\Rightarrow \hat{\underline{p}}$ is an odd operator:

$$\boxed{\hat{T}\hat{\underline{p}}\hat{T}^{-1} = -\hat{\underline{p}} \Longleftrightarrow \hat{T}\hat{\underline{p}} = -\hat{\underline{p}}\hat{T}} \; .$$

It follows than that $\hat{\underline{p}}\hat{T}|\underline{p}'\rangle = -\hat{T}\hat{\underline{p}}|\underline{p}'\rangle = -\underline{p}'\hat{T}|\underline{p}'\rangle$ which agrees with our earlier assumption that $\hat{T}|\underline{p}'\rangle$ is a momentum eigenket with eigenvalue $-\underline{p}'$.
Similarly we find that

$$\boxed{\hat{T}\hat{\underline{x}}\hat{T}^{-1} = \hat{\underline{x}}} \ .$$

and $\hat{T}|\underline{x}'\rangle = |\underline{x}'\rangle$ up to a phase factor $e^{i\delta}$ which is often taken to be unity.

Now we can verify the invariance of the fundamental commutator relation $[\hat{x}_i \, , \, \hat{p}_j]|\alpha\rangle = \boldsymbol{i}\hbar\delta_{ij}|\alpha\rangle$ where $|\alpha\rangle$ stands for every possible ket. Applying $\hat{T}$ to both sites yields

$$\hat{T}[\hat{x}_i \, , \, \hat{p}_j]\hat{T}^{-1}\hat{T}|\alpha\rangle = \hat{T}\boldsymbol{i}\hbar\delta_{ij}|\alpha\rangle \ .$$

Using the transformation properties of $\hat{\underline{x}}$ and $\hat{\underline{p}}$, and using $\hat{T}\boldsymbol{i} = -\boldsymbol{i}\hat{T}$ we find

$$\begin{aligned}[\hat{x}_i \, , \, -\hat{p}_j]\hat{T}|\alpha\rangle &= -\boldsymbol{i}\hbar\delta_{ij}\hat{T}|\alpha\rangle \\ [\hat{x}_i \, , \, \hat{p}_j] &= \boldsymbol{i}\hbar\delta_{ij} \ .\end{aligned}$$

From the invariance of the commutator under $\hat{T}$ we can sometimes determine if a operator must be odd or even.
The fundamental commutation relation is only preserved since $\hat{T}$ is anti-unitary. Similarly, in order to preserve

$$[\hat{J}_i \, , \, \hat{J}_j] = \boldsymbol{i}\hbar\varepsilon_{ijk}\hat{J}_k \ ,$$

the angular momentum operator $\hat{\underline{J}}$ must be odd under time-reversal.

$$\boxed{\hat{T}\hat{\underline{J}}\hat{T}^{-1} = -\hat{\underline{J}}}$$

This applies to orbital angular momentum and spin. For a spinless system with $\hat{\underline{J}} = \hat{\underline{x}} \times \hat{\underline{p}}$ this is consistent with $\hat{\underline{x}}$ being even and $\hat{\underline{p}}$ being odd.

1.2.3.3 Wave Functions

We consider a spinless particle to be in state $|\alpha\rangle$.
In position representation, we can expand

$$|\alpha\rangle = \int \mathrm{d}^3x' \ \langle\underline{x}'|\alpha\rangle|\underline{x}'\rangle \ .$$

Application of the time-reversal operator yields

$$\begin{aligned}\hat{T}|\alpha\rangle &= \int \mathrm{d}^3x' \ \langle\underline{x}'|\alpha\rangle^*\hat{T}|\underline{x}'\rangle \\ &= \int \mathrm{d}^3x' \ \langle\underline{x}'|\alpha\rangle^*|\underline{x}'\rangle\end{aligned}$$

$\Rightarrow \langle\underline{x}'|\alpha\rangle^*$ is the wave function of the time-reversed state, and we used the phase convention $\hat{T}|\underline{x}'\rangle = |\underline{x}'\rangle$.
We recover the following rule $\psi(\underline{x}') \overset{\hat{T}}{\longmapsto} \psi^*(\underline{x}')$, inferred earlier from looking at the Schrödinger equation.

In a rotationally invariant potential the angular part of the wave function is given by a spherical harmonic $Y_l^m(\theta,\varphi)$ with $Y_l^m \propto P_l^m(\cos\theta)\, e^{im\varphi}$. We find $Y_l^m(\theta,\varphi) \overset{\hat{T}}{\longmapsto} Y_l^{m*}(\theta,\varphi) = (-1)^m Y_l^{-m}(\theta,\varphi)$ since $P_l^m = (-1)^m P_l^{-m}$. We deduced that in general

$$\boxed{\hat{T}|l,m\rangle = (-1)^m |l,-m\rangle}\ .$$

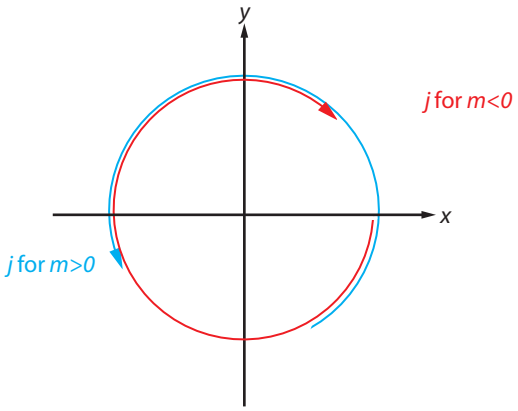

Figure 1.14: Probability current associated with a wave function of type $R_{nl}(r)Y_l^m(\theta,\varphi)$ (expected motion, e.g. of an electron; $j \propto \mathrm{Im}(\psi^*\nabla\psi)$)

When computing the probability current associated with a wave function of type $R_{nl}(r)Y_l^m(\theta,\varphi)$, one finds that for $m > 0$ the current flows in the counter clockwise direction within the x-y-plane (as seen from the positive z-axis). The wave function for the corresponding time-reversed state has the probability current flowing in the opposite direction, as m is reversed.

An interesting consequence of time-reversal symmetry is the following theorem:
We consider a time-reversal invariant Hamiltonian with a non-degenerate energy eigenket $|n\rangle$. Then the corresponding energy eigenfunction is real, or can be made real by multiplication with a phase factor independent of the position $\underline{x}$.

Proof: We start with

$$\hat{H}\hat{T}|n\rangle = \hat{T}\hat{H}|n\rangle = E_n\hat{T}|n\rangle\,,$$

and conclude that $|n\rangle$ and $\hat{T}|n\rangle$ have he same energy. Due to the assumption of non-degeneracy, $|n\rangle$ and $\hat{T}|n\rangle$ must represent the same state. The corresponding wave functions are $\langle\underline{x}'|n\rangle$ and $\langle\underline{x}'|n\rangle^*$. They must be the same $\langle\underline{x}'|n\rangle = \langle\underline{x}'|n\rangle^*$ since $\hat{\underline{x}}$ is even. $\square$

As a consequence the wave function of a non-degenerate bound state is always real. In the hydrogen atom, the eigenfunctions for states with $l \neq 0$, and $m \neq 0$ are complex because the spherical harmonics Y_l^m are complex. This does not contradict the above theorem because $|n;l,m\rangle$ and $|n;l,-m\rangle$ are degenerate.
Vice versa, if $\hat{H}$ is $\hat{T}$-invariant and we have a complex wave function, there need to be a degeneracy.
Similarly, the wave function of a plane wave $e^{\frac{i}{\hbar}\underline{p}\cdot\underline{x}}$ is complex, but degenerate with $e^{-\frac{i}{\hbar}\underline{p}\cdot\underline{x}}$.

For a spinless system, the wave function for the time-reversal state is simply obtained by complex conjugation (in the position representation).

Expanding a ket $|\alpha\rangle$ in position representation, $\hat{T}$ is the same as complex conjugation $\hat{K}$ because both have the same effect. When expressing in terms of momentum eigenkets however, we need to take into account $\hat{T}|\underline{p}'\rangle = |-\underline{p}'\rangle$ and obtain

$$\hat{T}|\alpha\rangle = \int \mathrm{d}^3p' \; |-\underline{p}'\rangle\langle\underline{p}'|\alpha\rangle^* = \int \mathrm{d}^3p' \; |\underline{p}'\rangle\langle-\underline{p}'|\alpha\rangle^* \; .$$

Apparently the momentum space wave function of the time-reversed state is not just the complex conjugation of the original wave function, but in addition we need to take $\phi^*(-\underline{p}')$, the complex conjugate with the momentum reversed.

1.2.3.4 Time-Reversal for a Spin-$\frac{1}{2}$ System

Consider an eigenket of $\hat{S} \cdot \hat{n}$:

$$|\hat{n}, +\rangle = e^{-\frac{i}{\hbar}\hat{S}_z\,\alpha} e^{-\frac{i}{\hbar}\hat{S}_y\,\beta}|+\rangle \; .$$

Since the rotation operator is given by $e^{-\frac{i}{\hbar}\underline{\varphi}\cdot\underline{\hat{S}}}$ this is a rotation of the $|+\rangle$ state which points in positive z-direction ($\hat{S}_z|+\rangle = \frac{\hbar}{2}|+\rangle$ and $\hat{S}_z|-\rangle = -\frac{\hbar}{2}|-\rangle$) to a position with polar angle β and azimuthal angle α.

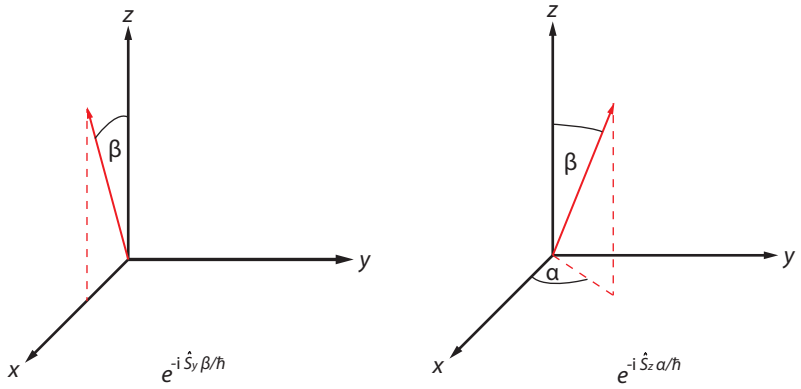

Figure 1.15: $e^{-\frac{i}{\hbar}\hat{S}_z\,\alpha}$ corresponds to a rotation by α around the z-axis and $e^{-\frac{i}{\hbar}\hat{S}_y\,\beta}$ is a rotation of β around the y-axis.

Because of $\hat{T}\hat{J} = -\hat{J}\hat{T}$ and the anti-unitary property of $\hat{T}$ we have

$$\hat{T}|\hat{n}, +\rangle = e^{-\frac{i}{\hbar}\hat{S}_z\alpha} e^{-\frac{i}{\hbar}\hat{S}_y\beta}|-\rangle$$

where $|+\rangle = |m = +1/2\rangle$, therefore $\hat{T}|+\rangle = \eta|-\rangle$

$$\hat{T}|\hat{n}, +\rangle = e^{-\frac{i}{\hbar}\hat{S}_z\alpha} e^{-\frac{i}{\hbar}\hat{S}_y\beta}\hat{T}|+\rangle = \eta|\hat{n}, -\rangle \; .$$

On the other hand, we can verify that

$$|\hat{n}, -\rangle = e^{-\frac{i}{\hbar}\hat{S}_z\alpha} e^{-\frac{i}{\hbar}\hat{S}_y(\beta+\pi)}|+\rangle \; .$$

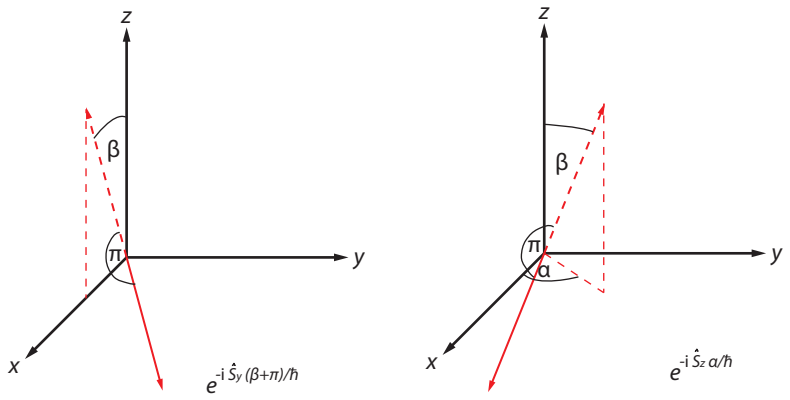

Figure 1.16: Additional factor $e^{-\frac{i}{\hbar}\pi\hat{S}_y}$ is needed for the $|\hat{n},-\rangle$ state.

We saw earlier that $\hat{T}=\hat{U}\hat{K}$ is a possible representation of $\hat{T}$. Remembering that $\hat{K}|+\rangle=|+\rangle$, $\hat{K}|-\rangle=|-\rangle$ does not change the base kets, we see that

$$\boxed{\hat{T}=\eta\, e^{-\frac{i}{\hbar}\pi\hat{S}_y}\hat{K}=-i\eta\left(\frac{2\hat{S}_y}{\hbar}\right)\hat{K}}$$

is the representation we are looking for.
Here we used that

$$\begin{aligned}e^{-\frac{i}{\hbar}\alpha\hat{S}_y}&=\sum_{n=0}^{\infty}\left(\frac{2\hat{S}_y}{\hbar}\right)^n\frac{(-i\alpha/2)^n}{n!}\\&=\sum_{m=0}^{\infty}\left(\frac{2\hat{S}_y}{\hbar}\right)^{2m}\frac{(\alpha/2)^{2m}}{(2m)!}(-i)^{2m}-i\,\frac{2\hat{S}_y}{\hbar}\sum_{n=0}^{\infty}\left(\frac{2\hat{S}_y}{\hbar}\right)^{2m}(-i)^{2m}\frac{(\alpha/2)^{2m+1}}{(2m+1)!}\,.\end{aligned}$$

With $\hat{S}_y^2=\frac{\hbar^2}{4}\,\mathbb{1}$ (remember this via: $\hat{S}^2=\hbar^2 s(s+1)=\hbar^2 3/4=\hat{S}_x^2+\hat{S}_y^2+\hat{S}_z^2\Rightarrow\hat{S}_z^2=\hbar^2/4$) we have $(2\hat{S}_y^2/\hbar)^2=\mathbb{1}$ and thus

$$\begin{aligned}e^{-\frac{i}{\hbar}\alpha\hat{S}_y}&=\sum_{m=0}^{\infty}\frac{(\alpha/2)^{2m}(-i)^{2m}}{(2m)!}-i\,\frac{2\hat{S}_y}{\hbar}\sum_{n=0}^{\infty}(-i)^{2m}\frac{(\alpha/2)^{2m+1}}{(2m+1)!}\\&=\sum_{m=0}^{\infty}(-1)^m\frac{(\alpha/2)^{2m}}{(2m)!}-i\,\frac{2\hat{S}_y}{\hbar}\sum_{n=0}^{\infty}(-1)^m\frac{(\alpha/2)^{2m+1}}{(2m+1)!}\\&=\cos\left(\frac{\alpha}{2}\right)-i\,\frac{2\hat{S}_y}{\hbar}\sin\left(\frac{\alpha}{2}\right).\end{aligned}$$

We found:

$$\boxed{e^{-\frac{i}{\hbar}\alpha\hat{S}_y}=\cos\left(\frac{\alpha}{2}\right)-i\,\frac{2\hat{S}_y}{\hbar}\sin\left(\frac{\alpha}{2}\right)}$$

and thus

$$e^{-\frac{i}{\hbar}\pi\hat{S}_y}=-i\,\frac{2\hat{S}_y}{\hbar}\,.$$

Along similar lines one finds the important result

$$\boxed{e^{-\frac{i}{\hbar}\alpha\,\hat{n}\cdot\hat{\underline{S}}} = \cos\left(\frac{\alpha}{2}\right) - \boldsymbol{i}\,\frac{2\,\hat{n}\,\cdot\,\hat{\underline{S}}}{\hbar}\,\sin\left(\frac{\alpha}{2}\right)} \ .$$

For spin-$\frac{1}{2}$ system holds

$$\hat{T} = -\boldsymbol{i}\eta\,\frac{2\hat{S}_y}{\hbar}\,\hat{K} \text{ and } \hat{S}_y \hat{=} \frac{\hbar}{2}\underline{\underline{\sigma}}^y \ , \ \underline{\underline{\sigma}}^y = \begin{pmatrix} 0 & -\boldsymbol{i} \\ \boldsymbol{i} & 0 \end{pmatrix} \ .$$

Therefore we have for the spin-$\frac{1}{2}$ system: $\hat{T} = -\boldsymbol{i}\eta\underline{\underline{\sigma}}^y\hat{K}$, and often one chooses $\eta = \boldsymbol{i}$ and thus

$$\boxed{\hat{T} = \underline{\underline{\sigma}}^y\hat{K}} \ .$$

In a homework problem, it was verified that if $\chi(\hat{n},+)$ is an eigenspinor of $\hat{n}\,\cdot\,\underline{\underline{\sigma}} = n_x\underline{\underline{\sigma}}^x + n_y\underline{\underline{\sigma}}^y + n_z\underline{\underline{\sigma}}^z$ with eigenvalue $+1$: $\hat{n}\cdot\underline{\underline{\sigma}}\,\chi(\hat{n},+) = \chi(\hat{n},+)$, then $-\boldsymbol{i}\underline{\underline{\sigma}}^y\,\chi^*(\hat{n},+) = \chi(\hat{n},-)$ with $\hat{n}\,\cdot\,\underline{\underline{\sigma}}\,\chi(\hat{n},-) = (-1)\chi(\hat{n},-)$ an eigenspinor pointing in the opposite direction. The appearance of $\hat{S}_y, \underline{\underline{\sigma}}^y$ is due to the fact that we use a basis $\{|+\rangle, |-\rangle\}$ of eigenspinors of $\hat{S}_z$, i.e. $\hat{S}_z$ is diagonal, and $\hat{S}_y, \underline{\underline{\sigma}}^y$ is purely imaginary.

$$\underline{\underline{\sigma}}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \ , \underline{\underline{\sigma}}^y = \begin{pmatrix} 0 & -\boldsymbol{i} \\ \boldsymbol{i} & 0 \end{pmatrix} \ , \underline{\underline{\sigma}}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \ .$$

We check $\hat{T}\underline{\underline{\sigma}}^{x,y,z} = -\underline{\underline{\sigma}}^{x,y,z}\hat{T}$:

- $\underline{\underline{\sigma}}^y$: $(-)$ sign from complex conjugation
- $\underline{\underline{\sigma}}^{x,z}$: $(-)$ sign from $\underline{\underline{\sigma}}^{x,z}\underline{\underline{\sigma}}^y = -\underline{\underline{\sigma}}^y\underline{\underline{\sigma}}^{x,z}$

We note that

$$e^{-\frac{i}{\hbar}\,\pi\,\hat{S}_y}|+\rangle = (+1)|-\rangle \text{ and } e^{-\frac{i}{\hbar}\,\pi\,\hat{S}_y}|-\rangle = (-1)|+\rangle$$

as can be seen in a component representation with $|+\rangle\hat{=}(1,0)$, $|-\rangle\,\hat{=}\,(0,1)$, and phase convention $\eta = 1$

$$\Rightarrow e^{-\frac{i}{\hbar}\,\pi\,\hat{S}_y}\hat{=} -\boldsymbol{i}\underline{\underline{\sigma}}^y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \ .$$

We are now in a position to work out the effect of $\hat{T}$ on the most general spin-$\frac{1}{2}$ ket

$$\begin{aligned} \hat{T}(c_+|+\rangle + c_-|-\rangle) &= \eta c_+^*|-\rangle + \eta c_-^*(-1)|+\rangle \\ \hat{T}^2(c_+|+\rangle + c_-|-\rangle) &= \eta\eta^* c_+(-1)|+\rangle + \eta\eta^* c_-(-1)|-\rangle \\ &= (-1)\,(c_+|+\rangle + c_-|-\rangle) \end{aligned}$$

Hence, we have for a spin-$\frac{1}{2}$ system

$$\boxed{\hat{T}^2 = -\mathbb{1}} \ .$$

This situation is very different for a spinless system, where $\hat{T}^2 = +\mathbb{1}$, which can be inferred from $\hat{T}|l,m\rangle = (-1)^m|l,-m\rangle$. Even more generally, we now demonstrate that

$$\begin{aligned} \hat{T}^2|j \text{ half-integer}\rangle &= -1\,|j \text{ half-integer}\rangle \\ \hat{T}^2|j \text{ integer}\rangle &= +1\,|j \text{ integer}\rangle \ . \end{aligned}$$

As a consequence, the eigenvalue of $\hat{T}^2$ is given by $(-1)^{2j}$. First, we note that even for general j we have

$$\hat{T} = \eta e^{-\frac{i}{\hbar}\pi \hat{J}_y}\hat{K}$$

since the from of the rotation operator does not depend on the specific value of j. We now expand a general ket $|\alpha\rangle$ in terms of $|j,m\rangle$ base kets

$$\begin{aligned}\hat{T}\left(\hat{T}|\alpha\rangle\right) &= \hat{T}\left(\hat{T}\sum_m |j,m\rangle\langle j,m|\alpha\rangle\right) = \hat{T}\left(\eta\sum_m e^{-\frac{i}{\hbar}\pi\hat{J}_y}|j,m\rangle\langle j,m|\alpha\rangle^*\right)\\ &= |\eta|^2 e^{-\frac{2i\pi}{\hbar}\hat{J}_y}\sum_m |j,m\rangle\langle j,m|\alpha\rangle = e^{-\frac{2i\pi}{\hbar}\hat{J}_y}|\alpha\rangle\\ \Rightarrow \hat{T}^2 &= e^{-2i\pi\hat{J}_y/\hbar}\ .\end{aligned}$$

However

$$e^{-2i\pi\hat{J}_y/\hbar}|j,m\rangle = (-1)^{2j}|j,m\rangle$$

due to the properties of angular momentum eigenkets under rotation. This can be understood for instance by expanding in an eigenbasis of $\hat{J}_y$ which satisfies $\hat{J}_y|j,m_y\rangle = \hbar m_y|j,m_y\rangle$ with $-j \le m_y \le j$ such that $\hat{J}_y$ can be replaced by an integer$\cdot\hbar$ for integer $j \Rightarrow e^{-2\pi i m_y} = 1$, and it is replaced by a half-integer$\cdot\hbar$ for half-integer $j \Rightarrow e^{-2\pi i m_y} = -1$.

Remark:
An integer j is obtained either by the orbital state $|l,m\rangle$ of a spinless particle, or by the "addition" (to be discussed later) of two spin-$\frac{1}{2}$ particles, for instance the spin state $\frac{1}{\sqrt{2}}(|+-\rangle \pm |-+\rangle)$ (corresponds to $m=0$, $+: j=1$ or $-: j=0$) or $|++\rangle$ ($j=1$, $m=1$) or $|--\rangle$ ($j=1$, $m=-1$) where $|m_1\,,\,m_2\rangle$ is used as a notation. Two times spin $\frac{1}{2}$ can be $j=0$ (one state, singlet) or $j=1$ (three states, triplet).
Similarly, a half-integer j may stand for a single electron or a three-electron system in any configuration. Generally, for a system made up of electrons only, any system with an odd (even) number of electrons has $\hat{T}^2 = -\mathbb{1}$ ($\hat{T}^2 = \mathbb{1}$). For this to happen, the electrons do not have to be in an eigenstate of $\hat{\underline{J}}^2$.

Remark on phase convention:
Inspired by the rule for angular momentum $\hat{T}|l,m\rangle = (-1)^m|l,-m\rangle$ often on chooses
$\hat{T}|j,m\rangle = (-1)^m|j,-m\rangle$ for integer j. This can be generalized to half-integer j by demanding $\hat{T}|j,m\rangle = i^{2m}|j,-m\rangle$. This corresponds to a choice of phase $\eta = i$.

1.2.3.5 Kramers Degeneracy

Consider a charged particle in a electrostatic potential $e\phi(\hat{\underline{x}})$. $\Rightarrow [\hat{T}\,,\,\hat{H}] = 0$ since $\hat{\underline{x}}$ is even under time-reversal. $\Rightarrow |n\rangle$ is an energy eigenstate with eigenvalue E_n, then $\hat{T}|n\rangle$ is an eigenstate with the same eigenvalue.

$$\hat{H}(\hat{T}|n\rangle) = \hat{T}(\hat{H}|n\rangle) = E_n(\hat{T}|n\rangle)$$

Does $\hat{T}|n\rangle$ represent the same state as $|n\rangle$?
Assume that it does represent the same state, $\hat{T}|n\rangle = e^{i\delta}|n\rangle$. Then

$$\hat{T}^2|n\rangle = \hat{T}(e^{i\delta}|n\rangle) = e^{-i\delta}e^{i\delta}|n\rangle = |n\rangle \Rightarrow \hat{T}^2 = +1$$

in contradiction to $\hat{T}^2 = -1$ for half-integer j. As a consequence, in a system with half-integer j, all energy levels are at least two-fold degenerate. This is called Kramers degeneracy.

Consider a free electron with spin.

$$\text{Dispersion: } \varepsilon(p) = \frac{\underline{p}^2}{2m} \text{ , state } |\underline{p}', m = \pm 1\rangle$$

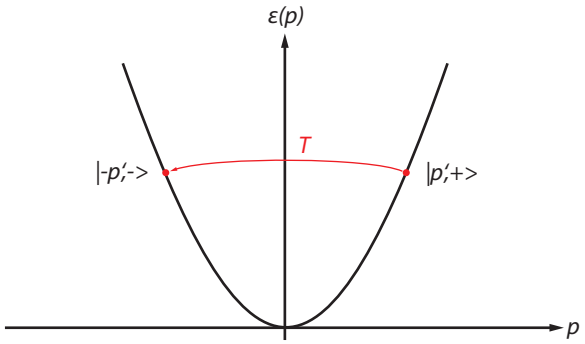

Figure 1.17: Parabolic dispersion of the free electron and action of time-reversal $\hat{T}$, the states $|\underline{p}', +\rangle$ and $|-\underline{p}', -\rangle$ are called Kramer pairs

Action of time-reversal yields $\hat{T}|\underline{p}', m\rangle \propto |-\underline{p}', -m\rangle$. In addition we have a parity symmetry $[\hat{H}\,, \hat{\Pi}] = 0$ and $\hat{\Pi}|\underline{p}', m\rangle = |-\underline{p}', m\rangle$. We consider $\hat{\Pi}\hat{T}|\underline{p}', m\rangle = |\underline{p}', -m\rangle$ therefore also $|\underline{p}', m\rangle$ and $|\underline{p}', -m\rangle$ are degenerate.
In the homework we will discuss

$$\hat{H} = \frac{\hat{p}^2}{2m} + \alpha\, \hat{p}\underline{\underline{\sigma}}^y + B_z \underline{\underline{\sigma}}^z \ .$$

There $\alpha\, \hat{p}\underline{\underline{\sigma}}^y$ is a "spin-orbit coupling" term.
(Motivation: 1D system needs confinement (potential) equivalent to a B_z field: Moving electron feels a effective B field that couples to the spin: $\underline{B} \propto \underline{E} \times \underline{v}$, $\underline{B} \cdot \underline{\sigma} = \alpha(\hat{e}_z \times \underline{p}) \cdot \underline{\sigma}$. "Left movers", "right movers", and no backscattering between both. This is relevant e.g. in spin quantum Hall edge states.)

2 Dirac Fermions

2.1 Graphene

Graphene is a two-dimensional variant of carbon, and can be experimentally prepared from Graphite by peeling of a single layer using scotch tape. This preparation was successfully performed in 2004 by K.S. Novoselov and A.K. Geim, who were awarded the 2010 Nobel prize in physics for proving that they had indeed studied single layers of Graphene.

Graphene is a two-dimensional hexagonal lattice of carbon atoms.

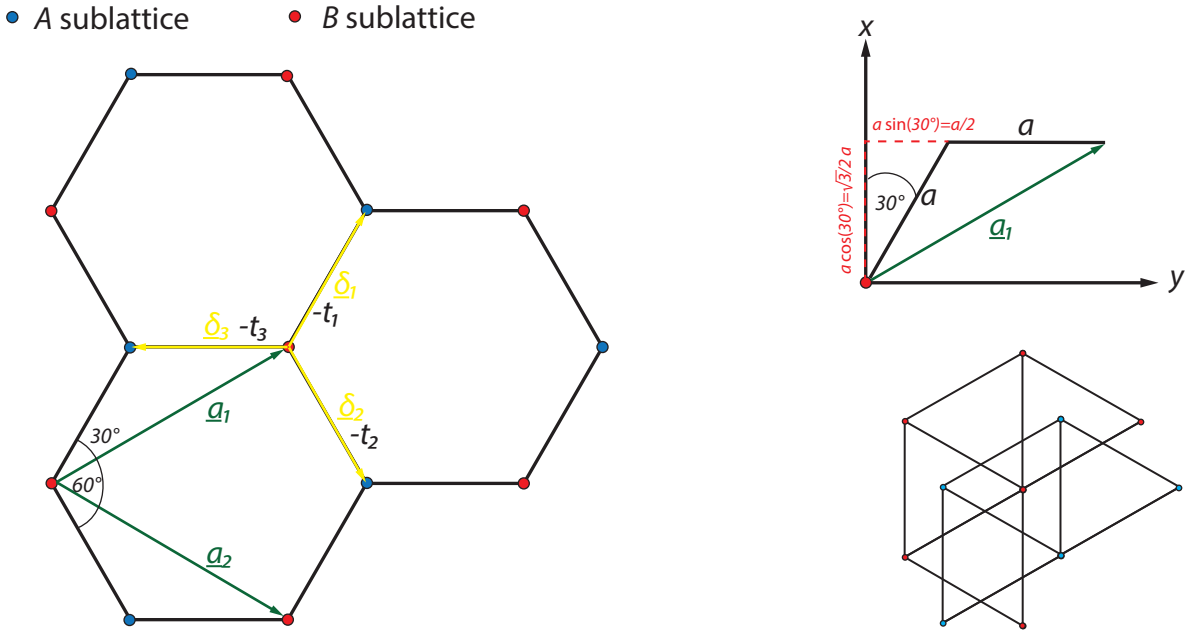

Figure 2.1: Graphene lattice, primitive and translation lattice vectors, diatomic unit cell

The Graphene lattice is composed of a triangular lattice (only A-sites for instance) with a diatomic unit cell. The underlying triangular lattice has the following translation vectors:

$$\underline{a}_1 = \frac{a}{2}\,(3, \sqrt{3}) \text{ and } \underline{a}_2 = \frac{a}{2}\,(3, -\sqrt{3})$$

where a is the bond length. In addition, there are reciprocal lattice vectors $\underline{b}_1$ and $\underline{b}_2$ defined by $\underline{a}_i \cdot \underline{b}_j = 2\pi\delta_{ij}$. One finds

$$\underline{b}_1 = \frac{2\pi}{3a}\,(1, \sqrt{3}) \text{ and } \underline{b}_2 = \frac{2\pi}{3a}\,(1, -\sqrt{3})\,.$$

A-sites can be moved into other A-sites via translation by an amount $\underline{a}_1$ or $\underline{a}_2$.
The Brillouin zone defines the allowed (distinguishable from each other) eigenvalues of the lattice translation operators

$$e^{i\underline{p}\cdot\underline{a}_1/\hbar} \text{ and } e^{i\underline{p}\cdot\underline{a}_2/\hbar}$$

given by $e^{i\underline{k}\cdot\underline{a}_1}$ and $e^{i\underline{k}\cdot\underline{a}_2}$, respectively.

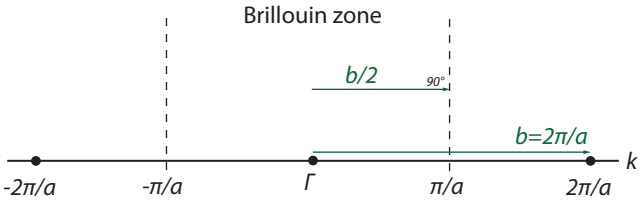

Figure 2.2: 1D reciprocal lattice and construction rule of the Brillouin zone

Remark:
The Brillouin zone is the Wigner-Seitz cell of the reciprocal lattice.

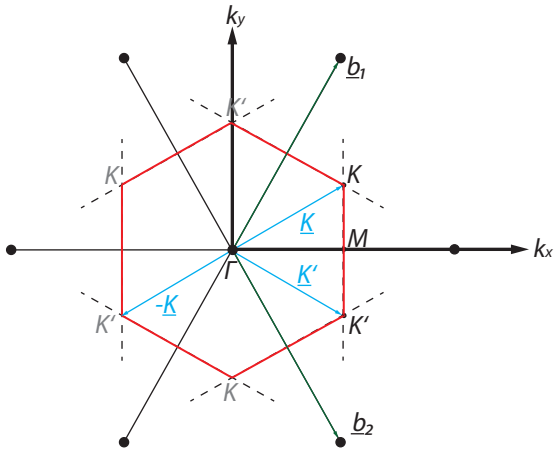

Figure 2.3: Hexagonal Brillouin zone with three-fold-rotation symmetry and special points

On finds for the K-point

$$\underline{K} = \frac{2\pi}{3a}\left(1\,,\,\frac{1}{\sqrt{3}}\right) \text{ and } \underline{K}' = \frac{2\pi}{3a}\left(1\,,\,-\frac{1}{\sqrt{3}}\right) .$$

These points are time-reversal partners of each other because $\underline{K} \xrightarrow{\hat{T}} -\underline{K}$ and $-\underline{K} = \underline{K}' - \underline{b}_1 - \underline{b}_2$.
Points are considered equivalent, if they can be connected by reciprocal lattice vectors, because $e^{i\underline{k}\cdot\underline{a}_1} = e^{i(\underline{k}+\underline{b}_1)\cdot\underline{a}_1} = e^{i\underline{k}\cdot\underline{a}_1}e^{2\pi i}$.
What is the dispersion relation $\varepsilon(\underline{k})$ of Graphene?
The simplest tight-binding model for Graphene contains hopping of electrons to nearest neighbor sites in the direction of the primitive vectors

$$\underline{\delta}_1 = \frac{a}{2}\,(1,\sqrt{3}) \;,\; \underline{\delta}_2 = \frac{a}{2}\,(1,-\sqrt{3}) \;, \text{ and } \underline{\delta}_3 = a\,(-1,0) \;.$$

We introduce Fourier transformed states such that (using the total number of lattice points N)

$$|\underline{k}, B\rangle = \frac{1}{\sqrt{N}} \sum_{n_1,n_2\in\mathbb{Z}} e^{\boldsymbol{i}(n_1\underline{a}_1+n_2\underline{a}_2)\cdot\underline{k}} \, |n_1\underline{a}_1 + n_2\underline{a}_2\rangle$$
$$|\underline{k}, A\rangle = \frac{1}{\sqrt{N}} \sum_{n_1,n_2\in\mathbb{Z}} e^{\boldsymbol{i}(n_1\underline{a}_1+n_2\underline{a}_2)\cdot\underline{k}} \, |n_1\underline{a}_1 + n_2\underline{a}_2 + \underline{\delta}_1\rangle \; .$$

Using this notation the to momentum-space transformed Hamiltonian is given by

$$\hat{H}(\underline{k}) = \sum_{\underline{k}} (|\underline{k}, A\rangle, |\underline{k}, B\rangle) \underbrace{\begin{pmatrix} 0 & h(\underline{k}) \\ h^*(\underline{k}) & 0 \end{pmatrix}}_{\underline{\underline{h}}(\underline{k})} \begin{pmatrix} \langle\underline{k}, A| \\ \langle\underline{k}, B| \end{pmatrix} \; .$$

The diagonal elements vanish because there is no hopping to nearest neighbors on the same sub-lattice. And the off-diagonal term is given by

$$h(\underline{k}) = \sum_{\underline{r}_j} e^{\boldsymbol{i}\underline{k}\cdot\underline{r}_j} H_{\underline{r}_0,\underline{r}_j} = -\sum_{i=1}^{3} t_i e^{\boldsymbol{i}\underline{k}\cdot\underline{\delta}_i} \; .$$

Where $H_{\underline{r}_0,\underline{r}_j} = \langle\underline{r}_j|\hat{H}|\underline{r}_0\rangle$ are matrix elements with respect to a basis of the Hilbert space. Unfortunately in this basis the Hamiltonian is not invariant under translation by a reciprocal lattice vector, i.e. $\underline{\underline{h}}(\underline{k}) \neq \underline{\underline{h}}(\underline{k} + \underline{G})$ with $\underline{G} = m_1\underline{b}_1 + m_2\underline{b}_2$ because $\underline{b}_i \cdot \underline{\delta}_j \neq 2\pi\delta_{ij}$.
Because of $\underline{a}_1 = \underline{\delta}_1 - \underline{\delta}_3$ and $\underline{a}_2 = \underline{\delta}_2 - \underline{\delta}_3$ a rescaling of $\sum t_i \, e^{\boldsymbol{i}\underline{k}\cdot\underline{\delta}_i}$ by $e^{-\boldsymbol{i}\underline{\delta}_3\cdot\underline{k}}$ restores the translation invariance. This can be achieved by transforming wave functions: $\langle k, B| \to \langle k, B|e^{\boldsymbol{i}\underline{k}\cdot\underline{\delta}_3}$.
$\Rightarrow$ We obtain

$$\underline{\underline{h}}(\underline{k}) = \begin{pmatrix} 0 & -t_1 e^{\boldsymbol{i}\underline{k}\cdot\underline{a}_1} - t_2 e^{\boldsymbol{i}\underline{k}\cdot\underline{a}_2} - t_3 \\ -t_1^* e^{-\boldsymbol{i}\underline{k}\cdot\underline{a}_1} - t_2^* e^{-\boldsymbol{i}\underline{k}\cdot\underline{a}_2} - t_3^* & 0 \end{pmatrix} \; .$$

We now consider the isotropic limit with $t_1 = t_2 = t_3 \equiv t \in \mathbb{R}$. In Graphene one can find $t \approx 2.8\text{eV}$. We expand around the points $\underline{K}$ and $\underline{K}' \hat{=} -\underline{K}$:

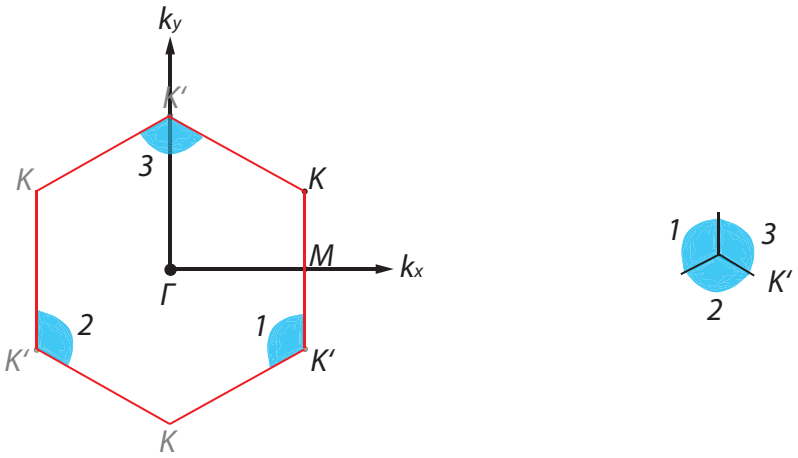

Figure 2.4: There is a full vicinity of $\underline{K}$ in the first Brillouin zone.

We parametrize $\underline{k} = \underline{K} + \underline{\kappa}$ or $\underline{k} = -\underline{K} + \underline{\kappa}$ and Taylor expand (around $\underline{K}$ or $\underline{K}'$ that is $\underline{\kappa} = 0$):

$$\Delta(\underline{\kappa}) = e^{\boldsymbol{i}(\underline{K}+\underline{\kappa})\cdot\underline{a}_1} + e^{\boldsymbol{i}(\underline{K}+\underline{\kappa})\cdot\underline{a}_2} + 1\,.$$

We only keep the terms to first order in $\underline{\kappa}$:

$$\Rightarrow \Delta(\underline{\kappa}) = e^{\boldsymbol{i}\underline{K}\cdot\underline{a}_1}(1 + \boldsymbol{i}\underline{\kappa}\cdot\underline{a}_1) + e^{\boldsymbol{i}\underline{K}\cdot\underline{a}_2}(1 + \boldsymbol{i}\underline{\kappa}\cdot\underline{a}_2) + 1 + o(\underline{\kappa}^2).$$

We use $\underline{K}\cdot\underline{a}_{1,2} = \frac{2\pi}{3a}\frac{3a}{2}\left(1, \frac{1}{\sqrt{3}}\right)\begin{pmatrix}1\\ \pm\frac{1}{\sqrt{3}}\end{pmatrix} = \pi(1 \pm 1/3) = \pi\begin{cases}4/3 & \text{for } \underline{a}_1\\ 2/3 & \text{for } \underline{a}_2\end{cases}$

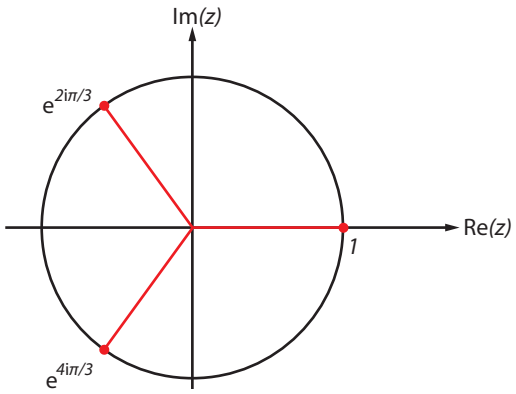

Figure 2.5: Sum of the constant terms $e^{4\boldsymbol{i}\pi/3} + e^{2\boldsymbol{i}\pi/3} + 1 = 0$ in $\Delta(\underline{\kappa})$

We have $e^{2\boldsymbol{i}\pi/3} = -\frac{1}{2} + \boldsymbol{i}\frac{\sqrt{3}}{2}$ and $e^{4\boldsymbol{i}\pi/3} = -\frac{1}{2} - \boldsymbol{i}\frac{\sqrt{3}}{2}$. Therefore the expansion is

$$\begin{aligned}
\Delta(\underline{\kappa}) &= e^{4\pi\boldsymbol{i}/3}\boldsymbol{i}\underline{\kappa}\cdot\underline{a}_1 + e^{2\pi\boldsymbol{i}/3}\boldsymbol{i}\underline{\kappa}\cdot\underline{a}_2\\
&= \left(-\frac{1}{2} - \boldsymbol{i}\frac{\sqrt{3}}{2}\right)\boldsymbol{i}\underline{\kappa}\cdot\underline{a}_1 + \left(-\frac{1}{2} + \boldsymbol{i}\frac{\sqrt{3}}{2}\right)\boldsymbol{i}\underline{\kappa}\cdot\underline{a}_2\\
&= -\frac{\boldsymbol{i}}{2}\underline{\kappa}\cdot(\underline{a}_1 + \underline{a}_2) + \frac{\sqrt{3}}{2}\underline{\kappa}\cdot(\underline{a}_1 - \underline{a}_2)\\
&= -\frac{\boldsymbol{i}}{2}\underline{\kappa}\cdot\frac{a}{2}(6,0) + \frac{\sqrt{3}}{2}\underline{\kappa}\cdot\frac{a}{2}(0,2\sqrt{3})\\
&= -\boldsymbol{i}\frac{3a}{2}\kappa_x + \frac{3a}{2}\kappa_y\\
&= -\boldsymbol{i}\,\frac{3a}{2}\,(\kappa_x + \boldsymbol{i}\kappa_y)
\end{aligned}$$

Therefore the Bloch-Hamiltonian expanded around $\underline{K}$ as a function of $\underline{\kappa}$ is given by

$$\underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) = \begin{pmatrix}0 & -t\Delta(\underline{\kappa})\\ -t\Delta^*(\underline{\kappa}) & 0\end{pmatrix} = \boldsymbol{i}\,\frac{3at}{2}\begin{pmatrix}0 & \kappa_x + \boldsymbol{i}\kappa_y\\ -\kappa_x + \boldsymbol{i}\kappa_y & 0\end{pmatrix}\,.$$

We now define $v_F \equiv \frac{3ta}{2\hbar} \approx 10^6\,\frac{\mathrm{m}}{\mathrm{s}}$ and absorb the phase factor $\boldsymbol{i}$ into the wave functions

$$\Rightarrow \underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) = \hbar v_F\begin{pmatrix}0 & \kappa_x + \boldsymbol{i}\kappa_y\\ \kappa_x - \boldsymbol{i}\kappa_y & 0\end{pmatrix} \equiv \hbar v_F\,\underline{\sigma}\cdot\underline{\kappa} \qquad (*)$$

where $\underline{\sigma} = (\underline{\underline{\sigma}}_x, \underline{\underline{\sigma}}_y)$ is the vector of Pauli matrices. We note that in the last step we have adopted an unusual definition of handedness ($\underline{\underline{\sigma}}_y \to -\underline{\underline{\sigma}}_y$) in order to conform with the usual definition of handedness on the Dirac-Hamiltonian at the $\underline{K}$-point in Graphene.
For the expansion around $\underline{K}' = -\underline{K}$:

$$\underline{K} \cdot \underline{a}_1 = \frac{4\pi}{3} \longrightarrow -\frac{4\pi}{3}$$
$$\underline{K} \cdot \underline{a}_2 = \frac{2\pi}{3} \longrightarrow -\frac{2\pi}{3}$$

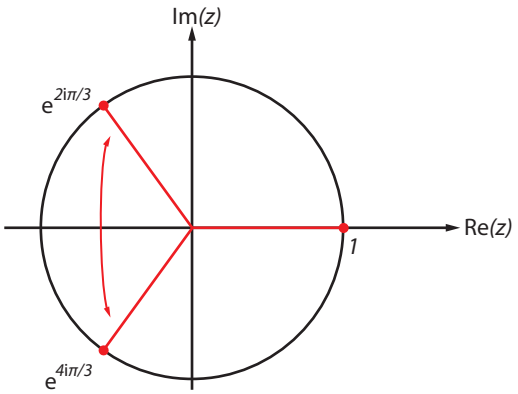

Figure 2.6: Again sum of the constant terms $e^{4i\pi/3} + e^{2i\pi/3} + 1 = 0$ in $\delta(\underline{\kappa})$ because the minus sign corresponds to a complex conjugation

Therefore, the expansion is

$$\Delta(\underline{\kappa}) \to \left(-\frac{1}{2} - \boldsymbol{i}\,\frac{\sqrt{3}}{2}\right) \boldsymbol{i}\underline{\kappa} \cdot \underline{a}_1 + \left(-\frac{1}{2} - \boldsymbol{i}\,\frac{\sqrt{3}}{2}\right) \boldsymbol{i}\underline{\kappa} \cdot \underline{a}_2 = \ldots = -\boldsymbol{i}\,\frac{3a}{2}\,(\kappa_x - \boldsymbol{i}\kappa_y)\,.$$

Hence, the Bloch Hamiltonian at the $\underline{K}'$ point is

$$\underline{\underline{h}}_{\underline{K}'}(\underline{\kappa}) = \underline{\underline{h}}^*_{\underline{K}} = \hbar v_F \underline{\sigma}^* \cdot \underline{\kappa} \text{ with } \underline{\sigma}^* = (\underline{\underline{\sigma}}_x, \underline{\underline{\sigma}}^*_y) = (\underline{\underline{\sigma}}_x, -\underline{\underline{\sigma}}_y)$$

since $\underline{\underline{\sigma}}_x$ is real and $\underline{\underline{\sigma}}_y$ is imaginary.
In order to find the eigenvalues $E_{\underline{\kappa}}$ of $\underline{\underline{h}}(\underline{\kappa})$, we use that $\underline{\underline{h}}^2(\underline{\kappa})$ has the same eigenfunctions as $\underline{\underline{h}}$ and eigenvalues $E^2_{\underline{\kappa}}$ (since $\underline{\underline{h}}\,|\underline{\kappa}\rangle = E_{\underline{\kappa}}|\underline{\kappa}\rangle \Rightarrow \underline{\underline{h}}\underline{\underline{h}}|\underline{\kappa}\rangle = E^2_{\underline{\kappa}}|\underline{\kappa}\rangle$).
Because $\underline{\underline{\sigma}}_x$ and $\underline{\underline{\sigma}}_y$ anti-commute $\underline{\underline{\sigma}}_x\underline{\underline{\sigma}}_y = -\underline{\underline{\sigma}}_y\underline{\underline{\sigma}}_x$, we find

$$\begin{aligned}
\underline{\underline{h}}^2(\underline{\kappa}) &= \hbar^2 v_F^2 [\kappa_x \underline{\underline{\sigma}}_x + \kappa_y \underline{\underline{\sigma}}_y]^2 \\
&= \hbar^2 v_F^2 \left[\kappa_x^2 \underline{\underline{\sigma}}_x^2 + \kappa_y^2 \underline{\underline{\sigma}}_y^2 + \kappa_x\kappa_y \underbrace{(\underline{\underline{\sigma}}_x\underline{\underline{\sigma}}_y + \underline{\underline{\sigma}}_y\underline{\underline{\sigma}}_x)}_{0}\right] \\
&= \hbar^2 v_F^2 [\kappa_x^2 + \kappa_y^2]\mathbb{1} = \hbar^2 v_F^2\, \underline{\kappa}^2 \mathbb{1}\,.
\end{aligned}$$

Hence, the energy eigenvalues are

$$\Rightarrow E_{\underline{\kappa}} = \pm\hbar v_F\,|\underline{\kappa}|\,.$$

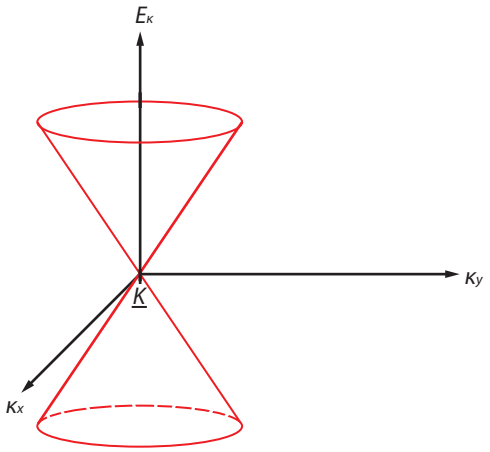

Figure 2.7: Dispersion at the $\underline{K}$-point

From a formal point of view, the Hamiltonian (*) is exactly that of an ultrarelativistic (or massless) particle of spin $\frac{1}{2}$, such as the neutrino (neglecting the rest mass which is very small and gives rise to neutrino oscillations).
However, the velocity of light c is here replaced by the Fermi-velocity v_F, smaller by a factor of about 300. The "left-handed neutrino described by (*) is not equivalent to the right-handed anti-neutrino living near $\underline{K}'$.
This opens up the possibility of observing many phenomena predicted (but not experimentally observed) in high energy physics in a solid state experiment. It is important to keep in mind that the Dirac excitations near $\underline{K}$ are *not* the anti-particles of those near $\underline{K}'$. Instead, the possible excitations near *one* Dirac point with energies $\pm\hbar v_F|\underline{\kappa}|$ are one another's anti-particles.
Eigenfunctions in the vicinity of the $\underline{K}$-point are given by (homework problem)

$$\psi^{\pm}_{\underline{K}}(\underline{\kappa}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta_{\underline{\kappa}}/2} \\ \pm e^{-i\theta_{\underline{\kappa}}/2} \end{pmatrix} \text{ with } \theta_{\underline{\kappa}} \equiv \arctan\left(\frac{\kappa_y}{\kappa_x}\right)$$

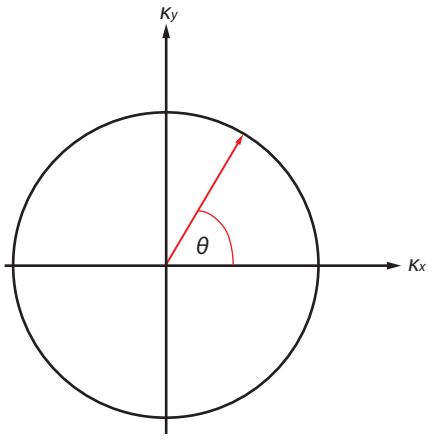

Figure 2.8: If the momentum rotates by 2π the $e^{i\theta_{\underline{\kappa}}/2}$ only gives a phase factor of -1, like known from electron spin

When $\underline{\kappa}$ rotates around the "Dirac-point" at $\underline{K}$, the phase of $\psi^{\pm}_{\underline{K}}$ changes by π, not by 2π, as characteristic for spin $\frac{1}{2}$ particles.
(We will find in a homework problem that in Graphene there exists a Landau level with $E_n = 0$.)

Remark
Assume electrons on A and B lattice sites had different energies. Then we can write

$$\underline{\underline{h}}(\underline{\kappa}) = \begin{pmatrix} \Delta\varepsilon/2 & -t\Delta(\underline{\kappa}) \\ -t\Delta^*(\underline{\kappa}) & -\Delta\varepsilon/2 \end{pmatrix} = \underline{\kappa} \cdot \underline{\sigma} + \frac{\Delta\varepsilon}{2}\,\underline{\underline{\sigma}}_z = \underline{d}(\underline{\kappa}) \cdot \underline{\sigma}\,.$$

Are there corrections to this result, for instance due to second-nearest neighbor (next-nearest neighbor) hopping with some matrix element t'? On the honeycomb lattice all next-nearest neighbor (nnn) are on the same sub-lattice as the original atom. This gives rise to diagonal terms in $\underline{\underline{h}}(\underline{k})$. Importantly such a term

$$\hat{H}_{\text{nnn}} = -\frac{t'}{2} \sum_{i,j=\text{nnn}} (|i,A\rangle\langle j,A| + |i,B\rangle\langle j,B| + \text{h.c.})$$

where $i, j \mathrel{\hat{=}} n_1\underline{a}_1 + n_2\underline{a}_2$ is exactly symmetric between A and B sub-lattices. Its Fourier transform $-t'f(\underline{k})$ appears as diagonal element in $\underline{\underline{h}}$, it is proportional to the unit matrix.

$$\underline{\underline{h}}'(\underline{k}) = \underline{\underline{h}}(\underline{k}) - t'f(\underline{k})\,\mathbb{1} \Longrightarrow \varepsilon'(\underline{k}) = \varepsilon(\underline{k}) - t'f(\underline{k})$$

$\Rightarrow$ only destroys the perfect symmetry of the solutions around $\varepsilon = 0$, but keeps the cones intact.
One finds

$$f(\underline{k}) = \frac{1}{2} \sum_{ij=\text{nnn}} \left(e^{i\underline{k}\cdot\underline{R}_{ij}} + \text{h.c.}\right) \equiv \sum_{i,j=\text{nnn}} \cos(\underline{k}\cdot\underline{R}_{ij}) = 2\cos(\sqrt{3}\,k_y a) + 4\cos\left(\frac{\sqrt{3}}{2}\,k_y\,a\right)\cos\left(\frac{3}{2}\,k_x\,a\right)$$

(homework problem). It turns out that the value of $-t'f(\underline{k})$ at the Dirac point is $+3t'$ and its gradients vanish. As a consequence up to an additional constant $3t'$, the form of the Hamiltonians $\underline{\underline{h}}_{\underline{K}}(\underline{\kappa})$, $\underline{\underline{h}}_{\underline{K}'}(\underline{\kappa})$ does not change.
Expanding up to $\mathcal{O}(\underline{\kappa}^2)$, the function $f(\underline{k} + \underline{\kappa})$ is isotropic around $\underline{K}$, but the original t-term introduces a "trigonal" dependence $\sim \sin(3\theta_{\underline{\kappa}})$. With $\theta_{\underline{\kappa}} = \arctan(\kappa_y/\kappa_x)$ as before. However, in the analysis of experiments, this term is usually neglected.
We now consider a shift of the energies of the sub-lattices.

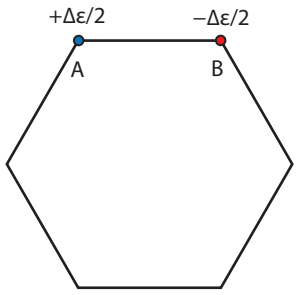

Figure 2.9: Shifts of the energies in the sub-lattices

Any kind of asymmetry in the Hamiltonian between the A and B sub-lattice will lift the degeneracies at the Dirac points, since the Hamiltonian can be written in the following form

$$\underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) = \begin{pmatrix} \Delta\varepsilon/2 & \hbar v_F(\kappa_x + \boldsymbol{i}\kappa_y) \\ \hbar v_F(\kappa_x - \boldsymbol{i}\kappa_y) & -\Delta\varepsilon/2 \end{pmatrix} = \underline{d}(\underline{\kappa}) \cdot \underline{\sigma} \text{ with } \underline{\sigma} = (\underline{\underline{\sigma}}_x, \underline{\underline{\sigma}}_y, \underline{\underline{\sigma}}_z)$$

with $d_x = \hbar v_F \kappa_x$, $d_y = \hbar v_F \kappa_y$, $d_z = \Delta\varepsilon/2$.
Here we have $\frac{1}{2}\{\underline{\underline{\sigma}}_i, \underline{\underline{\sigma}}_j\} = \delta_{ij}$ and thus $\underline{\underline{h}}^2_{\underline{K}}(\underline{\kappa}) = \hbar^2 v_F^2 \underline{\kappa}^2 + (\Delta\varepsilon/2)^2$. The eigenvalues are given by

$$E_\pm = \pm\sqrt{(\Delta\varepsilon/2)^2 + \hbar^2 v_F^2 \underline{\kappa}^2}\ .$$

We compare with the relativistic dispersion relation $E = \sqrt{m^2c^4 + p^2c^2}$ and identify $\underline{p} = \hbar\underline{\kappa}$ and $mc^2 = \Delta\varepsilon/2$. In the presence of a sub-lattice asymmetry, $\underline{\underline{h}}_{\underline{K}}(\underline{\kappa})$ describes massive relativistic particles.

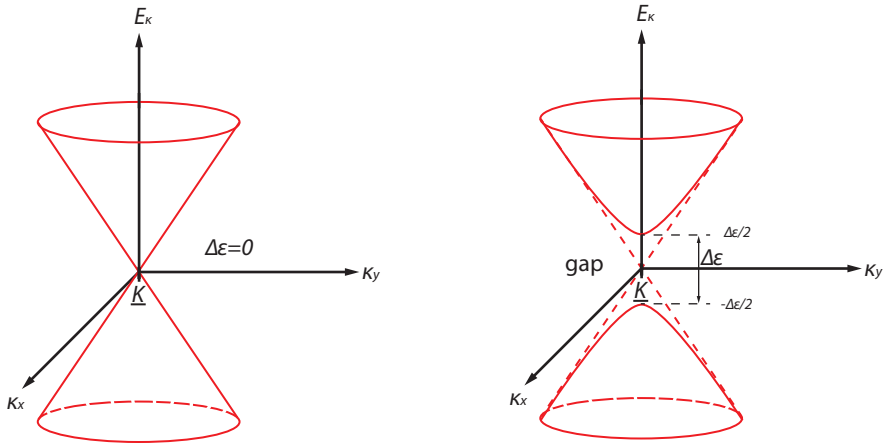

Figure 2.10: Dispersion relations in comparison

2.1.1 Symmetries of Graphene

In this section, we work with

$$\underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) = \hbar v_F \begin{pmatrix} 0 & \boldsymbol{i}\kappa_x - \kappa_y \\ -\boldsymbol{i}\kappa_x - \kappa_y & 0 \end{pmatrix} \text{ and } \underline{\underline{h}}_{\underline{K}'}(\underline{\kappa}) = \hbar v_F \begin{pmatrix} 0 & \boldsymbol{i}\kappa_x + \kappa_y \\ -\boldsymbol{i}\kappa_x + \kappa_y & 0 \end{pmatrix}\ .$$

Time-Reversal Transformation
Time-reversal changes (homework problem)

$$\underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) \xrightarrow{\hat{T}} (\underline{\underline{h}}_{-\underline{K}}(-\underline{\kappa}))^*$$

and we have $\underline{k} = \underline{K} + \underline{\kappa}$, $-\underline{k} = \underline{K}' - \underline{G}$. From this we have

$$\hat{T}\underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) = \underline{\underline{h}}^*_{\underline{K}'}(-\underline{\kappa}) = \hbar v_F \begin{pmatrix} 0 & -\boldsymbol{i}\kappa_x - \kappa_y \\ \boldsymbol{i}\kappa_x - \kappa_y & 0 \end{pmatrix}^* = \hbar v_F \begin{pmatrix} 0 & \boldsymbol{i}\kappa_x - \kappa_y \\ -\boldsymbol{i}\kappa_x - \kappa_y & 0 \end{pmatrix} = \underline{\underline{h}}_{\underline{K}}(\underline{\kappa})\ .$$

Our Hamiltonian has a time-reversal symmetry.

Parity Transformation

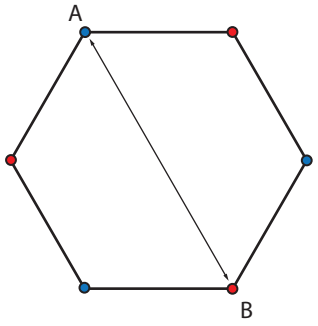

Figure 2.11: Action of a parity transformation on the Graphene lattice

A parity transformation changes $\underline{k}$ to $-\underline{k}$ and interchanges the A and B sub-lattice:

$$\begin{pmatrix} \langle \underline{k}, A| \\ \langle \underline{k}, B| \end{pmatrix} \overset{\text{sub-lat ch}}{\longrightarrow} \begin{pmatrix} \langle \underline{k}, B| \\ \langle \underline{k}, A| \end{pmatrix} = \underline{\underline{\sigma}}_x \begin{pmatrix} \langle \underline{k}, A| \\ \langle \underline{k}, B| \end{pmatrix} \ .$$

Therefore the transformation equation of the Hamiltonian is given by

$$\begin{aligned} \underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) \overset{\hat{\Pi}}{\longmapsto} \underline{\underline{\sigma}}_x \underline{\underline{h}}_{-\underline{K}}(-\underline{\kappa}) \underline{\underline{\sigma}}_x = \underline{\underline{\sigma}}_x \underline{\underline{h}}_{\underline{K}'}(-\underline{\kappa}) \underline{\underline{\sigma}}_x = \underline{\underline{\sigma}}_x \begin{pmatrix} 0 & -\boldsymbol{i}\kappa_x - \kappa_y \\ \boldsymbol{i}\kappa_x - \kappa_y & 0 \end{pmatrix} \underline{\underline{\sigma}}_x \\ = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -\boldsymbol{i}\kappa_x - \kappa_y \\ \boldsymbol{i}\kappa_x - \kappa_y & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -\boldsymbol{i}\kappa_x - \kappa_y & 0 \\ 0 & \boldsymbol{i}\kappa_x - \kappa_y \end{pmatrix} \\ = \begin{pmatrix} 0 & \boldsymbol{i}\kappa_x - \kappa_y \\ -\boldsymbol{i}\kappa_x - \kappa_y & 0 \end{pmatrix} = \underline{\underline{h}}_{\underline{K}}(\underline{\kappa}) \ . \end{aligned}$$

Our Hamiltonian is indeed invariant under parity transformation.

2.1.2 Local Stability of Dirac Points with Inversion and Time-Reversal

Time-reversal and parity separately do not impose any constraints on the Hamiltonian $\underline{\underline{h}}(\underline{k})$ because they both link a generic $\underline{k}$ to $-\underline{k}$, and thus do not impose any constraints for *generic* $\underline{k}$.
Remark:

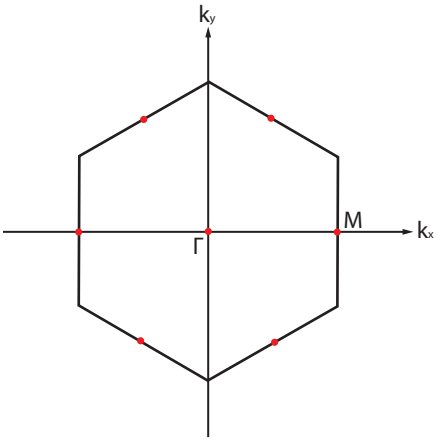

Figure 2.12: In the Brillouin zone there could be $\underline{k} = -\underline{k} + \underline{G}$ thus $\underline{k} \cong -\underline{k}$ would be non-generic. The $\underline{M}$-points are time-reversal invariant momenta and Γ is trivially time-reversal invariant. $\Rightarrow$ This are the 4 time-reversal invariant points on the Graphene reciprocal lattice

However the combination of time-reversal $\hat{T}$ and parity $\hat{\Pi}$ relates a momentum $\underline{k}$ to $\underline{k}$, and does impose a constraint on the Bloch-Hamiltonian for each $\underline{k}$ separately.

$$\hat{T}\colon \quad \underline{\underline{h}}(\underline{k}) \xrightarrow{\hat{T}} \hat{T}\underline{\underline{h}}(\underline{k})\hat{T}^{-1} = \underline{\underline{h}}^*(-\underline{k})$$
$$\hat{\Pi}\colon \quad \underline{\underline{h}}(\underline{k}) \xrightarrow{\hat{\Pi}} \hat{\Pi}\underline{\underline{h}}(\underline{k})\hat{\Pi}^{-1} = \underline{\underline{\sigma}}_x\underline{\underline{h}}(-\underline{k})\underline{\underline{\sigma}}_x$$

From the combined action of $\hat{T}$ and $\hat{\Pi}$ we find

$$\boxed{\underline{\underline{h}}(\underline{k}) = \underline{\underline{\sigma}}_x\underline{\underline{h}}^*(\underline{k})\underline{\underline{\sigma}}_x} \quad .$$

For a generic 2×2 Bloch-Hamiltonian of the form

$$\underline{\underline{h}}(\underline{k}) = \sum_{i=1}^{3} d_i(\underline{k})\underline{\underline{\sigma}}_i + \varepsilon(\underline{k})\mathbb{1}$$

with real $d_i(\underline{k})$ the above condition implies (dropping the explicit $\underline{k}$ dependence)

$$\sum_i d_i\underline{\underline{\sigma}}_i + \varepsilon \overset{!}{=} \underline{\underline{\sigma}}_x\left(\sum_i d_i\underline{\underline{\sigma}}_i + \varepsilon\right)^*\underline{\underline{\sigma}}_x = \underline{\underline{\sigma}}_x\left(d_x\underline{\underline{\sigma}}_x - d_y\underline{\underline{\sigma}}_y + d_z\underline{\underline{\sigma}}_z + \varepsilon\right)\underline{\underline{\sigma}}_x = d_x\underline{\underline{\sigma}}_x + d_y\underline{\underline{\sigma}}_y - d_z\underline{\underline{\sigma}}_z + \varepsilon \; .$$

This implies

$$d_z(\underline{k}) = -d_z(\underline{k}) \equiv 0 \; .$$

As a consequence, no $\underline{\underline{\sigma}}_z$ term can arise and open a gap directly. However, (small) additional $\underline{\underline{\sigma}}_x$ and $\underline{\underline{\sigma}}_y$ terms are allowed, giving rise to the generalized Hamiltonian

$$\underline{\underline{h}}'_{\underline{K}}(\underline{k}) = \kappa_x\underline{\underline{\sigma}}_x + \kappa_y\underline{\underline{\sigma}}_y + a_1\underline{\underline{\sigma}}_x + a_2\underline{\underline{\sigma}}_y = (\kappa_x + a_1)\underline{\underline{\sigma}}_x + (\kappa_y + a_2)\underline{\underline{\sigma}}_y$$

which only shifts the center of the Dirac cone to $\underline{K} - a_1\underline{\hat{e}}_x - a_2\underline{\hat{e}}_y$ in the Brillouin zone as long as a_1 and a_2 are small. For large perturbations obeying $\hat{T}$ and $\hat{\Pi}$ it is possible that the Dirac points merge and disappear.

2.1.3 Global Stability of Dirac Points

In this section we will only state the results. The calculations can be found in the book of B. Andrei Bernevig ("Topological Insulators and Topological Superconductors", Princeton University Press).
If additionally the threefold rotational symmetry of the honeycomb lattice is preserved, one can show that the location of the Dirac points at $\underline{K}$ and $\underline{K}'$ is fixed.

2.2 Relativistic Dirac Fermions

In this chapter (following the Book by Sakurai) we use so called natural units with $\hbar = c = 1$. Time is measured in length units. Velocity becomes a dimensionless number typically denoted by β. In addition, both momentum and mass are measured in units of energy, e.g. eV or MeV. Due to $\hbar = 1$, units of length and energy are tied together. For instance, the canonical commutation relation $[\hat{\underline{x}}\,, \hat{\underline{p}}] = \boldsymbol{i}$ tells us that the product of length and momentum is dimensionless and length is measured in units of inverse energy.

2.2.1 Klein-Gordon Equation

The Schrödinger equation can be obtained by using the non-relativistic dispersion relation $E = \frac{\underline{p}^2}{2m} + V(\underline{x})$ and making the replacements $E \mapsto \boldsymbol{i}\partial_t$ and $\underline{p} \mapsto -\boldsymbol{i}\nabla_{\underline{x}}$ from looking at plane waves $e^{\boldsymbol{i}\underline{k}\cdot\underline{x} - \boldsymbol{i}\omega t}$.
The relativistic dispersion relation is $E = \sqrt{p^2 + m^2}$. Making the same substitution
$\boldsymbol{i}\partial_t\psi = \sqrt{-\nabla^2 + m^2}\;\psi$ yields a differential equation with infinitely high derivatives which is not useful for our purposes. Considering the squared relation $E^2 = p^2 + m^2 \to -\partial_t^2\phi = (-\nabla^2 + m^2)\phi$ this can be written as the **Klein-Gordon equation**

$$(\partial_t^2 - \nabla^2 + m^2)\phi = 0$$

We use the 4-vector notation $t \mathrel{\hat{=}} x^0$, $\underline{x} \mathrel{\hat{=}} \underline{x}^i$

$$x^\mu \mathrel{\hat{=}} (x^0, \underline{x})\ .$$

The relativistic metric is given by

$$\eta^{ij} = \begin{pmatrix} 1 & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\ .$$

Remark:
In 3d we know:

- Scalars/scalar products are invariant under rotations

$$\underline{a} \cdot \underline{b} = a_1b_1 + a_2b_2 + a_3b_3 = (a_1, a_2, a_3) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

  $\to \mathbb{1}_3$ can be called a metric for the Euclidean $\mathbb{R}^3$. (This can change in other coordinate systems.)

- Formal definition: Rotation leaves metric invariant

For our 4-vector holds:

- Metric is η
- Lorentz transformation $\hat{L}$ keeps the metric invariant $\hat{L}^{-1}\eta\hat{L} = \eta$

Using the metric we differentiate between upper and lower indices: $\partial^\mu = \eta^{\mu\nu}\partial_\nu$ where the sum is implicit. Upper indices denote coordinates x^ν, and $\partial_\nu = \dfrac{\partial}{\partial x^\nu}$.
We have that $\partial^\mu\partial_\mu$ is invariant under Lorentz transformation since it is a scalar product, η is invariant, and

$$\partial^\mu\partial_\mu = \eta^{\mu\nu}\partial_\mu\partial_\nu = \partial_0^2 - \nabla^2 = \partial_t^2 - \nabla^2 \,.$$

The Klein-Gordon equation can be expressed as

$$(\partial^\mu\partial_\mu + m^2)\phi = 0$$

which is manifestly relativistically invariant.
In non-relativistic quantum mechanics, a state is completely described by the wave function $\psi(\underline{x}, t)$. As the Klein-Gordon equation is 2nd order in time, this does not work anymore, because as initial condition we need to know both $\phi(\underline{x}, t)$ and $\partial_t\phi(\underline{x}, t)$, in contradiction to the postulate that $\phi(\underline{x}, t)$ completely describes the state.
Introducing $\partial_t\phi = \chi$, one has $\partial_t\chi = -(-\nabla^2+m^2)\phi$, and can write a off-diagonal matrix equation

$$\partial_t \begin{pmatrix} \phi \\ \chi \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \nabla^2 - m^2 & 0 \end{pmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} \quad .$$

2.2.2 Dirac Equation

We consider a multi-component wave function $\underline{\Psi}(\underline{x}, t)$ which satisfies

$$\left(\boldsymbol{i}\underline{\underline{\gamma}}^\mu\partial_\mu - m\right)\underline{\Psi}(\underline{x}, t) = 0 \qquad (*)$$

with yet undetermined matrices $\underline{\underline{\gamma}}^\mu$, $\mu \in \{0, 1, 2, 3\}$. (This is similar to the Graphene case using $\kappa_i = -\boldsymbol{i}\partial_i$.) Demanding that

$$\frac{1}{2}\left(\underline{\underline{\gamma}}^\mu\underline{\underline{\gamma}}^\nu + \underline{\underline{\gamma}}^\nu\underline{\underline{\gamma}}^\mu\right) \equiv \frac{1}{2}\{\underline{\underline{\gamma}}^\mu, \underline{\underline{\gamma}}^\nu\} = \eta^{\mu\nu}$$

we find as before

$$(-\boldsymbol{i}\underline{\underline{\gamma}}^\mu\partial_\mu - m)(\boldsymbol{i}\underline{\underline{\gamma}}^\mu\partial_\mu - m)\underline{\Psi}(\underline{x}, t) = (\partial^\mu\partial_\mu + m^2)\underline{\Psi}(\underline{x}, t) = 0\,.$$

$\Rightarrow$ $\underline{\Psi}(\underline{x}, t)$ satisfies the Klein-Gordon equation, in addition to satisfying the Dirac equation.
$\Rightarrow$ $E^2 = p^2 + m^2$ is obeyed. The four quantities $\underline{\underline{\gamma}}^\mu$, $\mu \in \{0, 1, 2, 3\}$ are elements of a Clifford algebra defined by

i) $(\underline{\underline{\gamma}}^0)^2 = \mathbb{1}$

ii) $(\underline{\underline{\gamma}}^i)^2 = -\mathbb{1}$, $i \in \{1, 2, 3\}$

iii) $\underline{\underline{\gamma}}^\mu \underline{\underline{\gamma}}^\nu = -\underline{\underline{\gamma}}^\nu \underline{\underline{\gamma}}^\mu$ if $\mu \neq \nu$.

Due to the anti-commutation property, the matrices $\underline{\underline{\gamma}}^\mu$ are traceless (homework problem). We now substitute a relativistic plane wave into the Dirac equation

$$\underline{\Psi}(\underline{x}, t) = \underline{\Psi}_p \, e^{-\boldsymbol{i}\, p^\mu x_\mu} = \underline{\Psi}_p e^{\boldsymbol{i}(\underline{p}\cdot\underline{x} - Et)} \text{ with } p^\mu = (E, \underline{p})$$
$$(\underline{\underline{\gamma}}^\mu p_\mu - m)\underline{\Psi}_p = 0 = (\underline{\underline{\gamma}}^0 E - \underline{\underline{\gamma}}^i p_i - m)\underline{\Psi}_p \, .$$

Multiplying by $\underline{\underline{\gamma}}^0$ we find

$$E\underline{\Psi}_p = \left(\underline{\underline{\gamma}}^0 \underline{\underline{\gamma}} \cdot \underline{p} + \underline{\underline{\gamma}}^0 m\right) \underline{\Psi}_p \, ,$$

and identify the Dirac-Hamiltonian

$$\hat{H} = \underline{\alpha} \cdot \underline{p} + \beta m$$

with $\alpha_i \equiv \underline{\underline{\gamma}}^0 \underline{\underline{\gamma}}^i$ and $\beta = \underline{\underline{\gamma}}^0$. We have again, using $E \to \boldsymbol{i}\partial_t$, a eigenproblem $\boldsymbol{i}\partial_t \underline{\Psi}_p = \hat{H}\underline{\Psi}_p$. In the presence of a electrostatic potential, we find

$$\hat{H} = \underline{\alpha} \cdot \underline{p} + \beta m + e\phi(\underline{x}, t) \, .$$

A vector potential is included by making the usual substitution

$$\underline{p} \mapsto \underline{p} - e\underline{A} \, .$$

Remark:
$\frac{1}{2}\{\underline{\underline{\gamma}}^\mu, \underline{\underline{\gamma}}^\nu\} = \eta^{\mu\nu}$ cannot be realized using 2×2 matrices. We will use 4×4 matrices

$$\underline{\alpha}^i = \begin{pmatrix} 0 & \underline{\sigma}^i \\ \underline{\sigma}^i & 0 \end{pmatrix} \text{ and } \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \, .$$

2.2.2.1 Conserved Current

We argue that $\varrho = \underline{\Psi}^\dagger \underline{\Psi}$ can be interpreted as a probability density. There we have

$$\underline{\Psi} = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{pmatrix} \text{ and } \underline{\Psi}^\dagger = (\Psi_1^*, \Psi_2^*, \Psi_3^*, \Psi_4^*) \, .$$

One can show (homework problem): If $\underline{\Psi}$ solves the Dirac equation, the continuity equation holds

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot \underline{j} = 0 \text{ with } \underline{j} = \underline{\Psi}^\dagger \underline{\alpha} \underline{\Psi} \, .$$

That implies that ϱ changes only by flow into or out of a given region, and is conserved for this reason

$$0 = \partial_t \int \mathrm{d}^3 x \; \varrho(\underline{x}, t) \, .$$

Remark:
In the non-relativistic case we had $\underline{j} = \boldsymbol{i}/m \, \mathrm{Re}[\psi^*(-\boldsymbol{i}\nabla)\psi]$. In the relativistic case we need only

a matrix and no derivative because the Hamiltonian is only of first order in momentum and the current is one order lower. Some of the components of the vector $\underline{\Psi}$ have already the meaning of derivatives.

Instead of $\underline{\Psi}^\dagger$, the standard Hermitian adjoint of a column vector, one often uses $\overline{\underline{\Psi}} \equiv \underline{\Psi}^\dagger\beta = \underline{\Psi}^\dagger\underline{\underline{\gamma}}^0$ when forming the probability density and current. For simpler notation we will leave out the underlines $\overline{\underline{\Psi}} \equiv \overline{\Psi}$, $\underline{\underline{\gamma}}^\mu \equiv \gamma^\mu, ...$
Then

$$\varrho = \Psi^\dagger\Psi = \Psi^\dagger\gamma^0\gamma^0\Psi = \overline{\Psi}\gamma^0\Psi \text{ and } \underline{j} = \Psi^\dagger\gamma^0\gamma^0\underline{\alpha}\Psi = \overline{\Psi}\gamma^0\underline{\gamma}\Psi = \overline{\Psi}\gamma^i\Psi$$

such that

$$\frac{\partial}{\partial t}(\overline{\Psi}\gamma^0\Psi) + \nabla \cdot (\overline{\Psi}\underline{\gamma}\Psi) = \partial_\mu j^\mu = 0$$

with $j^\mu = \overline{\Psi}\gamma^\mu\Psi$ in a covariant notation.
The Dirac equation in momentum space is

$$0 = (\gamma^\mu p_\mu - m)\Psi \ .$$

We take the adjoint and insert a factor of γ^0

$$0 = \overline{\Psi}(\gamma^\mu p_\mu - m) \, ,$$

and find the following interpretation of the free particle current using associativity

$$j^\mu = \frac{1}{2}\left[(\overline{\Psi}\gamma^\mu)\Psi + \overline{\Psi}(\gamma^\mu\Psi)\right] \ .$$

Using the Dirac equation, we obtain

$$j^\mu = \frac{1}{2m}\left[(\overline{\Psi}\gamma^\mu)\gamma^\nu p_\nu\Psi + \overline{\Psi}\gamma^\nu p_\nu(\gamma^\mu\Psi)\right] \ .$$

Using $p^\mu = \eta^{\mu\nu}p_\nu$, we find

$$\Rightarrow j^\mu = \frac{1}{2m}\,\overline{\Psi}\,\underbrace{[\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu]}_{2\eta^{\mu\nu}}\,\Psi p_\nu = \frac{p^\mu}{m}\,\overline{\Psi}\Psi \ .$$

That is

$$j^0 = \frac{E}{m}\,\overline{\Psi}\Psi \quad , \quad \underline{j} = \frac{\underline{\underline{p}}}{m}\,\overline{\Psi}\Psi \ .$$

Taking into account relativistic mass enhancement by a Lorentz contraction factor $\gamma(v) = \frac{1}{\sqrt{1-(v/c)^2}}$

$$m(v) = \frac{m}{\sqrt{1-(v/c)^2}} = \gamma(v)m \ , \ \underline{p} = m(v)\,\underline{v} = \gamma(v)\,m\underline{v} \text{ and } \frac{E}{m} = \frac{E}{\gamma(v)m}\gamma(v) = \gamma(v)$$

$$\text{where } m(v)c^2 = E = \sqrt{m^2+p^2} \text{ and } \underline{p}/m = \underline{p}/(\gamma(v)m)\gamma(v) = \underline{v}\gamma(v)$$

and we have

$$j^0 = \gamma(v)\overline{\Psi}\Psi \qquad\qquad \underline{j} = \underline{v}\gamma(v)\overline{\Psi}\Psi$$

$\gamma(v)$ can be interpreted as describing the Lorentz contraction of the volume element.

Decomposing the four spinor components $\begin{pmatrix}\Psi_1\\ \Psi_2\\ \Psi_3\\ \Psi_4\end{pmatrix}$ into $\begin{pmatrix}\Psi_{\text{up}}\\ \Psi_{\text{down}}\end{pmatrix}$ with $\Psi_{\text{up}} = \begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}$ and $\Psi_{\text{down}} = \begin{pmatrix}\Psi_3\\ \Psi_4\end{pmatrix}$,

we obtain the final result

$$j^0 = \frac{E}{m}\,\overline{\Psi}\Psi = \gamma(v)\ \ [\Psi^\dagger_{\text{up}}\Psi_{\text{up}} - \Psi^\dagger_{\text{down}}\Psi_{\text{down}}]$$
$$\underline{j} = \frac{\underline{p}}{m}\,\overline{\Psi}\Psi = \gamma(v)\underline{v}[\Psi^\dagger_{\text{up}}\Psi_{\text{up}} - \Psi^\dagger_{\text{down}}\Psi_{\text{down}}]\ .$$

2.2.2.2 Free Particle Solutions

We first consider a free particle at rest with $\underline{p} = 0$. The Dirac equation simplifies to $\boldsymbol{i}\partial_t\Psi = \beta m\Psi = \gamma^0 m\Psi$ where γ^0 is diagonal such that the components of Ψ are uncoupled. There are four independent solutions

$$\Psi_1 = e^{-\boldsymbol{i}mt}\begin{pmatrix}1\\0\\0\\0\end{pmatrix}\ ,\quad \Psi_2 = e^{-\boldsymbol{i}mt}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}\ ,\quad \Psi_3 = e^{\boldsymbol{i}mt}\begin{pmatrix}0\\0\\1\\0\end{pmatrix}\ ,\quad \Psi_4 = e^{\boldsymbol{i}mt}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}\ .$$

The $e^{\boldsymbol{i}mp}$ is quite unusual because we had $e^{-\boldsymbol{i}Et/\hbar}$ with $E(p=0) = \sqrt{m^2+p^2}\big|_{m=0} = m$ factors. It seems that the solutions Ψ_3 and Ψ_4, spanning the space of Ψ_{down}, have a negative energy $-m$.
Next we look at free particle solutions with finite momentum $\underline{p} = p\hat{e}_z$. The eigenvalue problem $\hat{H}\Psi = E\Psi$ is no longer diagonal.

$$\begin{pmatrix}m & 0 & p & 0\\ 0 & m & 0 & -p\\ p & 0 & -m & 0\\ 0 & -p & 0 & -m\end{pmatrix}\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix} = E\begin{pmatrix}u_1\\u_2\\u_3\\u_4\end{pmatrix}$$

Both the equations for u_1, u_3 and u_2, u_4 couple together, but the two pairs of components are independent of each other. For the two pairs of components u_1, u_3 and u_2, u_4 we find eigenvalues $E = \pm\sqrt{m^2+p^2} = \pm E_p$.
We now construct the free particle spinors. For $E = +E_p$ we can start with $u_1 = 1$ (and $u_2 = u_4 = 0$), and obtain $u_3 = \frac{p}{E_p+m}$ or $u_2 = 1$ (and $u_1 = u_3 = 0$) with $u_4 = \frac{-p}{E_p+m}$.
In both cases, the upper component dominate in the non-relativistic limit.
Similarly, for negative energy solution $E = -p$, the nonzero components are either $u_3 = 1$ and $u_1 = \frac{-p}{E_p+m}$ or $u_4 = 1$ and $u_2 = \frac{p}{E_p+m}$.
For negative energy solutions, the lower component dominates in the non-relativistic limit.

We now consider the following operator $\underline{\Sigma}\cdot\hat{\underline{p}} = \Sigma_z$ (in our case $\underline{p} = p\hat{e}_z$, $\hat{p} = \hat{e}_z$) where $\underline{\Sigma}$ is a vector of 4×4 matrices

$$\underline{\Sigma} \equiv \begin{pmatrix}\underline{\sigma} & 0\\ 0 & \underline{\sigma}\end{pmatrix} \text{ with } \Sigma^z = \begin{pmatrix}\underline{\underline{\sigma}}^z & 0\\ 0 & \underline{\underline{\sigma}}^z\end{pmatrix}\ .$$

We expect this operator to project onto the spin in the direction of momentum (in the relativistic case we are not free to choose the quantization direction of spin but the spin is fully coupled

to p ; maximal spin-orbit coupling ; orbital angular momentum is not a good quantum number anymore). Spin is quantized in the direction of momentum, the states with positive and negative eigenvalues are called to have positive and negative *helicity*, respectively. Indeed, is is easy to see, by realizing the block-diagonal form, that the spin operator $\underline{s} = \frac{\hbar}{2}\underline{\Sigma}$ projects out positive (negative) helicity for the positive-energy solution with $u_1 \neq 0 \quad (u_2 \neq 0)$. In combination, we find

$$u_R^{(+)}(p) = \begin{pmatrix} 1 \\ 0 \\ \frac{p}{E_p+m} \\ 0 \end{pmatrix} \text{ and } u_L^{(+)}(p) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \frac{-p}{E_p+m} \end{pmatrix} \text{ for } E = E_p$$

with the subscript $R\,(L)$ denoting right (left) handedness (and upper $\pm$ denotes positive/negative energy solutions), i.e. positive or negative helicity . The negative energy solutions are given by

$$u_R^{(-)}(p) = \begin{pmatrix} \frac{-p}{E_p+m} \\ 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } u_L^{(-)}(p) = \begin{pmatrix} 0 \\ \frac{p}{E_p+m} \\ 0 \\ 1 \end{pmatrix} \text{ for } E = -E_p$$

Normalization is achieved dividing by $\frac{2E_p}{E_p+m}$, and the free particle wave functions are obtained multiplying by $e^{-p_\mu x^\mu}$.

2.2.2.3 Interpretation of Negative Energy Solutions

The problem is that there are infinitely many negative energy solutions, and the Hamiltonian is not bounded from below. The system could emit photons and lower its energy ad infinitum.
To make progress, we think about Graphene with a Fermi energy $E_F = 0$.

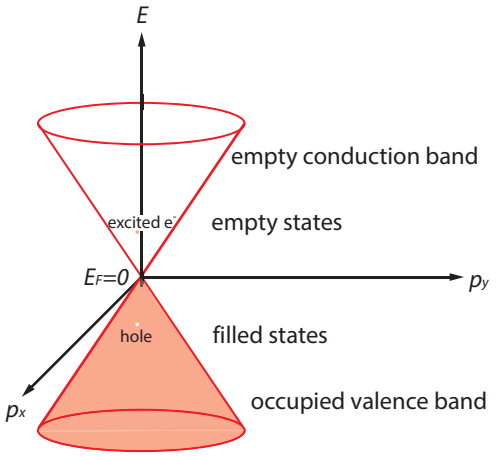

Figure 2.13: Graphene dispersion near the K point for Fermi energy $E_F = 0$, there is a lowest end of the band, at zero temperature the positive energy states are all empty (conduction band) and the negative energy states are all occupied (valence band), excitation of an electron into the conduction band leaves a hole in the valence band with opposite charge, mass and momentum

Removing an electron with momentum p from the occupied valence band creates a hole with

momentum $-p$ and charge $-e$. If the electron has energy $E = -E_p$, its excitations to the Fermi level costs energy $+E_p$, i.e. the hole created in the process has a positive energy $+E_p$. Dirac made use of the Pauli exclusion principle to argue that each of the infinitely many negative energy states is occupied by an electron, and that removal of the electron creates a positron ("hole", anti-particle of the electron) with positive energy. A high energy photon can promote an electron out of the "Dirac sea" (filled valence band) into the region of positive energies (conduction band).

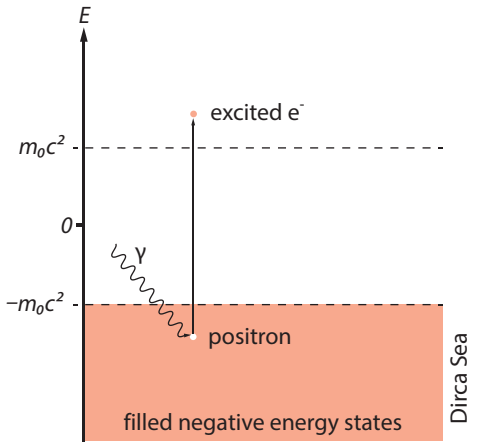

Figure 2.14: Dirac sea and excitation of an electron by a high energy photon γ

The positron was experimentally discovered by Carl Anderson in 1933. After this discovery, the Dirac equation was accepted as the correct relativistic wave equation.

2.2.2.4 Electromagnetic Interaction

A vector potential is introduced into the Dirac-Hamiltonian via the standard substitution

$$\hat{\underline{p}} = \hat{\underline{p}} - e\underline{A}$$

such that the Dirac equation becomes

$$\begin{pmatrix} m & \underline{\sigma} \cdot \hat{\underline{p}} \\ \underline{\sigma} \cdot \hat{\underline{p}} & -m \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

with $\Psi = (u, v) = (\Psi_1, \Psi_2, \Psi_3, \Psi_4)$. The two component spinor u represents the "upper" or "particle" component, whereas v represents the "lower" or "hole" component. At non-relativistic energies $E = K + m$, the kinetic energy $K \ll m$ (the rest energy), and the lower equation becomes $\underline{\sigma} \cdot \hat{\underline{p}} u = (E + m)v \approx 2mv$, which allows us to write the upper equation as

$$\frac{(\underline{\sigma} \cdot \hat{\underline{p}})(\underline{\sigma} \cdot \hat{\underline{p}})}{2m} u = Ku$$

We find $(\underline{a}\cdot\underline{\sigma})(\underline{b}\cdot\underline{\sigma}) = a_i\sigma_i b_j\sigma_j = \sum_{ij}[(1-\delta_{ij})a_ib_j\boldsymbol{i}\varepsilon_{ijk}\sigma_k + \delta_{ij}\mathbb{1}a_ib_i] = \underline{a}\cdot\underline{b} + \boldsymbol{i}\underline{\sigma}\cdot(\underline{a}\times\underline{b})$ and

$$\begin{aligned}\frac{1}{2m}(\underline{\sigma}\cdot\hat{\underline{p}})(\underline{\sigma}\cdot\hat{\underline{p}}) &= \frac{\hat{\underline{p}}^2}{2m} + \frac{\boldsymbol{i}\underline{\sigma}}{2m}(\hat{\underline{p}}\times\hat{\underline{p}})\\ (\hat{\underline{p}}\times\hat{\underline{p}})u &= (\boldsymbol{i}\nabla + e\underline{A})\times(\boldsymbol{i}\nabla u + e\underline{A}u)\\ &= \boldsymbol{i}e[\nabla\times(\underline{A}u) + (\underline{A}\times\nabla u)]\\ &= \boldsymbol{i}e(\nabla\times\underline{A})u = \boldsymbol{i}e\underline{B}u\end{aligned}$$

where $\underline{B} = \nabla\times\underline{A}$ is the magnetic field. Hence, we find the equation

$$\left[\frac{\hat{\underline{p}}^2}{2m} - \underline{\mu}\cdot\underline{B}\right]u = Ku \text{ with } \underline{\mu} = \frac{ge}{2m}\underline{S} \text{ and } \underline{S} = \frac{\hbar}{2}\underline{\sigma} \text{ and } g = 2\,.$$

This is the derivation for the electron spin and the way how it couples to a magnetic field.

2.2.2.5 Symmetries in the Dirac Equation

Consider a situation with external potential

$$\boldsymbol{i}\partial_t\Psi(\underline{x},t) = \hat{H}\Psi(\underline{x},t) \text{ with } \hat{H} = \underline{\alpha}\cdot\underline{p} + \beta m + V(\underline{x})$$

for some potential energy function $V(\underline{x})$. Due to the external potential, the Dirac equation cannot be brought into a covariant form.

Angular Momentum

In non-relativistic quantum mechanics, rotational invariance in 3 dimensions is centered on the observation that $[\hat{H}\,,\hat{\underline{L}}] = 0$ with $\hat{\underline{L}} = \hat{\underline{x}}\times\hat{\underline{p}}$ for a "central potential". This observation is based on the fact that $\hat{\underline{L}}$ commutes with $\hat{\underline{p}}^2$, and hence with the kinetic energy. In addition $\hat{\underline{L}}$ commutes with $\hat{\underline{x}}^2$, and hence with every potential $V(|\hat{\underline{x}}|)$. We now compare the commutator of $\hat{\underline{L}}$ with the free Dirac Hamiltonian $\hat{H} = \underline{\alpha}\cdot\hat{\underline{p}} + \beta m$. Since obviously $[\beta\,,\hat{\underline{L}}] = 0$, we focus on the commutator, using $[\hat{p}_k\,,\hat{p}_j] = 0$ and $[\hat{p}_l\,,\hat{x}_j] = -\boldsymbol{i}\delta_{lj}$,

$$[\underline{\alpha}\cdot\hat{\underline{p}}\,,\hat{L}_i] = [\alpha_l\hat{p}_l\,,\varepsilon_{ijk}\hat{x}_j\hat{p}_k] = \varepsilon_{ijk}\alpha_l[\hat{p}_l\,,\hat{x}_j]\hat{p}_k = -\boldsymbol{i}\varepsilon_{ijk}\alpha_j\hat{p}_k \neq 0$$

$\Rightarrow \hat{\underline{L}}$ does not commute with $\hat{H}$, and orbital angular momentum is not a good quantum number for spin-$\frac{1}{2}$ electrons (the reason is spin-orbit coupling in the relativistic case).
Next we consider the commutator of the spin operator $\underline{\Sigma}$ with the Hamiltonian. Using the definition

$$\underline{\Sigma} = \begin{pmatrix}\underline{\sigma} & 0\\ 0 & \underline{\sigma}\end{pmatrix} \text{ one sees that } \beta\Sigma_i = \Sigma_i\beta\,,$$

and $[\alpha_i\,,\Sigma_j] = 2\boldsymbol{i}\varepsilon_{ijk}\alpha_k$ (homework problem) and using $[\hat{p}_l\,,\Sigma_i] = 0$ since Σ_i is only a number in momentum space we have

$$[\underline{\alpha}\cdot\hat{\underline{p}}\,,\Sigma_i] = [\alpha_l\,,\Sigma_i]\hat{p}_l = 2\boldsymbol{i}\varepsilon_{ijk}\alpha_j\hat{p}_k\,.$$

We found

$$\begin{aligned}[\hat{H}\,,\hat{L}_i] &= -\boldsymbol{i}\varepsilon_{ijk}\alpha_j\hat{p}_k\\ [\hat{H}\,,\Sigma_i] &= 2\boldsymbol{i}\varepsilon_{ijk}\alpha_j\hat{p}_k\,.\end{aligned}$$

Although neither $\hat{\underline{L}}$ nor $\underline{\Sigma}$ by them self commute with $\hat{H}$, the combined operator

$$\boxed{\hat{\underline{J}} = \hat{\underline{L}} + \frac{\hbar}{2}\underline{\Sigma} = \underline{L} + \underline{S}}$$

does commute with $\hat{H}$ ($\hbar$ is reinserted here). The Dirac Hamiltonian conserves total angular momentum $\hat{\underline{J}}$, but not $\hat{\underline{L}}$ or $\hat{\underline{S}}$ individually ("spin-orbit coupling").

Parity

For a potential $V(\hat{\underline{x}}) = V(|\hat{\underline{x}}|)$ we expect solutions to be parity symmetric which means they are even or odd functions of $\underline{x}$: $\Psi(-\underline{x}) = \pm\Psi(\underline{x})$. However, parity not only changes $\hat{\underline{x}} \mapsto -\hat{\underline{x}}$ but also $\hat{\underline{p}} \mapsto -\hat{\underline{p}}$, and hence $\hat{H} = \underline{\alpha} \cdot \hat{\underline{p}} + \beta m$ changes its form under parity. Previously we defined $\hat{\Pi}$ with $\hat{\Pi}^\dagger \hat{\underline{x}} \hat{\Pi} = -\hat{\underline{x}}$ and $\hat{\Pi}^\dagger \hat{\underline{p}} \hat{\Pi} = -\hat{\underline{p}}$ and $\hat{\Pi}^\dagger \hat{\underline{L}} \hat{\Pi} = \hat{\underline{L}}$.
The full parity operator $\hat{\underline{\mathcal{P}}}$ needs to contain a unitary operator which acts in spinor space (due to spin-orbit coupling), and can hence be represented by a 4×4 matrix. We consider the form

$$\hat{\mathcal{P}} \equiv \hat{\Pi} U_p$$

and require to have the Dirac Hamiltonian independent under $\hat{\mathcal{P}}$ transformation. We need $U_p \underline{\alpha} U_p^\dagger = -\underline{\alpha}$ and $U_p \beta U_p^\dagger = \beta$ and $\hat{\mathcal{P}}^2 = 1$, since $\hat{\Pi}^2 = 1$ this is $U_p^2 = 1$. Since $\beta = \gamma^0$ and $\underline{\alpha} = \gamma^0 \underline{\gamma}$, the choice $U_p = \gamma^0$ is consistent with this requirement and

$$\boxed{\hat{\mathcal{P}} = \hat{\Pi}\gamma^0 \text{ , i.e. } \Psi(\underline{x}) \overset{\hat{\mathcal{P}}}{\longmapsto} \beta\Psi(-\underline{x})} \ .$$

Charge Conjugation

Motivation: We know that the "particle-like" solutions have positive energy $\Psi_{\text{part}}(\underline{x}, t) = \Psi_{E>0}(\underline{x}, t)$ and we propose that the "anti-particle" (charge $-e$) solutions are $\Psi_{\text{anti-part}}(\underline{x}, t) = \Psi^*_{E<0}(\underline{x}, t)$. Complex conjugations can be motivated by the Klein-Gordon equation with a vector potential $\hat{\underline{p}} - e\underline{A} = -\boldsymbol{i}\nabla - e\underline{A} = -\boldsymbol{i}(\nabla - \boldsymbol{i}e\underline{A})$ given by

$$\left[(\partial_\mu - \boldsymbol{i}eA_\mu)\,(\partial^\mu + \boldsymbol{i}eA^\mu) + m^2\right] \Psi_{\text{part}} = 0 \ .$$

Complex conjugation changes the sign of the electric charge, such that

$$\left[(\partial_\mu - \boldsymbol{i}(-e)A_\mu)\,(\partial^\mu + \boldsymbol{i}(-e)A^\mu) + m^2\right] \Psi_{\text{anti-part}} = 0 \ .$$

The anti-particle wave function behaves like that of a particle, but with opposite electric charge.

We consider the Dirac equation in presence of a vector potential $\underline{A}$

$$[\boldsymbol{i}\gamma^\mu \partial_\mu - e\gamma^\mu A_\mu - m]\,\Psi(\underline{x}, t) = 0 \ . \qquad (*)$$

We look for a new equation with $e \mapsto -e$ that relates the new wave function to the old one. Taking the complex conjugate of (*) yields

$$[-\boldsymbol{i}(\gamma^\mu)^* \partial_\mu - e(\gamma^\mu)^* A_\mu - m]\,\Psi^*(\underline{x}, t) = 0 \ .$$

To only change the sign in front of the e (and change the wave function), we need to find a matrix $\tilde{C}$ such that

$$\tilde{C}(\gamma^\mu)^* \tilde{C}^{-1} = -\gamma^\mu \ .$$

Therefore, we need to insert $\mathbb{1} = \tilde{C}^{-1}\tilde{C}$ in front of the wave function, and multiply the equation by $\tilde{C}$ from the left to obtain the result

$$[\boldsymbol{i}\gamma^\mu\partial_\mu - (-e)\gamma^\mu A_\mu - m]\,\tilde{C}\Psi^*(\underline{x},t) = 0\,.$$

Hence, $\tilde{C}\Psi^*(\underline{x},t)$ satisfies the "positron equation", if $\Psi(\underline{x},t)$ satisfies the "electron equation". We note that $\gamma^0,\gamma^1,\gamma^3$ are real matrices, but $(\gamma^2)^* = -\gamma^2$. Using $\frac{1}{2}\{\gamma^\mu,\gamma^\nu\} = \eta^{\mu\nu}$ we see that γ^2 anti-commutes with $\gamma^0,\gamma^1,\gamma^3$. We choose $\tilde{C} = \boldsymbol{i}\gamma^2$ where the phase is a convenient choice for later. $\Rightarrow$ The positron wave function corresponds to $\boldsymbol{i}\gamma^2\Psi^*(\underline{x},t)$.

Remark: An alternative way to express the "positron wave function" is

$$\overline{\Psi} = \Psi^\dagger\gamma^0 \Rightarrow \tilde{C}\Psi^*(\underline{x},t) = \boldsymbol{i}\gamma^2(\overline{\Psi}\gamma^0)^t = U_c(\overline{\Psi})^t$$

with $U_c \equiv \boldsymbol{i}\gamma^2\gamma^0$ because $(\gamma^0)^t = \gamma^0$.

We define the charge conjugation operator $\hat{\mathcal{C}}$ by

$$\boxed{\hat{\mathcal{C}}\Psi(\underline{x},t) = U_c(\overline{\Psi})^t \text{ which here is } \hat{\mathcal{C}} = \tilde{C}\hat{K} = \boldsymbol{i}\gamma^2\hat{K}}\quad .$$

Considering $\Psi(\underline{x},t) \propto e^{-\boldsymbol{i}p^\mu x_\mu}$ we see that $\hat{\mathcal{C}}$ effectively takes $\underline{x} \mapsto -\underline{x}$ and $t \mapsto -t$ since $p^\mu x_\mu = Et - \underline{p}\cdot\underline{x}$.

Time Reversal

For the Schrödinger equation we had the anti-unitary operator $\hat{T} = \hat{U}\hat{K}$ with complex conjugation $\hat{K}$ and unitary $\hat{U}$. $\hat{T}$ takes an arbitrary state ket $|\alpha\rangle$ into the time-reversed (motion-reversed) state

$$\hat{T}|\alpha\rangle = |\tilde{\alpha}\rangle \text{ with } \hat{T}\underline{\hat{p}}\hat{T}^{-1} = -\underline{\hat{p}}\ ,\ \hat{T}\underline{\hat{x}}\hat{T}^{-1} = \underline{\hat{x}} \text{ and } \hat{T}\underline{\hat{J}}\hat{T}^{-1} = -\underline{\hat{J}}\,.$$

Since we are in a spin-$\frac{1}{2}$ state, if $[\hat{H}\,,\,\hat{T}] = 0$ we say that the Hamiltonian is time-reversal invariant and every energy eigenstate has the same energy eigenvalue as its time-reversed partner $\hat{T}|n\rangle$. Acting twice on a spin-$\frac{1}{2}$ state yields $\hat{T}^2 = -\mathbb{1}$, and we found the explicit representation $\hat{T} = -\boldsymbol{i}\sigma_y\hat{K}$

$$\Rightarrow \hat{T}^2 = -\boldsymbol{i}\sigma_y\hat{K}(-\boldsymbol{i}\sigma_y\hat{K}) = -\boldsymbol{i}\sigma_y(+\boldsymbol{i})\sigma_y^*\hat{K}^2 = \sigma_y\sigma_y^* = -\mathbb{1}$$

since $\sigma_y^2 = \mathbb{1}$ and $\sigma_y^* = -\sigma_y$.
Consider the time dependent Dirac equation

$$\boldsymbol{i}\partial_t\Psi(\underline{x},t) = \left[-\boldsymbol{i}\gamma^0\underline{\gamma}\cdot\nabla + \gamma^0 m\right]\Psi(\underline{x},t)\,,$$

and denote the time-reversal operator for the Dirac equation as $\hat{\mathcal{T}} = U_T\hat{K}$. Inserting $\hat{\mathcal{T}}\hat{\mathcal{T}}^{-1}$ with $\hat{\mathcal{T}}^{-1} = (U_T\hat{K})^{-1} = \hat{K}^{-1}U_T^{-1} = \hat{K}U_T^{-1}$ in front of the wave function and multiplication by $\hat{\mathcal{T}}$ yields for the left hand site

$$\begin{aligned}\hat{\mathcal{T}}(\boldsymbol{i}\partial_t)\hat{\mathcal{T}}^{-1}\hat{\mathcal{T}}\Psi(\underline{x},t) &= U_T\hat{K}(\boldsymbol{i}\partial_t)\hat{K}U_T^{-1}U_T\Psi^*(\underline{x},t)\\ &= -\boldsymbol{i}\partial_t U_T\Psi^*(\underline{x},t) = \boldsymbol{i}\partial_{-t}\left[U_T\Psi^*(\underline{x},t)\right]\ .\end{aligned}$$

We want that the right hand site stays the same except $\Psi \mapsto U_T\Psi^*$, i.e. the Hamiltonian is $\hat{\mathcal{T}}$-invariant, and on the left hand site we want $\partial_t \mapsto \partial_{-t}$ and $\Psi \mapsto U_T\Psi^*$ (which propagates "back" in time). For $U_T\Psi^*(\underline{x},t)$ to satisfy the time-reversed form of the Dirac equation, the operator on the right hand site needs to satisfy (due to $[\hat{H}\,,\,\hat{\mathcal{T}}] \stackrel{!}{=} 0$)

$$\boxed{\hat{\mathcal{T}}(\boldsymbol{i}\gamma^0\underline{\gamma}\hat{\mathcal{T}}^{-1}) = \boldsymbol{i}\gamma^0\underline{\gamma} \text{ and } \hat{\mathcal{T}}\gamma^0\hat{\mathcal{T}}^{-1} = \gamma^0} \ .$$

First apply $\hat{\mathcal{T}}^{-1}$ from the left, and $\hat{\mathcal{T}}$ from the right to both of the equations. Next, apply $\hat{K}$ on both the left and right hand sites. Then we have

$$\hat{K}(\boldsymbol{i}\gamma^0\underline{\gamma})\hat{K} = \hat{K}\hat{\mathcal{T}}^{-1}(\boldsymbol{i}\gamma^0\underline{\gamma})\hat{\mathcal{T}}\hat{K} = U_T^{-1}(\boldsymbol{i}\gamma^0\underline{\gamma})U_T$$
$$\hat{K}\gamma^0\hat{K} = \hat{K}\hat{\mathcal{T}}^{-1}\gamma^0\hat{\mathcal{T}}\hat{K} = U_T^{-1}\gamma^0 U_T \ .$$

The second equation is equivalent to

$$\boxed{(\gamma^0)^* = \gamma^0 = U_T^{-1}\gamma^0 U_T} \ .$$

and the first one is

$$-\boldsymbol{i}(\gamma^0)^*(\underline{\gamma})^* = \boldsymbol{i}\underbrace{U_T^{-1}\gamma^0 U_T}_{(\gamma^0)^*}U_T^{-1}\underline{\gamma}U_T \ .$$

Multiplying with $(\gamma^0)^*$ yields

$$\boxed{-(\underline{\gamma})^* = U_T^{-1}\underline{\gamma}U_T} \ .$$

γ^2 is imaginary and $\gamma^0, \gamma^1, \gamma^3$ are real $\Rightarrow$ We need to find U_T which commutes with γ^0 and γ^2 and anti-commutes with γ^1 and γ^3.

$$[U_T\,,\,\gamma^{0,2}] = 0 \text{ and } \{U_T\,,\,\gamma^{1,3}\} = 0$$

can be accomplished by $U_T = \gamma^1\gamma^3$ up to a phase factor. One finds (homework problem)

$$\gamma^1\gamma^3 = \boldsymbol{i}\begin{pmatrix}\sigma_y & 0\\ 0 & \sigma_y\end{pmatrix} \ .$$

So we have

$$\boxed{\hat{\mathcal{T}} = \gamma^1\gamma^3\hat{K}} \ .$$

$\mathcal{CPT}$-Symmetry

It is interesting to consider the operator $\hat{\mathcal{C}}\hat{\mathcal{P}}\hat{\mathcal{T}}$ given by

$$\begin{aligned}\hat{\mathcal{C}}\hat{\mathcal{P}}\hat{\mathcal{T}}\Psi(\underline{x},t) &= \boldsymbol{i}\gamma^2\left[\hat{\mathcal{P}}\hat{\mathcal{T}}\Psi(\underline{x},t)\right]^*\\ &= \boldsymbol{i}\gamma^2\gamma^0\left[\hat{\mathcal{T}}\Psi(-\underline{x},t)\right]^*\\ &= \boldsymbol{i}\gamma^2\gamma^0\gamma^1\gamma^3\Psi(-\underline{x},t)\\ &= \boldsymbol{i}\gamma^0\gamma^1\gamma^2\gamma^3\Psi(-\underline{x},t) \equiv \gamma^5\Psi(-\underline{x},t)\end{aligned}$$

We defined

$$\gamma^5 \equiv \boldsymbol{i}\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix}0 & \mathbb{1}\\ \mathbb{1} & 0\end{pmatrix} \ .$$

γ^5 exchanges the upper two "particle like" with the down "anti-particle like" components of the wave functions. Such an operator is called a "chiral"-operator.
In context of the Dirac equation $\hat{\mathcal{C}}\hat{\mathcal{P}}\hat{\mathcal{T}}$ converts a free electron wave function into a positron wave function (datails as homework problem). In relativistic quantum field theory, $\hat{\mathcal{C}}\hat{\mathcal{P}}\hat{\mathcal{T}}$ is equivalent to a total symmetry between matter and anti-matter. $\hat{\mathcal{C}}\hat{\mathcal{P}}\hat{\mathcal{T}}$ can be shown to be equivalent to Lorentz symmetry.

3 Review of Angular Momentum Addition

As a motivation we will consider two examples before generalizing the results in a semi-classical model. We are interested in the addition of angular momentum because terms like $\hat{\underline{L}} \cdot \hat{\underline{S}}$ often appear in Hamiltonians we consider.

3.1 Examples

A. One Spin-$\frac{1}{2}$ Particle with Orbital and Spin Angular Momentum
We denote spin-up and -down with $\pm$ and decompose kets in orbital part $|\underline{x}'\rangle$, and spin part $|\pm\rangle$ via a direct product $\otimes$ of two vector spaces

$$|\underline{x}', \pm\rangle = |\underline{x}'\rangle \otimes |\pm\rangle \text{ or } |j_1, m_1\rangle \otimes |j_2, m_2\rangle = |j_1, j_2; m_1, m_2\rangle \ .$$

The rotation operator with angular momentum $\hat{\underline{J}}$ for rotation around axis $\underline{n}$ by an angle φ is given as

$$D(\underline{\varphi}) = \exp\left[-\frac{\boldsymbol{i}}{\hbar}\hat{\underline{J}} \cdot \underline{n}\,\varphi\right] \text{ with } \underline{\varphi} = \varphi\underline{n}$$

where we write

$$\hat{\underline{J}} = \hat{\underline{L}} + \hat{\underline{S}} = \hat{\underline{L}} \otimes \mathbb{1}_s + \mathbb{1}_o \otimes \hat{\underline{S}} \ .$$

$\mathbb{1}_0$ is the identity in orbital space and $\mathbb{1}_s$ is identity in spin space, i.e. they only act on orbital kets and spin kets, respectively. Obviously we have $[\hat{\underline{L}}\,,\,\hat{\underline{S}}] = 0$ because the operators act on different spaces and using the Baker-Hausdorff formula we find

$$D(\underline{\varphi}) = \exp\left[-\frac{\boldsymbol{i}}{\hbar}\hat{\underline{L}} \cdot \underline{n}\,\varphi\right] \otimes \exp\left[-\frac{\boldsymbol{i}}{\hbar}\hat{\underline{S}} \cdot \underline{n}\,\varphi\right] = D^{(\text{orb})}(\underline{\varphi}) \otimes D^{(\text{spin})}(\underline{\varphi}) \ .$$

We write wave functions as vectors with spin-up and spin-down component

$$\langle \underline{x}', \pm|\alpha\rangle = \Psi_\pm(\underline{x}') \text{ "=" } \begin{pmatrix} \Psi_+(\underline{x}') \\ \Psi_-(\underline{x}') \end{pmatrix} \ .$$

Then $|\Psi_\pm(\underline{x}')|^2$ is the probability of finding the particle with spin $\pm$ at $\underline{x} = \underline{x}'$.

B. Two Spin-$\frac{1}{2}$ Particles without Orbital Angular Momentum
The total spin is denoted by $\hat{\underline{S}}$ and given by

$$\hat{\underline{S}} = \hat{\underline{S}}_1 + \hat{\underline{S}}_2 = \hat{\underline{S}}_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \hat{\underline{S}}_2$$

where $\mathbb{1}_1$ and $\mathbb{1}_2$ is identity for subspace 1 and 2, respectively. Hence, we again have $[\hat{\underline{S}}_1\,,\,\hat{\underline{S}}_2] = 0$. Within one and the same subspace, we have the usual commutator algebra for angular momentum

$$[\hat{S}_{1,i}\,,\,\hat{S}_{1,j}] = \boldsymbol{i}\hbar\varepsilon_{ijk}\hat{S}_{1k}$$
$$[\hat{S}_{2,i}\,,\,\hat{S}_{2,j}] = \boldsymbol{i}\hbar\varepsilon_{ijk}\hat{S}_{2k} \ .$$

We see that in this case the total spin (added) from two spins is again a spin imbedded in the known algebra, since using $\hat{S}_i = \hat{S}_{1,i} + \hat{S}_{2,i}$ we have

$$[\hat{S}_i\ ,\ \hat{S}_j] = \boldsymbol{i}\hbar\varepsilon_{ijk}\hat{S}_k\ .$$

Hence, we already know the eigenvalues of $\hat{\underline{S}}^2$ and $\hat{S}_z$ because they were deduced only using the commutator algebra:

$$\begin{array}{rll} \hat{\underline{S}}^2 = (\hat{\underline{S}}_1 + \hat{\underline{S}}_2)^2 & \text{has eigenvalues} & s(s+1)\hbar^2 \\ \hat{S}_z = \hat{S}_{1,z} + \hat{S}_{2,z} & \text{has eigenvalues} & m\hbar \\ \hat{S}_{1,z} & \text{has eigenvalues} & m_1\hbar \\ \hat{S}_{2,z} & \text{has eigenvalues} & m_2\hbar \end{array}$$

To describe a general spin state one can pick any two compatible observables. In this case, we have two choices

i) Use eigenstates of $\hat{S}_{1,z}, \hat{S}_{2,z}$ ($|m_1, m_2\rangle$ representation) with basis

$$|+,+\rangle\ ,\ |+,-\rangle,\ |-,+\rangle,\ |-,-\rangle\ .$$

ii) Use eigenstates of $\hat{\underline{S}}^2$ and $\hat{S}_z$ (in $|s = s_1 \pm s_2, m = m_1 \pm m_2\rangle$ representation) with

- Triplet state $s = 1$:

$$\begin{aligned} |s=1, m=1\rangle &= |++\rangle \\ |s=1, m=0\rangle &= \frac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right) \\ |s=1, m=-1\rangle &= |--\rangle \end{aligned}$$

- Singlet state $s = 0$:

$$|s=0, m=0\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$$

The coefficients in the basis transformation between i) and ii) are (simple) Clebsch-Gordon coefficients.
We define ladder operator $\hat{\underline{S}}_\pm$ as

$$\hat{\underline{S}}_\pm = \hat{\underline{S}}_{1,\pm} + \hat{\underline{S}}_{2,\pm} = (\hat{S}_{1,x} \pm \boldsymbol{i}S_{1,y}) + (\hat{S}_{2,x} \pm \boldsymbol{i}S_{2,y})$$

where $\hat{\underline{S}}_{i,\pm}$ only affects the ith entry in the ket since it only acts on the i-subspace.
The action on our state kets in ii) is

$$\hat{\underline{S}}_-|++\rangle = \hat{\underline{S}}_-|s=1, m=1\rangle = \sqrt{(1+1)(1-1+1)}|s=1, m=0\rangle = \sqrt{2}|s=1, m=0\rangle$$

and in i) we have

$$\begin{aligned} \hat{\underline{S}}_-|++\rangle = (\hat{\underline{S}}_{1-} + \hat{\underline{S}}_{2,-})|++\rangle &= \sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)}\,|-+\rangle + \sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)}\,|+-\rangle \\ &= |-+\rangle + |+-\rangle \end{aligned}$$

which coincides with our considerations above.
We see that using the ladder operators we can express

$$\begin{aligned}\hat{\underline{S}}^2 &= (\hat{\underline{S}}_1 + \hat{\underline{S}}_2)^2 = \hat{\underline{S}}_1^2 + \hat{\underline{S}}_2^2 + 2\hat{\underline{S}}_1 \cdot \hat{\underline{S}}_2 \\ &= \hat{\underline{S}}_1^2 + \hat{\underline{S}}_2^2 + 2\left[\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y} + \hat{S}_{1,z}\hat{S}_{2,z}\right] \\ &= \hat{\underline{S}}_1^2 + \hat{\underline{S}}_2^2 + 2\hat{S}_{1,z}\hat{S}_{2,z} + \hat{S}_{1,+}\hat{S}_{2,-} + \hat{S}_{1,-}\hat{S}_{2,+} \ .\end{aligned}$$

Formal Theory for Addition of Angular Momentum

We want to consider the formal theory in a general case of two angular momenta $\hat{\underline{J}}_1, \hat{\underline{J}}_2$ in the semi-classical model. We have the commutator algebra

$$\begin{aligned}[\hat{J}_{1,i}\ ,\ \hat{J}_{1,j}] &= \boldsymbol{i}\hbar\varepsilon_{ijk}J_{1,k} \\ [\hat{J}_{2,i}\ ,\ \hat{J}_{2,j}] &= \boldsymbol{i}\hbar\varepsilon_{ijk}J_{2,k} \\ [\hat{J}_{1,i}\ ,\ \hat{J}_{2,j}] &= 0 \ .\end{aligned}$$

The operator for infinitesimal rotations around the axis $\underline{n}$ by an angle ϕ is given by

$$\begin{aligned}\left(\mathbb{1} - \frac{\boldsymbol{i}\hat{\underline{J}}_1 \cdot \underline{n}\,\varphi}{\hbar}\right) \otimes \left(\mathbb{1} - \frac{\boldsymbol{i}\hat{\underline{J}}_1 \cdot \underline{n}\,\varphi}{\hbar}\right) + \mathcal{O}(\varphi^2) &= \mathbb{1} - \frac{\boldsymbol{i}(\hat{\underline{J}}_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \hat{\underline{J}}_2) \cdot \underline{n}\varphi}{\hbar} + \mathcal{O}(\varphi^2) \\ &\equiv \mathbb{1} - \frac{\boldsymbol{i}\hat{\underline{J}} \cdot \underline{n}\,\varphi}{\hbar} + \mathcal{O}(\varphi^2) \ .\end{aligned}$$

We identify the total angular momentum, the generator of rotation, as

$$\hat{\underline{J}} = \hat{\underline{J}}_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes \hat{\underline{J}}_2 = \hat{\underline{J}}_1 + \hat{\underline{J}}_2 \ .$$

For finite rotation angles φ we use the commutator $[\hat{J}_{1,i}\ ,\ \hat{J}_{2,j}] = 0$ in the Baker-Hausdorff formula to obtain

$$D_1(\underline{\varphi}) \otimes D_2(\underline{\varphi}) = \exp\left[-\frac{\boldsymbol{i}\hat{\underline{J}}_1 \cdot \underline{n}\,\varphi}{\hbar}\right] \otimes \exp\left[-\frac{\boldsymbol{i}\hat{\underline{J}}_2 \cdot \underline{n}\,\varphi}{\hbar}\right] = \exp\left[-\frac{\boldsymbol{i}\hat{\underline{J}} \cdot \underline{n}\,\varphi}{\hbar}\right] = D(\underline{\varphi}) \ .$$

We again have the commutator algebra

$$[\hat{\underline{J}}_i\ ,\ \hat{\underline{J}}_j] = \boldsymbol{i}\hbar\varepsilon_{ijk}\hat{\underline{J}}_k$$

which is why $\hat{\underline{J}}$ is again a angular momentum.
We have two choices of bases:

i) Use eigenstates of $\hat{\underline{J}}_1^2\ ,\ \hat{\underline{J}}_2^2\ ,\ \hat{J}_{1,z}\ ,\ \hat{J}_{2,z}$ and find

$$\begin{aligned}\hat{\underline{J}}_1^2|j_1, j_2; m_1, m_2\rangle &= j_1(j_1+1)\hbar^2|j_1, j_2; m_1, m_2\rangle \\ \hat{\underline{J}}_2^2|j_1, j_2; m_1, m_2\rangle &= j_2(j_2+1)\hbar^2|j_1, j_2; m_1, m_2\rangle \\ \hat{J}_{1,z}|j_1, j_2; m_1, m_2\rangle &= m_1\hbar|j_1, j_2; m_1, m_2\rangle \\ \hat{J}_{2,z}|j_1, j_2; m_1, m_2\rangle &= m_2\hbar|j_1, j_2; m_1, m_2\rangle\end{aligned}$$

ii) Use eigenstates of $\underline{\hat{J}}^2$, $\underline{\hat{J}}_1^2$, $\underline{\hat{J}}_2^2$ and $\hat{J}_z$

$$\begin{aligned}
\underline{\hat{J}}_1^2|j_1,j_2;j,m\rangle &= j_1(j_1+1)\hbar^2|j_1,j_2;j,m\rangle \\
\underline{\hat{J}}_2^2|j_1,j_2;j,m\rangle &= j_2(j_2+1)\hbar^2|j_1,j_2;j,m\rangle \\
\underline{\hat{J}}^2|j_1,j_2;j,m\rangle &= j(j+1)\hbar^2|j_1,j_2;j,m\rangle \\
\hat{J}_z|j_1,j_2;j,m\rangle &= m\hbar|j_1,j_2;j,m\rangle
\end{aligned}$$

We want again to consider the base transformation i)$\leftrightarrow$ ii) inserting an identity (completeness relation)

$$|j_1,j_2;j,m\rangle = \underbrace{\sum_{m_1}\sum_{m_2}|j_1,j_2;m_1,m_2\rangle\langle j_1,j_2;m_1,m_2|}_{\mathbb{1}}\,|j_1,j_2;j,m\rangle\ .$$

Here $\mathbb{1}$ is the identity in ket-space with fixed j_1, j_2.
The elements of the transformation matrix $\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle$ are the Clebsch-Gordon coefficients.

Claim: The coefficients vanish unless $m = m_1 + m_2$.
Proof: We consider

$$(\hat{J}_z - \hat{J}_{1,z} - \hat{J}_{2,z})|j_1,j_2;j,m\rangle = 0\ .$$

Applying $\langle j_1,j_2;m_1,m_2|$ from the left and letting $\hat{J}_z$ act to the right on the ket, and $\hat{J}_{1,z}^\dagger = \hat{J}_{1,z}$, $\hat{J}_{2,z}^\dagger = \hat{J}_{2,z}$ to the left yields

$$\begin{aligned}
\langle j_1,j_2;m_1,m_2|(\hat{J}_z - \hat{J}_{1,z} - \hat{J}_{2,z})|j_1,j_2;j,m\rangle &= 0 \\
(m - m_1 - m_2)\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle &= 0\ . \quad \square
\end{aligned}$$

Claim: The Clebsch-Gordon coefficients vanish unless

$$|j_1 - j_2| \le j \le j_1 + j_2\ .$$

Proof: Can be found in Sakurai.

The matrix formed by the Clebsch-Gordon coefficients is unitary due to the properties of the kets. We pick the elements to be real. Hence, the matrix is orthogonal ($A^t = A^{-1}$) and we have

$$\begin{aligned}
\sum_j\sum_m \langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle \underbrace{\langle j_1,j_2;m_1',m_2'|j_1,j_2;j,m\rangle}_{(\langle j_1,j_2;j,m|j_1,j_2;m_1',m_2'\rangle)^*} &= \delta_{m_1,m_1'}\delta_{m_2,m_2'} \\
\sum_{m_1}\sum_{m_2}\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle\langle j_1,j_2;m_1,m_2|j_1,j_2;j',m'\rangle &= \delta_{j,j'}\delta_{m,m'}\ .
\end{aligned}$$

Picking $j = j'$ and $m' = m = m_1 + m_2$ we find

$$\sum_{m_1}\sum_{m_2}|\langle j_1,j_2;m_1,m_2|j_1,j_2;j,m\rangle|^2 = 1\ .$$

In the literature one finds alternative notations for $\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle$ like

$$\langle j_1, m_2; j_2, m_2 | j_1, j_2; j, m\rangle \ , \ C(j_1, j_2, j; m_1, m_2, m) \ , \ C_{j_1,j_2}(j, m; m_1, m_2)$$

or the Wigner 3-j-symbol:

$$\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle = (-1)^{j_1 - j_2 + m} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} .$$

3.2 Recursion Relation for the Clebsch-Gordon Coefficients

For fixed j_1, j_2 and j, the coefficients with different m_1, m_2 and m are related by recursion relations:

$$\hat{J}_\pm |j_1, j_2; j, m\rangle = (\hat{J}_{1,\pm} + \hat{J}_{2,\pm}) \sum_{m_1, m_2} |j_1, j_2; m_1, m_2\rangle \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle \ .$$

We use that

$$\begin{aligned} \hat{J}_+ |j, m\rangle &= \sqrt{(j-m)(j+m+1)}\hbar |j, m+1\rangle \\ \hat{J}_- |j, m\rangle &= \sqrt{(j+m)(j-m+1)}\hbar |j, m-1\rangle \end{aligned}$$

to obtain

$$\begin{aligned} \sqrt{(j \mp m)(j \pm m + 1)} |j_1, j_2; j, m \pm 1\rangle = \sum_{m_1', m_2'} \Big[& \sqrt{(j_1 \mp m_1')(j, \pm m_1' + 1)} |j_1, j_2; m_1' \pm 1, m_2'\rangle \\ & + \sqrt{(j_2 \mp m_2')(j_2 \pm m_2' + 1)} |j_1, j_2; m_1', m_2' \pm 1\rangle \Big] \\ & \cdot \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle \end{aligned}$$

We relabeled m_1, m_2 just to indicate that $-j_1 \leq m_1 \leq j_1$ might not hold anymore. We now multiply by $\langle j_1, j_2; m_1, m_2|$ from the left hand site, and use orthonormality, i.e. non-vanishing contributions from right hand site only possible with

$$\begin{array}{rlcl} \text{first term} & m_1 = m_1' \pm 1 & , & m_2 = m_2' \\ \text{second term} & m_1 = m_1' & , & m_2 = m_2' \pm 1 \ . \end{array}$$

This is

$$\begin{aligned} \sqrt{(j \mp m)(j \pm m + 1)} & \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m \pm 1\rangle \\ & = \sqrt{(j_1 \mp m_1 + 1)(j_1 \pm m_1)} \langle j_1, j_2; m_1 \mp 1, m_2 | j_1, j_2; j, m\rangle \\ & \quad + \sqrt{(j_2 \mp m_2 + 1)(j_2 \pm m_2)} \langle j_1, j_2; m_1, m_2 \mp 1 | j_1, j_2; j, m\rangle \ . \qquad (*) \end{aligned}$$

The condition on the sum of z-components has now become $m_1 + m_2 = m \pm 1$ due to the action of $\hat{J}_\pm$. We interpret (*) graphically in the m_1-m_2-plane .

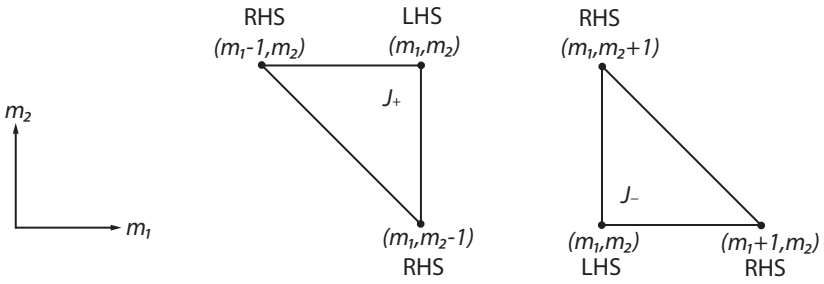

Figure 3.1: Graphic representations of the recursion relation where the points represent the three sums in (*)

The recursion relation (*) together with normalization condition, uniquely determines the Clebsch-Gordon coefficients up to a phase factor.

Strategy
Due to the fact that j_1, j_2, and j are fixed, the allowed region in the m_1-m_2-plane is limited by the inequalities

$$|m_1| \leq j_1 \ , \ |m_2| \leq j_2 \text{ and } \ -j \leq m_1 + m_2 \leq j \ .$$

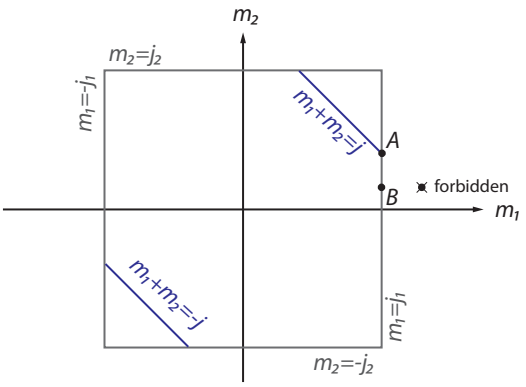

Figure 3.2: Allowed regions where the sums are not vanishing determined by the inequalities above

We may start with the upper right hand corner, denoted by A.

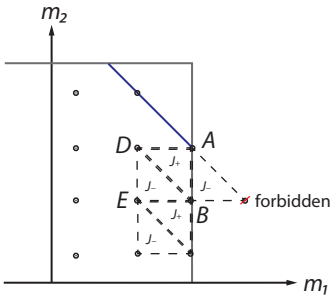

Figure 3.3: Forbidden region, iterative calculation of the points starting from A

We first apply the $\hat{J}_-$ recursion relation with $(m_1, m_2 \pm 1)$ corresponding to A. The recursion relation connects A to B only, as the site $(m_1 + 1, m_2)$ is forbidden by the constraint $m_1 \leq j_1$. We obtain the Clebsch-Gordon coefficient of B in terms of the coefficient of A. In the next step, we consider the triangle defined by the points A, B, and D. Application of $\hat{J}_+$ allows to determine the coefficient of D, than E, and so on. After some afford, we know all the coefficients expressed in terms of the coefficient in A. The overall normalization is provided by

$$\sum_{m_1,m_2} |\langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle|^2 = 1\,,$$

and the overall sign is fixed by convention.

As an example, we consider the addition of orbital and spin momentum of a single angular spin-$\frac{1}{2}$ particle. We have

$$\begin{array}{ll} j_1 = l \text{ (integer)} & , \; m_1 = m_l \\ j_2 = s = \frac{1}{2} & , \; m_1 = m_s = \pm\frac{1}{2}\,. \end{array}$$

The allowed values for j are given by $j = l \pm \frac{1}{2}$ or $j = \frac{1}{2}$ only if $l = 0$ which can be deduced from $|j_1 - j_2| \leq j \leq j_1 + j_2$. $\Rightarrow$ There are two possible j-values. As an example we consider $l = 1$ and obtain in the spectroscopic notation $p_{3/2},\ p_{1/2}$ where p denotes $l = 1$.

Using $m = m_1 + m_2 \Rightarrow m_1 = m - m_2$ we can write

$$\begin{aligned} |j_1, j_2; j, m\rangle &= \sum_{m_1,m_2} \langle j_1, j_2; m_1, m_2 | j_1, j_2; j, m\rangle |j_1, j_2; m_1, m_2\rangle \\ &= \sum_{m_2} \langle j_1, j_2; m - m_2, m_2 | j_1, j_2; j, m\rangle |j_1, j_2; m - m_2, m_2\rangle\ . \end{aligned}$$

Goal: Find the transformation matrix in

$$\begin{pmatrix} |j_1 = l + \frac{1}{2}, m\rangle \\ |j_1 = l - \frac{1}{2}, m\rangle \end{pmatrix} = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} |m_l = m - \frac{1}{2}, m_s = \frac{1}{2}\rangle \\ |m_l = m + \frac{1}{2}, m_s = -\frac{1}{2}\rangle \end{pmatrix} \qquad (*)$$

where we used the notation $|j_1 = l, j_2 = \frac{1}{2}; j = l + \frac{1}{2}, m\rangle \equiv |j = l + \frac{1}{2}, m\rangle$.

Strategy: Using the recursion relation

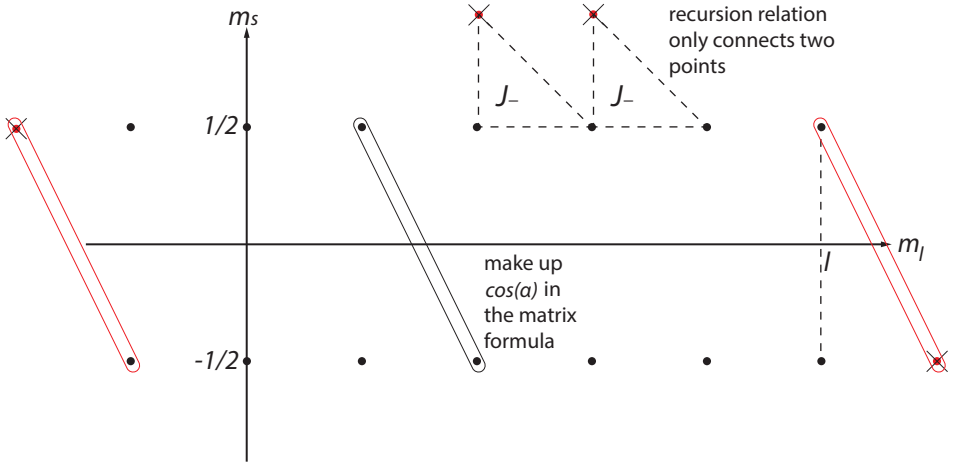

Figure 3.4: Recursion relation in m_s-m_l-plane for $j_1 = l$ and $j_2 = s = \frac{1}{2}$

We focus on the case $j = l + \frac{1}{2}$ (the upper row) here. Since $m_s \leq \frac{1}{2}$, we use the $\hat{J}_-$-recursion relation in such a way that we always stay in the upper row $m_s = m_2 = +\frac{1}{2}$, while the m_l-value changes by one unit within each $\hat{J}_-$-triangle. This is

$$\sqrt{(j+m)(j-m+1)}\langle m_l, m_s = \tfrac{1}{2}|j, m-1\rangle = \sqrt{(j_1+m_1+1)(j_1-m_1)}\langle m_l+1, m_s = +\tfrac{1}{2}|j, m\rangle$$

Note that on the left we have $m_l + \frac{1}{2} = m - 1$ and on the right $m_l + 1 + \frac{1}{2} = m$ which is the same. Substitute $m \to m + 1$ and use $j = l + \frac{1}{2}$, and $j_1 = l$ to obtain

$$\sqrt{(j+m+1)(j-m)}\langle m_l, \tfrac{1}{2}|l+\tfrac{1}{2}, m\rangle = \sqrt{(l+m_l+1)(l-m_l)}\langle m_l+1, \tfrac{1}{2}|l+\tfrac{1}{2}, m+1\rangle$$

We now use $m_l = m - \frac{1}{2}$ due to $m_l + \frac{1}{2} = m$ in the upper row. We consider

$$\sqrt{(l+\tfrac{1}{2}+m+1)(l+\tfrac{1}{2}-m)}\langle m-\tfrac{1}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m\rangle = \sqrt{(l+m+\tfrac{1}{2})(l-m+\tfrac{1}{2})}\langle m+\tfrac{1}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m+1\rangle$$
$$\sqrt{l+\tfrac{1}{2}+m+1}\langle m-\tfrac{1}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m\rangle = \sqrt{l+m+\tfrac{1}{2}}\langle m+\tfrac{1}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m+1\rangle \ .$$

Hence, we have

$$\langle m-\tfrac{1}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m\rangle = \sqrt{\frac{l+m+\frac{1}{2}}{l+m+\frac{3}{2}}}\langle m+\tfrac{1}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m+1\rangle \ .$$

Next we can express $\langle m+\frac{1}{2}, \frac{1}{2}|l+\frac{1}{2}, m+1\rangle$ in terms of $\langle m+\frac{3}{2}, \frac{1}{2}|l+\frac{1}{2}, m+2\rangle$ and so on. This can be continued until m_l reaches l, the maximum possible value

$$\begin{aligned}
\langle m-\tfrac{1}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m\rangle &= \sqrt{\frac{l+m+\frac{1}{2}}{l+m+\frac{3}{2}}}\sqrt{\frac{l+m+\frac{3}{2}}{l+m+\frac{5}{2}}}\langle m+\tfrac{3}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m+2\rangle \\
&= \sqrt{\frac{l+m+\frac{1}{2}}{l+m+\frac{3}{2}}}\sqrt{\frac{l+m+\frac{3}{2}}{l+m+\frac{5}{2}}}\sqrt{\frac{l+m+\frac{5}{2}}{l+m+\frac{7}{2}}}\langle m+\tfrac{5}{2}, \tfrac{1}{2}|l+\tfrac{1}{2}, m+3\rangle \\
&= \sqrt{\frac{l+m+\frac{1}{2}}{l+l+1}}\langle l, \tfrac{1}{2}|l+\tfrac{1}{2}, l+\tfrac{1}{2}\rangle \ .
\end{aligned}$$

We used that the denominator always cancels the next nominator, so we are only left with the first numerator and last denominator with $m_l = l = m + \frac{1}{2}$. This is the maximum value of m_l and m_s, i.e. $m_l = l$ and $m_s = \frac{1}{2} \Rightarrow m = m_l + m_s = l + \frac{1}{2}$. This is possible only for $j = l + \frac{1}{2}$, not for $j = l - \frac{1}{2}$.
The recursion relations stop since

$$|j_1, j_2; m_1 = j_1, m_2 = j_2\rangle = |j_1, j_2; j = j_1 + j_2, m = j\rangle$$
$$|j_1, j_2; m_1 = -j_1, m_2 = -j_2\rangle = |j_1, j_2; j = j_1 + j_2, m = -j\rangle$$

due to the missing of a partner (see Fig. 2.18) at the ends.

$$\Rightarrow |m_1 = l, m_2 = +\tfrac{1}{2}\rangle = e^{i\delta}|j = l + \tfrac{1}{2}, m = l + \tfrac{1}{2}\rangle$$

We take $e^{i\delta} = 1$ by convention and have $\langle l, \frac{1}{2} | l + \frac{1}{2}, l + \frac{1}{2} \rangle = 1$.
Using this, we have

$$\langle m - \tfrac{1}{2}, \tfrac{1}{2} | l + \tfrac{1}{2}, m \rangle = \sqrt{\frac{l + m + \frac{1}{2}}{2l + 1}} \; .$$

We are close to finding the desired transformation (*): (The z component of the angular momentum needs to be conserved: $m = m_1 + m_2 = m + \frac{1}{2} - \frac{1}{2} = m - \frac{1}{2} + \frac{1}{2}$)

$$|j = l + \tfrac{1}{2}, m\rangle = \sqrt{\frac{l + m + \frac{1}{2}}{2l + 1}} |m_l = m - \tfrac{1}{2}, m_s = +\tfrac{1}{2}\rangle + \; \mathbf{?} \; |m_l = m + \tfrac{1}{2}, m_s = -\tfrac{1}{2}\rangle$$
$$|j = l - \tfrac{1}{2}, m\rangle = \; \mathbf{?} \; |m_l = m - \tfrac{1}{2}, m_s = +\tfrac{1}{2}\rangle + \; \mathbf{?} \; |m_l = m + \tfrac{1}{2}, m_s = -\tfrac{1}{2}\rangle \; .$$

We know comparing with the matrix relation (*) that

$$\cos\alpha = \sqrt{\frac{l + m + \frac{1}{2}}{2l + 1}} \Longrightarrow \sin^2\alpha = 1 - \cos^2\alpha = \frac{2l + 1 - (l + m + \frac{1}{2})}{2l + 1} \Longrightarrow \sin^2\alpha = \frac{l - m + \frac{1}{2}}{2l + 1} \; .$$

We now use the idea that the coefficient represented by $\sin\alpha$: $\langle m_l = m + \frac{1}{2}, m_s = -\frac{1}{2} | j = l + \frac{1}{2}, m \rangle$ has to be positive because all $j = l + \frac{1}{2}$ states can be reached by applying $\hat{J}_-$ sucessively to $|j = l + \frac{1}{2}, m = l + \frac{1}{2}\rangle$, and the matrix elements of $\hat{J}_-$ are positive by convention. $\Rightarrow$ We choose the positive sign when taking the square root.
The transformation matrix is thus given by

$$\begin{pmatrix} \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} & \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} \\ -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} & \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} \end{pmatrix} \; .$$

We can use this result to define spin angular wave functions in two component notation $\chi_+ = (1, 0)$, $\chi_- = (0, 1)$:

$$\begin{aligned} \mathcal{Y}_l^{j=l\pm\frac{1}{2},m}(\theta,\varphi) &= \pm\sqrt{\frac{l \pm m + \frac{1}{2}}{2l + 1}} \, \mathrm{Y}_l^{m-\frac{1}{2}}(\theta,\varphi) \, \chi_+ + \sqrt{\frac{l \mp m + \frac{1}{2}}{2l + 1}} \, \mathrm{Y}_l^{m+\frac{1}{2}}(\theta,\varphi) \, \chi_- \\ &= \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \pm\sqrt{l \pm m + \frac{1}{2}} \, \mathrm{Y}_l^{m-\frac{1}{2}}(\theta,\varphi) \\ \sqrt{l \mp m + \frac{1}{2}} \, \mathrm{Y}_l^{m+\frac{1}{2}}(\theta,\varphi) \end{pmatrix} \; . \end{aligned}$$

The $\mathcal{Y}_l^{j=l\pm\frac{1}{2},m}$ are simultaneous eigenfunctions of $\hat{\underline{L}}^2, \hat{\underline{S}}^2, \hat{\underline{J}}^2$ and $\hat{J}_z$. As a consequence, they are also eigenfunctions of $\hat{\underline{L}}^2 \cdot \hat{\underline{S}}^2$ since $\hat{\underline{L}} \cdot \hat{\underline{S}} = \frac{1}{2}\left(\hat{\underline{J}}^2 - \hat{\underline{L}}^2 - \hat{\underline{S}}^2\right)$. ($\rightarrow \hat{\underline{J}}$ is a good quantum number as we have spin-orbit coupling $\hat{\underline{L}} \cdot \hat{\underline{S}}$ in the Hamiltonian). The eigenvalues of $\hat{\underline{L}} \cdot \hat{\underline{S}}$ are

$$\frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - \underbrace{s(s+1)}_{3/4}\right] = \begin{cases} \frac{l\hbar^2}{2} & \text{for } j = l + \frac{1}{2} \\ -\frac{(l+1)^2\hbar^2}{2} & \text{for } j = l - \frac{1}{2} \end{cases} \; .$$

4 Identical Particles

Due to the Heisenberg uncertainty principle, it is not possible to keep track of individual particles:

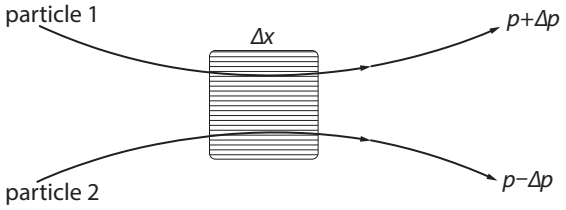

Figure 4.1: If the spacial resolution is good enough to differentiate the particles then we cannot say which one goes up and down after the scattering, due to momentum uncertainty. If the momentum resolution is good enough then we cannot track the particle in the marked region due to the position uncertainty.

When they perform a scattering process and come close to each other, $\Delta x_i \, \Delta p_i \geq \hbar/2$ tells us that we don't know the particle's locations well enough to keep them apart, and/or know their momenta well enough to predict where they will go.
To describe a two-particle system in ket-space, we use a direct product $|k'\rangle \otimes |k''\rangle$ or short $|k'\rangle|k''\rangle$. Since particles are indistinguishable, $|k''\rangle|k'\rangle$ has to classify the same state, and all kets

$$c_1|k'\rangle|k''\rangle + c_2|k''\rangle|k'\rangle$$

have to be considered. To derive c_1 and c_2, we define the permutation operator

$$\hat{P}_{12}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle \ .$$

We have $\hat{P}_{12} = \hat{P}_{21}$ and $(\hat{P}_{12})^2 = \mathbb{1}$. We now introduce observables $\hat{A}_1$ and $\hat{A}_2$ representing the state of particle 1 or particle 2. Examples are the spins $\underline{\hat{S}}_1$ or $\underline{\hat{S}}_2$.

$$\hat{A}_1|a'\rangle|a''\rangle = a'|a'\rangle|a''\rangle$$
$$\hat{A}_2|a'\rangle|a''\rangle = a''|a'\rangle|a''\rangle$$

From the first equation, we obtain by application of $\hat{P}_{12}$ and insertion of $\mathbb{1} = \hat{P}_{12}^{-1}\hat{P}_{12}$

$$\begin{aligned}\hat{P}_{12}\hat{A}_1|a'\rangle|a''\rangle &= a'\hat{P}_{12}|a'\rangle|a''\rangle = a'|a''\rangle|a'\rangle \\ &= \hat{P}_{12}\hat{A}_1\hat{P}_{12}^{-1}\hat{P}_{12}|a'\rangle|a''\rangle = \hat{P}_{12}\hat{A}_1\hat{P}_{12}^{-1}|a''\rangle|a'\rangle \ .\end{aligned}$$

This is consistent with the eigenvalue equation for $\hat{A}_2$ only if $\hat{P}_{12}\hat{A}_1\hat{P}_{12}^{-1} = \hat{A}_2$.
The Hamiltonian of two interacting identical particles is given by

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + V_{\text{pair}}(|\underline{\hat{x}}_1 - \underline{\hat{x}}_2|) + V_{\text{ext}}(\underline{\hat{x}}_1) + V_{\text{ext}}(\underline{\hat{x}}_2) \ .$$

We find $\hat{P}_{12}\hat{H}\hat{P}_{12}^{-1} = \hat{H} \Rightarrow [\hat{P}_{12}\,,\,\hat{H}] = 0$. As a consequence of the Heisenberg equation of motion, $\hat{P}_{12}$ is a constant of motion. Because $\hat{P}_{12}^2 = \mathbb{1}$, the allowed eigenvalues are ± 1. $\Rightarrow$ If

the two particle state ket is anti-symmetric or symmetric initially, it will remain so at all times. The eigenstates of $\hat{P}_{12}$ are

$$|k'k''\rangle_+ \equiv \frac{1}{\sqrt{2}}\left[|k'\rangle|k''\rangle + |k''\rangle|k'\rangle\right]$$
$$|k'k''\rangle_- \equiv \frac{1}{\sqrt{2}}\left[|k'\rangle|k''\rangle - |k''\rangle|k'\rangle\right] \ .$$

In addition we can define symmetrizer and anti-symmetrizer

$$\hat{S}_{12} \equiv \frac{1}{2}\left[1 + \hat{P}_{12}\right]$$
$$\hat{A}_{12} \equiv \frac{1}{2}\left[1 - \hat{P}_{12}\right] \ .$$

Applying this operators to an arbitrary two-particle state yields

$$\left.\begin{matrix}\hat{S}_{12}\\ \hat{A}_{12}\end{matrix}\right\}\left[c_1|k'\rangle|k''\rangle + c_2|k''\rangle|k'\rangle\right] = \frac{1}{2}\left[c_1|k'\rangle|k''\rangle + c_2|k''\rangle|k'\rangle\right] \pm \frac{1}{2}\left[c_1|k''\rangle|k'\rangle + c_2|k'\rangle|k''\rangle\right]$$
$$= \frac{c_1 \pm c_2}{2}\left[|k'\rangle|k''\rangle \pm |k''\rangle|k'\rangle\right] \ .$$

4.1 Symmetrization Postulate

We describe interchange of particles by a π-rotation of one particle around the other (followed by a translation).

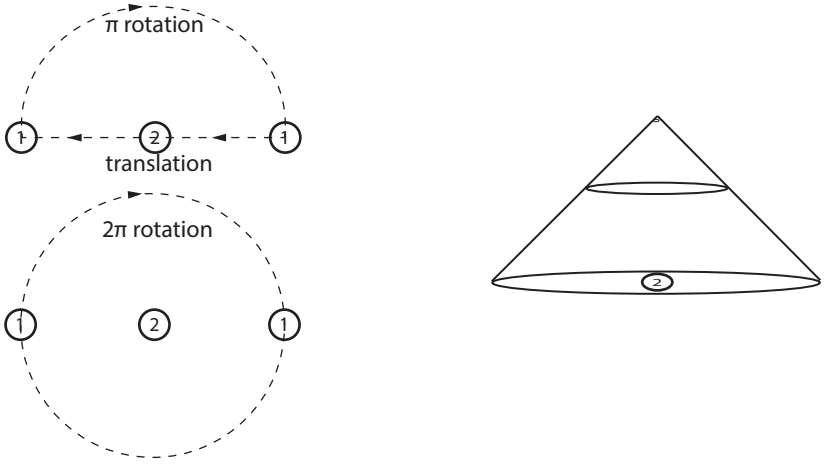

Figure 4.2: π-rotation and translation (we often consider translational invariant systems) as a way to describe interchanging the particles; 2π rotation is identity in three dimensions

In three spacial dimension the loop corresponding to the two-fold interchange of two particles can be contracted to a point, i.e. it is topological equivalent to the identity operation. $\Rightarrow$ Physical interchanging particles can be identified with the action of $\hat{P}_{12}$ with $\hat{P}_{12}^2 = \mathbb{1}$.
The indistinguishability of quantum particles makes it plausible that many particle states should

be eigenstates of $\hat{P}_{12}$, and due to $\hat{P}_{12}^2 = \mathbb{1}$ there are only two possibilities:

$$\hat{P}_{ij}|N \text{ identical bosons}\rangle = +|N \text{ identical bosons}\rangle$$
$$\hat{P}_{ij}|N \text{ identical fermions}\rangle = -|N \text{ identical fermions}\rangle \ .$$

Particles whose wave function is symmetric under exchange are called *bosons*, particles with an anti-symmetric wave function are called *fermions*.

Note:
If the motion of particles is restricted to two spatial dimension, a two-fold exchange is no longer equivalent to the identity. This gives the possibility for

$$|\underline{r}_1, \underline{r}_2\rangle = e^{\pm i\theta}|\underline{r}_2, \underline{r}_1\rangle \text{ with } \theta \neq \{0, \pi\} \ .$$

Particles satisfying such generalized statistics are called *anyons* and are believed to exist in the fractional quantum Hall state.

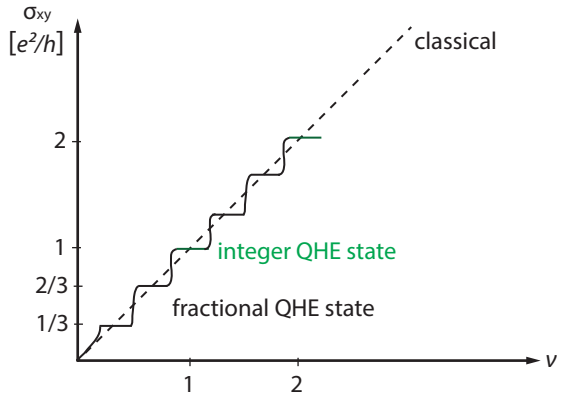

Figure 4.3: The Hall conductivity in the QHE state is quantized $\sigma_{xy} = \nu\frac{e^2}{\hbar}$ where $\nu \approx \frac{p}{2q+1}$, $p, q \in \mathbb{N}$ is the filling fraction (for $\nu = 1$ all states in each Landau level are filled, and e.g. $\nu = 1/3$ says that $1/3$ of the states in the Landau level are filled). Classically we have $\sigma_{xy} = \nu\frac{e^2}{h} = \frac{2\pi n\hbar}{eB}\frac{e^2}{h} = \frac{ne}{B}$ where we used that ν is here the electron density divided by the number of the places in the Landau level $\nu = \frac{n}{1/(2\pi l_B^2)}$. The quasi-particles are anyons with charge $\frac{1}{2q+1}\,e$ which is a fraction of the elementary charge.

In addition there exists an even more exotic possibility of non-Abelian exchange statistics. In the presence of N quasi-particles ($N \in 2\mathbb{N}$), the ground state has a 2^n-fold degeneracy for fixed particle positions (we do not mean the translational degeneracy), i.e. there are (for $N = 4$) 4 different ground state wave functions with energy E_0 where $E_i \geq E_0 + \Delta$ with excitation gap Δ:

$$\begin{aligned}
\varphi_1(R_1, R_2, R_3, R_4) \ &, \ \hat{H}\varphi_1 = E_0\varphi_1 \\
\varphi_2(R_1, R_2, R_3, R_4) \ &, \ \hat{H}\varphi_2 = E_0\varphi_2 \\
\varphi_3(R_1, R_2, R_3, R_4) \ &, \ \hat{H}\varphi_3 = E_0\varphi_3 \\
\varphi_4(R_1, R_2, R_3, R_4) \ &, \ \hat{H}\varphi_4 = E_0\varphi_4 \ .
\end{aligned}$$

The exchange of two particles corresponds to unitary operations in the 4-dimensional ground state sector of the Hilbert space.

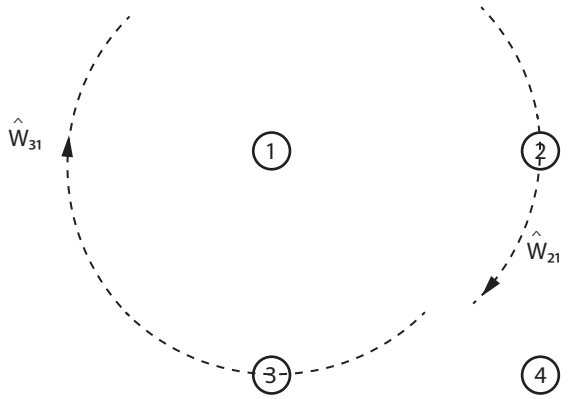

Figure 4.4: Rotations/interchanges $\hat{W}_{32}, \hat{W}_{21}$ of the particles in the ground state space with wave functions $\varphi = c_1\varphi_1 + c_2\varphi_2 + c_3\varphi_3 + c_4\varphi_4$ interpreted as 4×4 matrix actions $W_{3,1}, W_{2,1}$ on $\underline{\varphi} = (c_1, c_2, c_3, c_4)$

The unitary transformations $\hat{W}_{32}, \hat{W}_{21}$ can be represented as 4×4 unitary matrices $W_{3,1}, W_{2,1}$. Since in general matrix multiplication is non-commutative (matrices form a non-Abelian group), such particles are called *non-Abelian anyons*. The transformations $\hat{W}_{31}$ and $\hat{W}_{21}$ are topological in nature ("topological protected") since they do not depend on the detail of the particular path but only on its topology ("which particle goes around which other particle"). Non-Abelian anyons are believed to be realized in the fractional quantum Hall state at $\nu = \frac{5}{2}$ and in superconductor-semiconductor-heterostructures with strong spin orbit coupling.

Back to fermions and bosons: there exists a remarkable connection between the spin and the statistics of particles. Half-integer-spin particles are fermions and integer-spin particles are bosons.
In this context, particles can be composites: a ^{3}He nucleus is a fermion in the same way as a electron e^- or a proton is, and a ^{4}He nucleus is a boson such as a photon, the π-meson or the Z^0 gauge boson. The *spin-statistics theorem* is believed to be an exact law of nature with no known exceptions. In relativistic quantum field theory it can be proved that half-integer-spin particles cannot be bosons and that integer-spin particles cannot be fermions.
A consequence of fermionic statistics is the Pauli exclusion principle: two electrons (fermions) cannot occupy the same quantum state. This follows because a state like $|k'\rangle|k'\rangle$ is automatically symmetric, which is not possible for fermions.
The important difference between fermions, bosons and "classical" particles can be illustrated by considering two free particles which occupy states $|k'\rangle, |k''\rangle$:

- Fermions: $\frac{1}{\sqrt{2}}\left(|k'\rangle|k''\rangle - |k''\rangle|k'\rangle\right)$
- Bosons: $|k'\rangle|k'\rangle$, $|k''\rangle|k''\rangle$ or $\frac{1}{\sqrt{2}}\left(|k'\rangle|k''\rangle + |k''\rangle|k'\rangle\right)$
- "Classical:" $|k'\rangle|k'\rangle$, $|k''\rangle|k''\rangle$, $|k'\rangle|k''\rangle$, $|k''\rangle|k'\rangle$
  (Entropy of classical particles is not extensive)

4.2 Two Electron System

We specify base kets and bras by $\underline{x}_1, \underline{x}_2$, and the spin quantum numbers m_{s_1}, and m_{s_2} such that

$$\Psi = \sum_{m_{s_1}, m_{s_2}} C(m_{s_1}, m_{s_2}) \, \langle \underline{x}_1, m_{s_1}; \underline{x}_2, m_{s_2} | \alpha \rangle \ .$$

If the Hamiltonian commutes with $\hat{\underline{S}}^2_{\rm tot}$ with $\hat{\underline{S}}_{\rm tot} = \hat{\underline{S}}_1 + \hat{\underline{S}}_2$, i.e. $[\hat{\underline{S}}^2_{\rm tot} \, , \, \hat{H}] = 0$, energy eigenstates can be chosen as eigenstates of $\hat{\underline{S}}^2_{\rm tot}$, and if expressed as $\Psi = \phi(\underline{x}_1, \underline{x}_2)\chi(m_{s_1}, m_{s_2})$, the spin function χ is one of the following possibilities

$$\chi(m_{s_1}, m_{s_2}) = \begin{cases} \left.\begin{array}{l} \chi_{++} \\ \frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+}) \\ \chi_{--} \end{array}\right\} & \text{triplet (sym.) } S_{\rm tot} = 1 \\ \left.\begin{array}{l} \frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+}) \end{array}\right\} & \text{singlet (anti-sym.) } S_{\rm tot} = 0 \end{cases}$$

Here $\chi_{+-} = \delta_{m_{s_1}, \frac{1}{2}} \delta_{m_{s_2}, -\frac{1}{2}}$, and so on. Fermi-Dirac statistics for the electrons require

$$\langle \underline{x}_1, m_{s_1}; \underline{x}_2, m_{s_2} | \alpha \rangle = - \langle \underline{x}_2, m_{s_2}; \underline{x}_1, m_{s_1} | \alpha \rangle \ .$$

We decompose the permutation operator $\hat{P}_{12}$ according to $\hat{P}^{(\rm space)}_{12} \hat{P}^{(\rm spin)}_{12}$, interchanging the position and the spin coordinates, respectively. We can express $\hat{P}^{(\rm spin)}_{12}$ as

$$\hat{P}^{(\rm spin)}_{12} = \frac{1}{2} \left(1 + \frac{4}{\hbar^2} \, \hat{\underline{S}}_1 \cdot \hat{\underline{S}}_2 \right) ,$$

due to

$$\hat{\underline{S}}_1 \cdot \hat{\underline{S}}_2 = \begin{cases} \hbar^2/4 & \text{triplet} \\ -3\hbar^2/4 & \text{singlet} \end{cases} \Longrightarrow \begin{array}{l} \hat{P}^{(\rm spin)}_{12} |\text{triplet}\rangle = (+1)|\text{triplet}\rangle \\ \hat{P}^{(\rm spin)}_{12} |\text{singlet}\rangle = (-1)|\text{single}\rangle \end{array} \ .$$

Using this decomposition, the transformation $|\alpha\rangle \mapsto \hat{P}_{12}|\alpha\rangle$ gives rise to

$$\phi(\underline{x}_1, \underline{x}_2) \overset{\hat{P}_{12}}{\longmapsto} \phi(\underline{x}_2, \underline{x}_1) \text{ and } \chi(m_{s_1}, m_{s_2}) \overset{\hat{P}_{12}}{\longmapsto} \chi(m_{s_2}, m_{s_1}) \ .$$

$\Rightarrow$ If the space part of the wave function is symmetrical (anti-symmetrical), then the spin part must be anti-symmetrical (symmetrical). $\Rightarrow$ The spin triplet part has to be combined with an anti-symmetrical space part, the spin singlet part has to be combined with a symmetrical space part.
The probability for finding electron 1 within a volume element d^3x_1 around position $\underline{x}_1$, and electron 2 within a volume element d^3x_2 around $\underline{x}_2$ is $|\phi(\underline{x}_1, \underline{x}_2)|^2 \mathrm{d}^3x_1 \mathrm{d}^3x_2$.
What influence does the statistics of particles have on observable quantities? If the interaction of particles is not important, and in the absence of a Zeeman field, the Schrödinger equation is given by

$$\left[-\frac{\hbar^2}{2m} \nabla^2_1 - \frac{\hbar^2}{2m} \nabla^2_1 + V_{\rm ext}(\underline{x}_1) + V_{\rm ext}(\underline{x}_2) \right] \Psi(\underline{x}_1, \underline{x}_2) = E \Psi(\underline{x}_1, \underline{x}_2) \ .$$

The spatial part of the wave function $\Psi(\underline{x}_1, \underline{x}_2)$ is now separable into the form $\omega_A(\underline{x}_1)\omega_B(\underline{x}_2)$. Since $\hat{\underline{S}}^2_{\rm tot}$ trivially commutes with the Hamiltonian, we can choose the spin part of the wave

function to be an eigenstate of the total spin $\hat{\underline{S}}_{\text{tot}}$, i.e. a singlet or triplet state, which both have a definite symmetry property under $\hat{P}_{12}^{(\text{spin})}$. Accordingly, the space part must be a symmetrical or anti-symmetrical combination

$$\phi(\underline{x}_1, \underline{x}_2) = \frac{1}{\sqrt{2}} \left[\omega_A(\underline{x}_1)\omega_B(\underline{x}_2) \pm \omega_A(\underline{x}_2)\omega_B(\underline{x}_1)\right]$$

where the upper sign applies for the spin singlet, and the lower sign for the triplet.
The probability for observing the two electrons around $\underline{x}_1$ and $\underline{x}_2$ is given by

$$|\phi(\underline{x}_1, \underline{x}_2)|^2 = \frac{1}{2}\Big\{ |\omega_A(\underline{x}_1)|^2|\omega_B(\underline{x}_2)|^2 + |\omega_A(\underline{x}_2)|^2|\omega_B(\underline{x}_1)|^2 \pm \underbrace{2\text{Re}\Big[\omega_A(\underline{x}_1)\omega_B(\underline{x}_2)\omega_A^*(\underline{x}_2)\omega_B^*(\underline{x}_1)\Big]}_{\substack{\text{"Exchange density" due to the} \\ \text{exchange of coordinates } \underline{x}_1 \text{ and } \underline{x}_2 \\ \text{in } \omega_A \text{ and } \omega_A^*,\ \omega_B \text{ and } \omega_B^*}} \Big\}$$

For electrons in a spin triplet state, the probability of finding both electrons in the same point in space $\underline{x}_1 = \underline{x}_2$ vanishes. Electrons in a spin triplet state tend to avoid each other. However, when the two electrons are in a singlet state, there is an enhanced probability of finding the electrons at the same point in space.
Remark:
If ω_A and ω_B are non-zero only in spatially well separated regions, there is no need to (anti-) symmetrize the wave function, as the exchange density vanishes.

4.3 The Helium Atom

The Hamiltonian for two electrons moving in the Coulomb field of two protons is given by

$$\hat{H} = \frac{\hat{\underline{p}}_1^2}{2m} + \frac{\hat{\underline{p}}_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

with $r_1 \equiv |\underline{x}_1|$, $r_2 \equiv |\underline{x}_2|$ and $r_{12} \equiv |\underline{x}_1 - \underline{x}_2|$ where the positive nucleus has the charge $2e$ and is located at (0,0,0).

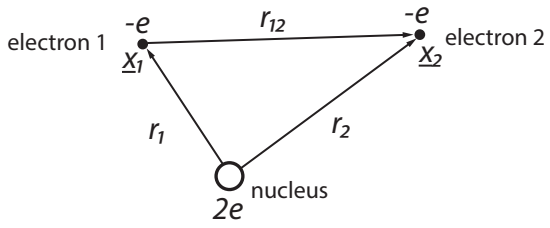

Figure 4.5: Definitions of quantities for the helium atom

We first assume that the e^2/r_{12} term is absent. Then the wave functions would just be the product of two hydrogen wave functions with $Z = 1$ changed into $Z = 2$. $\hat{\underline{S}}_{\text{tot}}^2$ commutes with $\hat{H}$, so we choose the spin state to be either singlet or triplet. We consider the case where one electron is in the ground state, and the other one in an excited state with quantum numbers (n, l, m)

$$\Rightarrow \phi(\underline{x}_1, \underline{x}_2) = \frac{1}{\sqrt{2}} \left[\Psi_{100}(\underline{x}_1)\Psi_{nlm}(\underline{x}_2) \pm \Psi_{100}(\underline{x}_2)\Psi_{nlm}(\underline{x}_1)\right] \ . \qquad (*)$$

For the ground state, both electrons are in the state $n = 1, l = 0$. $\Rightarrow$ The space function is necessarily symmetrical, and only the spin singlet wave function is allowed:

$$\Psi_{100}(\underline{x}_1)\Psi_{100}(\underline{x}_2)\chi_{\text{singlet}} = \frac{Z^3}{\pi a_0^3}\,\mathrm{e}^{-Z(r_1+r_2)/a_0}\chi_{\text{singlet}} \quad \text{with } Z = 2.$$

The energy of this "unperturbed" wave function is

$$E = 2 \cdot \underbrace{4}_{Z^2} \cdot \left(-\frac{e^2}{2a_0}\right) = -108.8\text{eV}\,,$$

about 30% larger than the experimental value: $E_{\text{exp}} = -78.8\text{eV}$ since we neglected e^2/r_{12}.
We now treat the Coulomb interaction between the electons in first order perturbation theory, i.e. we compute the expectation value of e^2/r_{12} with regards to the wave function (*). In this way, one finds the energy shift

$$\Delta_{(1s)^2} = \langle\frac{e^2}{r_{12}}\rangle_{(1s)^2} = \iint \underbrace{\frac{Z^6}{\pi^2 a_0^6}\,\mathrm{e}^{-\frac{2Z(r_1+r_2)}{a_0}}}_{\Psi_{100}(\underline{x}_1)\Psi_{100}(\underline{x}_2)} \frac{e^2}{r_{12}}\,\mathrm{d}^2x_1\mathrm{d}^2x_2\,.$$

The term under the integral can be understood as interaction of different charge densities $\varrho_C(\underline{x}_1)\varrho_C(\underline{x}_2)/r_{12}$ (but electrons in the "charge clouds" are not interacting).

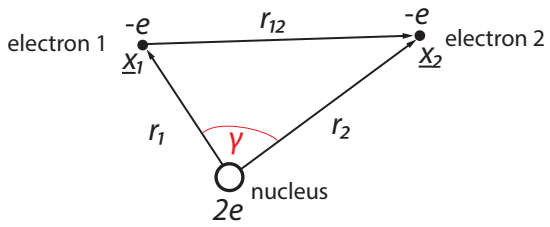

Figure 4.6: Definitions of the angle and the distances

A useful coordinate system to calculate the integral uses the angle γ between $\underline{x}_1$ and $\underline{x}_2$, and $\underline{x}_1 \cdot \underline{x}_2 = r_1 r_2 \cos\gamma$ to obtain

$$r_{12} = |\underline{x}_1 - \underline{x}_2| = \sqrt{(\underline{x}_1 - \underline{x}_2)^2} = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\gamma}\,.$$

Denoting $r_< = \min\{r_1, r_2\}$ and $r_> = \max\{r_1, r_2\}$ we can write

$$\begin{aligned} r_{12} &= r_>\sqrt{1 - 2\frac{r_<}{r_>}\cos\gamma + \left(\frac{r_<}{r_>}\right)^2} \\ \Rightarrow \frac{1}{r_{12}} &= \frac{1}{r_>}\frac{1}{\sqrt{1 - 2\frac{r_<}{r_>}\cos\gamma + \left(\frac{r_<}{r_>}\right)^2}}\,. \end{aligned}$$

Comparison with the generating function of the Legendre polynomials $\frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x)t^n$ yields

$$\Rightarrow \frac{1}{r_{12}} = \sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}\,P_l(\cos\gamma)\,.$$

To perform the angular integration, it is useful to use the addition theorem for spherical harmonics

$$P_l(\cos\gamma) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} \mathrm{Y}_l^{m*}(\theta_1,\phi_1)\mathrm{Y}_l^m(\theta_2,\phi_2)\,.$$

Interpret the "constant factor" in the integral as $\mathrm{Y}_0^0 = \frac{1}{\sqrt{4\pi}}$. Due to the orthogonality between spherical harmonics, the angular integration is straight forward

$$\int \mathrm{Y}_l^m(\theta_i,\phi_i)\mathrm{d}\Omega_i = \sqrt{4\pi}\int \frac{1}{\sqrt{4\pi}}\mathrm{Y}_l^m(\theta_i,\phi_i)\mathrm{d}\Omega_i = \sqrt{4\pi}\delta_{l,0}\delta_{m,0}\,.$$

The radial integration is elementary but tedious, it leads to

$$\int_0^\infty \left[\int_0^{r_1} \frac{1}{r_1}\,\mathrm{e}^{-\frac{2Z}{a_0}(r_1+r_2)} r_2^2\mathrm{d}r_2 + \int_{r_1}^\infty \frac{1}{r_1}\mathrm{e}^{-\frac{2Z}{a_0}(r_1+r_2)} r_2^2\mathrm{d}r_2\right] r_1^2\mathrm{d}r_1 = \frac{5}{128}\,\frac{a_0^5}{Z^5}\,.$$

Combining everything, we obtain for $Z = 2$:

$$\Delta_{(1s)^2} = \underbrace{\frac{Z^6e^2}{\pi^2 a_0^6}}_{\text{Normalization}} \underbrace{4\pi}_{Ad.Th.} \underbrace{(\sqrt{4\pi})^2}_{1/\mathrm{Y}_0^0} \underbrace{\frac{5}{128}\frac{a_0^5}{Z^5}}_{\text{Radial integral}} = \frac{5}{2}\frac{e^2}{2a_0}\,.$$

Adding this energy shift to the zeroth order energy, we find

$$E_{\text{calc.}} = \left(-8+\frac{5}{2}\right)\frac{e^2}{2a_0} \approx -74.8\text{eV}\,.$$

However, we can do even better when treating the nuclear charge Z in the wave function as a variational parameter, i.e. use the wave function

$$\langle \underline{x}_1, \underline{x}_2|\widetilde{0}\rangle = \left(\frac{Z_{\text{eff}}^3}{\pi a_0^3}\right)\mathrm{e}^{-Z_{\text{eff}}(r_1+r_2)/a_0}$$

to compute the expectation value of the Hamiltonian and then minimizing with regards to Z_{eff}. This is the Ritz variation method.

$$\langle\hat{H}\rangle = \langle\widetilde{0}|\frac{\hat{p}_1^2}{2m}+\frac{\hat{p}_2^2}{2m}|\widetilde{0}\rangle - \langle\widetilde{0}|\frac{Ze^2}{r_1}+\frac{Ze^2}{r_2}|\widetilde{0}\rangle + \langle\widetilde{0}|\frac{e^2}{r_{12}}|\widetilde{0}\rangle$$

where we have to distinguish Z in the Hamiltonian from Z_{eff} in the wave function. We can write $\frac{Z}{Z_{\text{eff}}}\langle\widetilde{0}|\frac{Z_{\text{eff}}e^2}{r_1}+\frac{Z_{\text{eff}}e^2}{r_2}|\widetilde{0}\rangle$ to make use of the assumed eigenfunction. One finds in the end

$$\langle\hat{H}\rangle = \left(2\frac{Z_{\text{eff}}^2}{2} - 2ZZ_{\text{eff}} + \frac{5}{8}Z_{\text{eff}}\right)\frac{e^2}{a_0}$$

with the minimum found for $Z_{\text{eff}} = 2-\frac{5}{16} = 1.6875$ which is smaller than Z as expected from the argument that one electron partially "screens" the nuclear charge seen by the other electron. Using $Z_{\text{eff}} = 2-\frac{5}{16}$, we find for the energy $E_{\text{cal}} = -77.5\text{eV}$, already quite close to $E_{\text{exp}} = -78.8\text{eV}$, given the crudeness of the trial wave function. [A. Unsöld, Ann. Phys. **82**, 355 (1927)]

For the discussion of excited states, we consider symmetrized wave functions with the building block (1s)(nl), and write the energy of such states as

$$E_{n,l,\pm} = E_{100} + E_{nlm} + \Delta E_{\pm} \text{ with } \Delta E_{\pm} = I_{n,l} \pm J_{n,l} \ .$$

In first-order perturbation theory, ΔE is obtained by evaluating the expectation value of $\frac{e^2}{r_{12}}$, which we can decompose according to

$$\langle \frac{e^2}{r_{12}} \rangle = I_{n,l} \pm J_{n,l},$$

where I and J are called Coulomb integral and exchange integral, respectively. The upper (lower) sign goes with the singlet (triplet) state. I and J are given by

$$I = \int \mathrm{d}^3\underline{x}_1 \mathrm{d}^3\underline{x}_2 |\Psi_{100}(\underline{x}_1)|^2 |\Psi_{nlm}(\underline{x}_2)|^2 \frac{e^2}{r_{12}}$$

where we can think of $|\Psi_{100}(\underline{x}_1)|^2 = \varrho_{100}(\underline{x}_1)$ and $|\Psi_{nlm}(\underline{x}_2)|^2 = \varrho_{nlm}(\underline{x}_2)$ as charge densities, and

$$J = \int \mathrm{d}^3\underline{x}_1 \mathrm{d}^3\underline{x}_2 \Psi_{100}(\underline{x}_1)\Psi_{nlm}(\underline{x}_2) \frac{e^2}{r_{12}} \Psi^*_{100}(\underline{x}_2)\Psi^*_{nlm}(\underline{x}_1)$$

which cannot be interpreted using charge densities, its due to the exchange statistics. Obviously I is non-negative, and it can be shown that J is non-negative as well.
$\Rightarrow$ For the same configuration of orbitals the spin singlet states lies energetically higher than the triplet state.

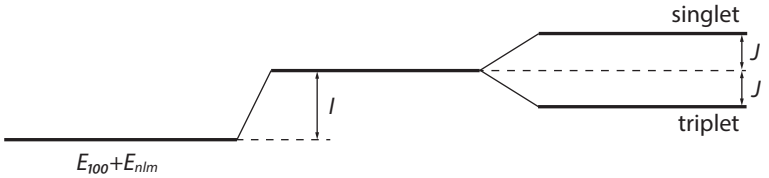

Figure 4.7: Shift of the unperturbed energy states by the exchange and Coulomb integral

In the singlet case, the space wave function is symmetrical and the electrons can get close to each other $\Rightarrow$ have a strong mutual Coulomb repulsion $\Rightarrow$ high energy.
In the triplet case, the space wave function is anti-symmetrical, and the electrons avoid each other $\Rightarrow$ have a weaker Coulomb repulsion $\Rightarrow$ smaller energy.
Helium in the singlet state is known as para-helium, helium in the triplet state is known as ortho-helium. Although the original Hamiltonian was spin-independent without an explicit $\hat{\underline{S}}_1 \cdot \hat{\underline{S}}_2$-term, the electrons with parallel spins have lower energy due to the effects of Fermi-Dirac statistics.
The explanation of the apparent spin dependence of the helium energy levels is due to Heisenberg. Along similar lies, Heisenberg could explain the occurrence of ferromagnetism in solids. Electrons with parallel spins avoid each other spatially and heave a lower energy for this reason.

4.4 Multiparticle States

We now define the action of the permutation operator for states with N identical particles

$$\hat{P}_{ij} = |k'\rangle|k''\rangle\cdots|k^i\rangle\cdots|k^j\rangle\cdots = |k'\rangle|k''\rangle\cdots|k^j\rangle|k^{i+1}\rangle\cdots|k^i\rangle\cdots \ .$$

We still have $\hat{P}_{ij}^2 = 1$ as before, such that the allowed eigenvalues are ± 1. In general, $[\hat{P}_{ij}\ ,\ \hat{P}_{kl}] \neq 0$.
We work out explicitly the example of three identical particles: There are $3! = 6$ possible kets of the form $|k'\rangle|k''\rangle|k'''\rangle$, where k', k'', and k''' are all different from each other. However, there is only one totally symmetrical (+), and one totally anti-symmetrical (-) linear combination

$$|k'k''k'''\rangle_\pm = \frac{1}{\sqrt{6}}\Big\{|k'\rangle|k''\rangle|k'''\rangle \pm |k''\rangle|k'\rangle|k'''\rangle + |k''\rangle|k'''\rangle|k'\rangle \pm |k'''\rangle|k''\rangle|k'\rangle + |k'''\rangle|k'\rangle|k''\rangle \pm |k'\rangle|k'''\rangle|k''\rangle\Big\}$$

which are simultaneous eigenkets of $\hat{P}_{12}, \hat{P}_{13}$, and $\hat{P}_{23}$. It follows that there are four independent kets which are neither totally symmetrical nor totally anti-symmetrical (six ways to choose the $\pm$ but only all $+$ is symmetrical and all $-$ is anti-symmetrical). So far we assumed that k', k'', and k''' are all different from each other. When two coincide, we can only form a totally symmetrical state

$$|k'k'k''\rangle_+ = \frac{1}{\sqrt{3}}\left\{|k'\rangle|k'\rangle|k''\rangle + |k'\rangle|k''\rangle|k'\rangle + |k''\rangle|k'\rangle|k'\rangle\right\}$$

where the normalization factor can be interpreted as $\sqrt{\frac{2!}{3!}}$. In a more general case, the normalization factor is $\sqrt{\frac{N_1!N_2!\cdots N_n!}{N!}}$ where N is the total number of particles, and N_i is the number of times $|k^i\rangle$ occurs.

4.4.1 Second Quantization

Second quantization is a different approach to keeping track of multi-particle states, which is also the foundation of quantum field theory. Historically the term was coined to describe the idea that the wave function of single-particle quantum mechanics is turned into an operator, which is subject to its own canonical quantization, such that the quantization rule is enforced a second time. However, "second quantization" is completely equivalent to solving the many particle Schrödinger equation (but allows for powerful approximation to be found). We define a multi-particle state vector as $|n_1, n_2, ..., n_i, ...\rangle$, where n_i defines the number of particles with eigenvalue k_i for some operator. Such state vectors are element of a new typ of vector space, called Fock-space, which has the necessary permutation symmetry built in.
We begin by describing two special cases of states in Fock-space, the first of which is $|0, ..., 0\rangle \equiv |0\rangle$, which does not contain any particles and is called "vacuum". The second special case is $|0, ..., 0, n_i = 1, 0, ...\rangle = |k_i\rangle$, which has exactly one particle in the state with eigenvalue k_i.
We now need to build multi-particle states in such a way that permutation symmetry is respected. It turns out that the creation and annihilation (ladder) operators as defined for the harmonic oscillator are the right tool for this. We define a "field operator" $\hat{a}_i^\dagger$ that increases the number of particles in the state with eigenvalue k_i by one, i.e.

$$\hat{a}_i^\dagger|n_1, ..., n_i, ...\rangle \propto |n_1, ..., n_i + 1, ...\rangle,$$

where the correct normalization will be determined later. We postulate that applying a particle creation operator $\hat{a}_i^\dagger$ to the vacuum creates a properly normalized single-particle state $\hat{a}_i^\dagger|0\rangle = |k_i\rangle$ (and $\langle 0|\hat{a}_i = \langle k_i|$).

$$1 = \langle k_i|k_i\rangle = (\langle 0|\hat{a}_i)(\hat{a}_i^\dagger|0\rangle) = \langle 0|\hat{a}_i\hat{a}_i^\dagger|0\rangle = \langle 0|\underbrace{\hat{a}_i|k_i\rangle}_{|0\rangle}$$

We see that $\hat{a}_i|k\rangle_i = |0\rangle$, so that $\hat{a}_i$ is a particle annihilation operator.

$$\hat{a}_i|n_1, ..., n_i, ...\rangle \propto |n_1, ..., n_i - 1, ...\rangle$$

with $\hat{a}_i|0\rangle = 0$ and $\hat{a}_i|k_j\rangle = \delta_{ij}|0\rangle$. These postulates almost fully define the field operator, but do not incorporate permutation symmetry yet. For discussing permutation symmetry, we create a two-particle state by applying two creation operators and demand

$$|k^i k^j\rangle = \hat{a}_i^\dagger\hat{a}_j^\dagger|0\rangle = \pm\hat{a}_j^\dagger\hat{a}_i^\dagger|0\rangle = |k^j k^i\rangle \ .$$

Here, the + (−) sign applies for bosons (fermions). Using the same logic for the application of two creation operators to a general multi-particle states leads to

$$\hat{a}_i^\dagger\hat{a}_j^\dagger - \hat{a}_j^\dagger\hat{a}_i^\dagger = 0 = [\hat{a}_i^\dagger\ ,\ \hat{a}_j^\dagger] \qquad \text{(bosons)}$$
$$\hat{a}_i^\dagger\hat{a}_j^\dagger + \hat{a}_j^\dagger\hat{a}_i^\dagger = 0 = \{\hat{a}_i^\dagger\ ,\ \hat{a}_j^\dagger\}\ . \qquad \text{(fermions *)}$$

Taking the adjoint of the relations yields

$$0 = [\hat{a}_i\ ,\ \hat{a}_j] \qquad \text{(bosons)}$$
$$0 = \{\hat{a}_i\ ,\ \hat{a}_j\} \qquad \text{(fermions)}$$

We note that the Pauli exclusion principle is incorporated into this formalism since (*) implies $\hat{a}_i^\dagger\hat{a}_i^\dagger = 0$.
What are the commutation rules between $\hat{a}_i$ and $\hat{a}_i^\dagger$? We would like to define a number operator $\hat{N}_i = \hat{a}_i^\dagger\hat{a}_i$ counting the number of particles in single-particle state $|k_i\rangle$. From working with the harmonic oscillator, we know that this is possible when $[\hat{a}_i\ ,\ \hat{a}_i^\dagger] = 1$. We claim that a self-consistent picture for both bosons and fermions can be built this way, replacing the commutator with the anti-commutator for fermions:

$$\delta_{ij} = [\hat{a}_i\ ,\ \hat{a}_j^\dagger] \qquad \text{(bosons)}$$
$$\delta_{ij} = \{\hat{a}_i\ ,\ \hat{a}_j^\dagger\}\ . \qquad \text{(fermions)}$$

$\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i$ is the number of particles in state $\hat{k}_i$, and $\hat{N} = \sum_i \hat{a}_i^\dagger\hat{a}_i$ the total number of particles in the system.

4.4.1.1 Single Particle Operators in Second Quantization

We assume that the single-particle states $|k_i\rangle$ are eigenstates of an "additive" single particle operator $\hat{K} = \sum_{j=1}^N \hat{k}_j$, e.g. momentum or kinetic energy.
For a multi-particle state $|\Psi\rangle = |n_1, n_2, ..., n_i, ...\rangle$, we expect the eigenvalue of $\hat{K}$ to be $\sum_i n_i k_i$

where the sum is over states in the single particle Hilbert space (not over particles). This can be easily accomplished when using

$$\hat{\mathcal{K}} = \sum_i k_i \hat{N}_i = \sum_i k_i \hat{a}_i^\dagger \hat{a}_i \ .$$

If needed, this can be transformed to a different basis.

- Tight binding Hamiltonian

$$\hat{H} = \sum_{\underline{k}} \varepsilon(\underline{k}) \hat{a}_{\underline{k}}^\dagger \hat{a}_{\underline{k}} \qquad (**)$$

from $|n\rangle = \sum_l \mathrm{e}^{\boldsymbol{i}kl}|l\rangle$, $\hat{c}_{\underline{k}} = \sum_k \mathrm{e}^{\boldsymbol{i}kl}\hat{c}_l$, and

$$\hat{H} = -t \sum_l \Big(|l+1\rangle\langle l| + |l\rangle\langle l+1| \Big) = \sum_{\underline{k}} \varepsilon(\underline{k}) \, |\underline{k}\rangle\langle\underline{k}|$$

is equivalent to (**) in the single particle subspace

$$\hat{\mathcal{H}} = -t \sum_l \left(\hat{c}_{l+1}^\dagger \hat{c}_l + \hat{c}_l^\dagger \hat{c}_{l+1} \right)$$

5 Time Dependent Perturbation Theory

5.1 Sudden Perturbation

We decompose the Hamiltonian according to $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1(t)$, and assume that $\hat{H}_0$ has known eigenstates $|m\rangle, |n\rangle$ with eigenvalues E_m, E_n. λ is a small number, and we are interested in finding the solution to linear order in λ. We assume that $\hat{H}_1(t)$ vanishes for $t \leq t_0$. Hence, for $t \leq t_0$, the system is described by the Schrödinger equation

$$\boldsymbol{i}\hbar \frac{\partial}{\partial t} |\Psi^{(0)}(t)\rangle = \hat{H}_0 |\Psi^{(0)}(t)\rangle \,,$$

with the initial condition $|\Psi(t)\rangle = |\Psi^{(0)}(t)\rangle$ for $t \leq t_0$.

Brief reminder:

- **Schrödinger picture** $|\Psi_S(t)\rangle$, $\hat{A}_S$
- **Heisenberg picture** $|\Psi_H\rangle$, $\hat{A}_H(t)$

These pictures are related by the transformation

$$|\Psi_S(t)\rangle = \mathrm{e}^{-\frac{\boldsymbol{i}}{\hbar}\hat{H}} |\Psi_H\rangle \text{ and } \hat{A}_H(t) = \mathrm{e}^{\frac{\boldsymbol{i}}{\hbar}\hat{H}\,t} \hat{A}_S \mathrm{e}^{-\frac{\boldsymbol{i}}{\hbar}\hat{H}\,t} = \hat{U}^\dagger \hat{A}_S \hat{U} \,,$$

if $\hat{H}$ does not explicitly depend on time.
If $\hat{H}$ does depend explicitly on time, one finds

$$\hat{U}(t, t_0 = 0) = \mathrm{e}^{-\boldsymbol{i}\frac{\hat{H}\,t}{\hbar}} \longrightarrow \hat{T}\mathrm{e}^{-\boldsymbol{i}\int_0^t \mathrm{d}t'\, \hat{H}(t')/\hbar}$$

where $\hat{T}$ is the time ordering operator

$$\hat{T}\hat{A}(t_1)\hat{B}(t_2) = \begin{cases} \hat{A}(t_1)\hat{B}(t_2) & \text{for } t_1 > t_2 \\ \hat{B}(t_2)\hat{A}(t_1) & \text{for } t_2 > t_1 \end{cases} .$$

The sign in $\hat{U}$ can be remembered by noting that the time evolution has to satisfy the Schrödinger equation

$$\boldsymbol{i}\hbar\partial_t \mathrm{e}^{-\boldsymbol{i}\hat{H}t/\hbar} = \hbar\boldsymbol{i}(-\boldsymbol{i})\,\frac{\hat{H}}{\hbar}\,\mathrm{e}^{-\boldsymbol{i}\hat{H}t/\hbar} = \hat{H}\,\mathrm{e}^{-\boldsymbol{i}\hat{H}t/\hbar}$$

so it needs to be a $(-)$.
Using

$$|\Psi_S(t)\rangle = \mathrm{e}^{-\boldsymbol{i}\hat{H}t/\hbar}|\Psi_H\rangle \,, \quad \langle\Psi_S(t)| = \langle\Psi_H|\mathrm{e}^{\boldsymbol{i}\hat{H}t/\hbar}$$

the expectation value in the Schrödinger picture

$$\langle\hat{A}\rangle = \langle\Psi_S(t)|\hat{A}|\Psi_S(t)\rangle = \langle\Psi_H|\mathrm{e}^{\boldsymbol{i}\hat{H}t/\hbar}\hat{A}\mathrm{e}^{-\boldsymbol{i}\hat{H}t/\hbar}|\Psi_H\rangle = \langle\Psi_H|\hat{A}_H(t)|\Psi_H\rangle$$

coincides with the one in the Heisenberg picture.

- **Dirac interaction picture** $\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t)$

  $\hat{A}_D(t) = \mathrm{e}^{\boldsymbol{i}\hat{H}_{0,S}t/\hbar}\hat{A}_S\mathrm{e}^{-\hat{H}_{0,S}t/\hbar}$ and $|\Psi_D(t)\rangle = \mathrm{e}^{\boldsymbol{i}\hat{H}_{0,S}t/\hbar}|\Psi_S(t)\rangle = \mathrm{e}^{-\boldsymbol{i}\int_0^t \mathrm{d}t'\,\hat{H}_{1,D}(t')/\hbar}|\Psi_D(0)\rangle$

  with $|\Psi_D(0)\rangle = |\Psi_S(0)\rangle = |\Psi_H\rangle$, where we used the time evolution in the Dirac picture and the fact that $\hat{H}_1$ can depend on time where $\hat{H}_0$ is time independent ($\hat{H}_{0,D} = \hat{H}_{0,S}$ and time evolution $\hat{U}_D|\Psi_D(0)\rangle = |\Psi_D(t)\rangle$ satisfies the Schrödinger equation in the Dirac picture). Transforming the Schrödinger equation into the interaction picture yields

  $$\boldsymbol{i}\hbar\frac{d}{dt}|\psi_D(t)\rangle = H_{1,D}(t)|\psi_D(t)\rangle\,,$$

  where $H_{1,D}(t) = \mathrm{e}^{\boldsymbol{i}H_{0,S}t/\hbar}H_{1,S}\mathrm{e}^{-\boldsymbol{i}H_{0,S}t/\hbar}$.

We now transform into the interaction picture

$$|\Psi_D(t)\rangle = \mathrm{e}^{\boldsymbol{i}\hat{H}_0t/\hbar}|\Psi(t)\rangle\ .$$

As an example we consider a system which was initially, at $t = t_0$, in an eigenstate $|m\rangle$ of $\hat{H}_0$.

$$|m(t \le t_0)\rangle = \mathrm{e}^{-\boldsymbol{i}\hat{H}_0t/\hbar}|m\rangle = \mathrm{e}^{-\boldsymbol{i}E_mt/\hbar}|m\rangle\ .$$

The action of $\hat{H}_1$ for times $t > t_0$, gives rise to a time evolution $|\Psi_m(t)\rangle = \sum_n\langle n(t)|\Psi_m(t)\rangle|n(t)\rangle$ where $\langle n(t)|\Psi_m(t)\rangle$ is the amplitude to find $|\Psi_m(t)\rangle$ in state $|n\rangle$. $|\langle n(t)|\Psi_m(t)\rangle|^2$ is the probability to find $|\Psi_m(t)\rangle$ in state $|n(t)\rangle$, called the "transmission probability from $|m\rangle$ to $|n\rangle$".

$$\langle n(t)|\Psi_m(t)\rangle = \langle n|\mathrm{e}^{\boldsymbol{i}\hat{H}_0t/\hbar}|\Psi_m(t)\rangle = \langle n|\Psi_{m,D}(t)\rangle\,.$$

Expanding the time evolution of $|\Psi_{m,D}(t)\rangle$ to first order in λ, we find usign the notation $|\Psi_{m,D}(0)\rangle = |m\rangle$ that $|\Psi_{m,D}(t)\rangle = |m\rangle - \dfrac{\boldsymbol{i}}{\hbar}\lambda\displaystyle\int_{t_0}^{t}\mathrm{d}\tilde{t}\ \hat{H}_{1,D}(\tilde{t})|m\rangle$, and since $|m\rangle$ is eigenstate of $\hat{H}_0$ and $H_{1,D}(t) = \mathrm{e}^{\boldsymbol{i}H_{0,S}t/\hbar}H_{1,S}\mathrm{e}^{-\boldsymbol{i}H_{0,S}t/\hbar}$:

$$\langle n(t)|\Psi_m(t)\rangle = \delta_{nm} - \frac{\boldsymbol{i}}{\hbar}\lambda\int_{t_0}^{t}\mathrm{d}\tilde{t}\,\mathrm{e}^{\boldsymbol{i}(E_n-E_m)\tilde{t}/\hbar}\langle n|\hat{H}_1(\tilde{t})|m\rangle\ .$$

The transition probability is given by

$$P_{m,n}(t) = |\langle n(t)|\Psi_m(t)\rangle|^2 = \left|\frac{\lambda}{\hbar}\int_{t_0}^{t}\mathrm{d}\tilde{t}\ \mathrm{e}^{\boldsymbol{i}\,(E_n-E_m)\tilde{t}/t}\langle n|\hat{H}_1(\tilde{t})|m\rangle\right|^2\ .$$

We now set $\lambda = 1$. We first specialize in $\hat{H}_1(t) = \hat{V}\theta(t)$, $t_0 = 0$ and $\lambda = 1$.

$$\begin{aligned}\Rightarrow P_{m,n}(t) &= \frac{1}{\hbar^2}\left|\int_0^t\mathrm{d}\tilde{t}\ \mathrm{e}^{\boldsymbol{i}(E_n-E_m)\tilde{t}/\hbar}\langle n|\hat{V}|m\rangle\right|^2\\ &= \frac{1}{\hbar^2}\left|\frac{\mathrm{e}^{\boldsymbol{i}\omega_{nm}t}-1}{\boldsymbol{i}\omega_{nm}}\right|^2\ \left|\langle n|\hat{V}|m\rangle\right|^2\end{aligned}$$

with $\omega_{nm} = \frac{E_n - E_m}{\hbar}$

$$\Rightarrow P_{m,n}(t) = \frac{1}{\hbar^2} \left| \mathrm{e}^{\frac{i\omega_{nm}}{2\hbar}} \right|^2 \cdot \left| \frac{\mathrm{e}^{\boldsymbol{i}\omega_{nm}t/2} - \mathrm{e}^{-\boldsymbol{i}\omega_{nm}t/2}}{\boldsymbol{i}\omega_{nm}} \right|^2 \left| \langle n|\hat{V}|m\rangle \right|^2$$
$$= \frac{1}{\hbar^2} \left(\frac{\sin(\omega_{nm}t/2)}{\omega_{nm}/2} \right)^2 \left| \langle n|\hat{V}|m\rangle \right|^2 .$$

For $t \to \infty$ the expression $\frac{\sin^2(\alpha t)}{\pi \alpha^2 t}$ is a representation of the delta function $\delta(\alpha)$. For large times t (actually large $\omega_{nm}t$ while $P_{mn} \ll 1$, i.e. $\left|\langle n|\hat{V}|m\rangle\right|^2$ small) we find

$$P_{mn}(t) \cong t \, \frac{\pi}{\hbar^2} \, \delta\left(\frac{\omega_{nm}}{2}\right) \left| \langle n|\hat{V}|m\rangle \right|^2$$
$$= t \, \frac{2\pi}{\hbar} \, \delta(E_n - E_m) \left| \langle n|\hat{V}|m\rangle \right|^2 .$$

The transition rate, i.e. the transition probability per unit time is given by

$$\Gamma_{mn} = \frac{2\pi}{\hbar} \, \delta(E_n - E_m) \left| \langle n|\hat{V}|m\rangle \right|^2 .$$

There $\delta(E_n - E_m)$ ensures energy conservation.
If the eigenvalues E_n form a continuum (or quasi-continuum) and if the matrix element $\langle n|\hat{V}|m\rangle$ depends only weakly on n, we can introduce the density of states (number of states per unit energy ϱ) and obtain for the total transition rate

$$\sum_n \Gamma_{mn} = \int \mathrm{d}E_n \, \varrho(E_n) \, \Gamma_{mn} = \varrho(E_m) \frac{2\pi}{\hbar} \left| \langle n|\hat{V}|m\rangle \right|^2 . \qquad (!)$$

This relation is known as Fermi's golden rule. It was derived in 1928 by Wolfgang Pauli and because of the usefulness of the relation E. Fermi coined the term golden rule in 1950.
Next, we consider the case of periodic perturbations.

$$\hat{H}_1(t) = \theta(t) \left[\hat{F}\mathrm{e}^{-\boldsymbol{i}\omega t} + \hat{F}^\dagger \mathrm{e}^{\boldsymbol{i}\omega t} \right]$$
$$\langle n(t)|\Psi_m(t)\rangle = -\frac{\boldsymbol{i}}{\hbar} \int_0^t \mathrm{d}\tilde{t} \;\; \left[\mathrm{e}^{\boldsymbol{i}(\omega_{nm}-\omega)\tilde{t}} \langle n|\hat{F}|m\rangle + \mathrm{e}^{\boldsymbol{i}(\omega_{nm}+\omega)\tilde{t}} \langle n|\hat{F}^\dagger|m\rangle \right]$$

And hence

$$|\langle n(t)|\Psi_m(t)\rangle|^2 = t \, \frac{2\pi}{\hbar} \left[\delta(\omega_{nm} - \omega) \left| \langle n|\hat{F}|m\rangle \right|^2 + \delta(\omega_{nm} + \omega) \left| \langle n|\hat{F}^\dagger|m\rangle \right|^2 \right] .$$

The mixed term does not contribute due to the incompatible delta-functions.

$$\Rightarrow \Gamma_{nm} = \frac{2\pi}{\hbar} \left[\underbrace{\delta(E_n - E_m - \hbar\omega)}_{\text{absor.}} \left| \langle n|\hat{F}|m\rangle \right|^2 + \underbrace{\delta(E_n - E_m + \hbar\omega)}_{\text{stm. em.}} \left| \langle n|\hat{F}^\dagger|m\rangle \right|^2 \right] .$$

In addition spontaneous emission of an excited atomic state due to vacuum fluctuations in the electromagnetic field is possible and discussed in the problem sets.

5.2 Adiabatic Theorem

Adiabatic Process:
The Hamiltonian of the system changes gradually, such that the system can adopt its configuration to the changed Hamiltonian. If the system starts in an eigenstate of the original Hamiltonian, it will end in the corresponding eigenstate of the final Hamiltonian.

Diabatic Process:
A rapid change of the Hamiltonian ("quench") preserves the system from adapting its configuration during the process, hence the spacial and spin probability density remains unchanged (same state but no longer an eigenstate).

Reminder:
For a time independent Hamiltonian, the time-dependent Schrödinger equation $\boldsymbol{i}\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ can be turned into the time-independent Schrödinger equation via a product ansatz

$$|\Psi_n(t)\rangle = \mathrm{e}^{-\frac{\boldsymbol{i}}{\hbar}E_n t}|\Psi_n\rangle \text{ , with } \hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle,$$

and the general solution of the time-dependent problem is

$$|\Psi(t)\rangle = \sum_n c_n|\Psi_n\rangle \mathrm{e}^{-\frac{\boldsymbol{i}}{\hbar}E_n t} \text{ with } c_n = \langle\Psi_n|\Psi(t=0)\rangle \ .$$

A time-dependent Hamiltonian $\hat{H}(t)$ has at every instance of time eigenfunctions and eigenvalues

$$\hat{H}(t)|\Psi_n(t)\rangle = E_n(t)|\Psi_n(t)\rangle \qquad (*)$$

with $\sum_n |\Psi_n(t)\rangle\langle\Psi_n(t)| = \mathbb{1}$ and $\langle\Psi_n(t)|\Psi_n(t)\rangle = \delta_{nm}$. Note that the $|\Psi_n(t)\rangle$ are not solutions of the time-dependent Schrödinger equation in general.
Ansatz:

$$|\Psi(t)\rangle = \sum_n c_n(t)|\Psi_n(t)\rangle \mathrm{e}^{\boldsymbol{i}\theta_n(t)} \text{ with } \theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\mathrm{d}t'$$

to determine $c_n(t)$. Substitution into the Schrödinger equation $\boldsymbol{i}\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ yields

$$\sum_n c_n\hat{H}|\Psi_n(t)\rangle \mathrm{e}^{\boldsymbol{i}\theta_n(t)} = \boldsymbol{i}\hbar\sum_n \left[\dot{c}_n|\Psi_n\rangle + c_n|\dot{\Psi}_n\rangle + \boldsymbol{i}c_n|\Psi_n\rangle\dot{\theta}_n\right] \mathrm{e}^{\boldsymbol{i}\theta_n(t)}$$

with $|\dot{\Psi}_n\rangle = \partial_t|\Psi_n(t)\rangle$ and $\dot{\theta}_n = -E_n/\hbar$ and $\hat{H}|\Psi_n(t)\rangle = E_n(t)|\Psi_n(t)\rangle$ due to $(*)$. We are left with

$$\sum_n \dot{c}_n|\Psi_n(t)\rangle \mathrm{e}^{\boldsymbol{i}\theta_n} = -\sum_n c_n|\dot{\Psi_n}(t)\rangle \mathrm{e}^{\boldsymbol{i}\theta_n} \ .$$

We multiply by $\langle\Psi_m(t)|$ from the left

$$\dot{c}_m = -\sum_n c_n\langle\Psi_m(t)|\dot{\Psi}_n(t)\rangle \, \mathrm{e}^{\boldsymbol{i}(\theta_n-\theta_m)} \ . \qquad (**)$$

We now compute the time derivative of (*) as

$$\left(\partial_t\hat{H}(t)\right)|\Psi_n(t)\rangle + \hat{H}|\dot{\Psi_n}(t)\rangle = \dot{E}_n(t) + E_n|\dot{\Psi_n}(t)\rangle \ .$$

We again multiply from the left with $\langle\Psi_m(t)|$, assuming $m \neq n$, and obtain

$$\langle\Psi_m(t)|(\partial_t\hat{H})|\Psi_n(t)\rangle + E_m\langle\Psi_m(t)|\dot{\Psi_n}(t)\rangle = \dot{E}_n(t)\underbrace{\langle\Psi_m|\Psi_n\rangle}_{=0} + E_n\langle\Psi_m(t)|\dot{\Psi_n}(t)\rangle$$

$$\langle\Psi_m(t)|\dot{\Psi_n}(t)\rangle = \frac{\langle\Psi_m(t)|(\partial_t\hat{H}(t))|\Psi_n(t)\rangle}{E_n(t) - E_m(t)}$$

Inserting this into (**) gives (we have to consider $m = n$ in the sum separately) the exact result

$$\dot{c}_m = -c_m\langle\Psi_m(t)|\dot{\Psi_m}(t)\rangle - \sum_{n\neq m} c_n \frac{\langle\Psi_m(t)|(\partial_t\hat{H})|\Psi_n(t)\rangle}{E_n(t) - E_m(t)} \, \mathrm{e}^{\boldsymbol{i}(\theta_n - \theta_m)} \, .$$

In the adiabatic approximation, we assume that the time derivative of the Hamiltonian $\partial_t\hat{H}$ is extremely small, and the sum will not contribute (small means that the matrix element $\langle\Psi_m(t)|(\partial_t\hat{H})|\Psi_n(t)\rangle \ll E_n - E_m$ which depends on the spacing of the energy levels). Then,

$$\dot{c}_m(t) = -c_m(t)\langle\Psi_m(t)|\dot{\Psi_m}(t)\rangle$$

which can be solved yielding

$$c_m(t) = c_m(0)\,\mathrm{e}^{-\int_0^t \mathrm{d}t' \, \langle\Psi_m(t')|\dot{\Psi_m}(t')\rangle} \equiv c_m(0)\,\mathrm{e}^{\boldsymbol{i}\gamma_m(t)} \, .$$

In the last step, the **geometric phase**

$$\gamma_m(t) = \boldsymbol{i}\int_0^t \mathrm{d}t' \, \langle\Psi_m(t')|\dot{\Psi_m}(t')\rangle$$

was defined.

Remarks:
In the adiabatic approximation, the system is always in an instantaneous eigenstate. ($|\Psi^{(m)}(t)\rangle$ is an eigenstate of the time dependent Schrödinger equation, $c_m(0) = 1$ and $c_{n\neq m}(0) = 0$ and $|\Psi_m(t)\rangle$ is instantaneous eigenstate)

$$|\Psi^{(m)}(t)\rangle = |\Psi_m(t)\rangle \mathrm{e}^{\boldsymbol{i}\gamma_m(t)}\,\mathrm{e}^{\boldsymbol{i}\theta_m(t)} \text{ and } |\Psi^{(m)}(0)\rangle = |\Psi_m\rangle \, ,$$

where $\hat{H}(t)|\Psi_m(t)\rangle = E_m(t)|\Psi_m(t)\rangle$. The phase convention for $|\Psi_m(t)\rangle$ is chosen in the ansatz $|\Psi(t)\rangle = \sum_n c_n(t)|\Psi_n(t)\rangle \mathrm{e}^{-\frac{\boldsymbol{i}}{\hbar}\int_0^t \mathrm{d}t' \, E_n(t')}$ so that the $|\Psi_n(t)\rangle$ evolve explicitly in time. This is contained in the $\mathrm{e}^{\boldsymbol{i}\gamma_m(t)}$ phase at the end.

$\gamma_m(t)$ is real, since $\langle\Psi_m|\dot{\Psi_m}\rangle$ is imaginary which can be shown by taking the time-derivative of $1 = \langle\Psi_m(t)|\Psi_m(t)\rangle$

$$\Rightarrow 0 = \langle\dot{\Psi_m}|\Psi_m\rangle + \langle\Psi_m|\dot{\Psi_m}\rangle = \langle\Psi_m|\dot{\Psi_m}\rangle + \langle\Psi_m|\dot{\Psi_m}\rangle^* = 2\mathrm{Re}\langle\Psi_m|\dot{\Psi_m}\rangle \, .$$

5.3 Berry Phase

We now consider the example of a spin with magnitude S in a time-dependent magnetic field $\underline{B}(t)$. The spin has a magnetic momentum $\frac{g\mu_B}{\hbar}\hat{\underline{S}}$, and $\hat{H}(\underline{B}) = -g\mu_B\underline{B}(t)\cdot\hat{\underline{S}}/\hbar$, with energy eigenvalues $E_m = -g\mu_B Bm$, and $-S \leq m \leq S$ using a quantization axis parallel to the $\underline{B}$ field. Under adiabatic changes of the magnetic field direction, the spin keeps its quantum number m, but the quantization axis rotates with the magnetic field. We denote the spin-quantization direction by $\underline{n}$ (with $\underline{B} = \underline{n}B$), and instantaneous eigenstates by $|m(t)\rangle$ (but the quantum number m does not depend on time, better would be $|m, \underline{n}(t)\rangle \equiv |m(t)\rangle$) with $\hat{S}_{z'}$ (z' axis is parallel to $\underline{n}$) $\Rightarrow \hat{S}_{z'}|m(t)\rangle = m\hbar|m(t)\rangle$. We move the direction of $\underline{B}$ along a closed loop $\mathcal{C}$, and compute γ_m.

$$\gamma_m(\mathcal{C}) = \boldsymbol{i}\int_0^T \langle m(t)|\left(\partial_t|m(B(t))\rangle\right)\mathrm{d}t = \boldsymbol{i}\int_0^T \langle m(t)|\nabla_B|m(B(t))\rangle\frac{\mathrm{d}B}{\mathrm{d}t}\,\mathrm{d}t$$

$$\Rightarrow \gamma_m(\mathcal{C}) = \boldsymbol{i}\oint_{\mathcal{C}}\langle m|\nabla_B m(B)\rangle\,\mathrm{d}\underline{B}$$

where $|\nabla_B m(B)\rangle \equiv \nabla_B|m(B)\rangle$. Hence, $\gamma_m(\mathcal{C})$ depends only on the geometry.
We use Stokes theorem to write this as a surface integral

$$\gamma_m(\mathcal{C}) = -\iint_{S(\mathcal{C})}\underline{V}_m(\underline{B})\cdot\mathrm{d}\underline{S}$$

with $\underline{V}_m(\underline{B}) = \mathrm{Im}\left(\nabla_B\times\langle m(\underline{B})|\nabla_B m(\underline{B})\rangle\right)$ where we used that the matrix element is fully imaginary. We use $\nabla\times[f(x)\nabla g] = (\nabla f)\times(\nabla g)$ to write

$$\underline{V}_m(\underline{B}) = \mathrm{Im}\left(\langle\nabla_B m(\underline{B})|\times|\nabla_B m(\underline{B})\rangle\right) = \mathrm{Im}\sum_{m\neq m'}\langle\nabla_B m(\underline{B})|m'(\underline{B})\rangle\times\langle m'(\underline{B})|\nabla_B m(\underline{B})\rangle\,.$$

Here we used that $\langle m|\nabla_B m\rangle$ is purely imaginary so that the product will not contribute taking the imaginary part. We now compute $\langle m'|\nabla_B m\rangle$ by taking the gradient of the eigenvalue equation

$$\hat{H}(\underline{B})|m(\underline{B})\rangle = E_m|m(\underline{B})\rangle$$

$$\Rightarrow (\nabla_B\hat{H})|m(\underline{B})\rangle + \hat{H}|\nabla_B m(\underline{B})\rangle = (\nabla_B E_m)|m(\underline{B})\rangle + E_m|\nabla_B m(\underline{B})\rangle$$

Multiply from the left with $\langle m'(\underline{B})|$, $m \neq m'$

$$\Rightarrow \langle m'(\underline{B})|\nabla_B m(\underline{B})\rangle = \frac{\langle m'(\underline{B})|\nabla_B\hat{H}|m(\underline{B})\rangle}{E_m - E_{m'}}\,.$$

Using $\nabla_B\hat{H} = -g\mu_B\hat{S}/\hbar$ with $\nabla_{\underline{x}}(\underline{x}\cdot\underline{a}) = \underline{a}$ yields

$$\underline{V}_m(\underline{B}) = \mathrm{Im}\sum_{m'\neq m}\frac{\langle m(\underline{B})|\hat{\underline{S}}/\hbar|m'(\underline{B})\rangle\times\langle m'(\underline{B})|\hat{\underline{S}}/\hbar|m(\underline{B})\rangle}{B^2(m'-m)^2}\,.$$

We now use the direction of the magnetic field as instantaneous z-axis ("z'-axis") for spin quantization. Then, $\hat{S}_{z'}$ does not contribute to the sum, as it leaves $m_{z'}$ unchanged, due to

$\hat{S}_{z'}|m(\underline{B})\rangle = m_{z'}\hbar|m(\underline{B})\rangle$.
Only $\hat{S}_{x'}$ and $\hat{S}_{y'}$ give rise to contributions for $m' = m \pm 1$. We now use the matrix elements

$$\langle S, m \pm 1|\hat{S}_{x'}/\hbar|S, m\rangle = \frac{1}{2}\sqrt{(S \mp m)(S \pm m + 1)}$$
$$\langle S, m \pm 1|\hat{S}_{y'}/\hbar|S, m\rangle = \frac{\mp \boldsymbol{i}}{2}\sqrt{(S \mp m)(S \pm m + 1)}$$

In this way, we obtain for the components of $\underline{V}_m$

$$(\underline{V}_m(\underline{B}))_{x'} = 0 \ , \ (\underline{V}_m(\underline{B}))_{y'} = 0 \text{ and } (\underline{V}_m(\underline{B}))_{z'} = \frac{m}{B^2} \ .$$

The x' and y' component are easy, because they are $\sim \hat{S}_{z'}$ in the cross product.
We check the z' component for the case $S = \frac{1}{2},\ m = \frac{1}{2},\ m' = -\frac{1}{2}$

$$\langle 1/2, m - 1|\hat{S}_{y'}/\hbar|1/2, m\rangle = \frac{\boldsymbol{i}}{2}\sqrt{(1/2 + 1/2) \cdot (1/2 - 1/2 + 1)} = \frac{\boldsymbol{i}}{2}$$
$$\langle 1/2, m|\hat{S}_{x'}/\hbar|1/2, m - 1\rangle = \frac{1}{2}\sqrt{(1/2 + 1/2) \cdot (1/2 - 1/2 + 1)} = \frac{1}{2} \ .$$

There are two contributions $\hat{S}_{x'} \times \hat{S}_{y'}$ and $\hat{S}_{y'} \times \hat{S}_{x'}$. $\Rightarrow$ in total one finds $\mathrm{Im}(2 \cdot 1/2 \cdot \boldsymbol{i}/2) = 1/2 = m = m/B^2$.

We now established that

$$\gamma_m(\mathcal{C}) = -m \iint_{S(\mathcal{C})} \frac{\hat{B}}{B^2} \ \cdot \mathrm{d}\underline{B} = -m \int_{\mathcal{C}} \mathrm{d}\Omega = -m\Omega(\mathcal{C})$$

where $\Omega(\mathcal{C})$ denotes the solid angle which is enclosed by the trajectory $\mathcal{C}$.
Mathematically, it is important that there exists a degenerate point of the Hamiltonian at the origin of the coordinate system.

In the problem sets we show that the Aharonov–Bohm phase can be understood as a Berry phase with $\gamma_m = 2\pi\frac{\Phi_B}{\Phi_0}$, where $\Phi_0 = h/e$ is the flux quantum.

6 Topological Phases and Anions

6.1 Introduction

Consider a regular lattice with N sites in one spatial dimensions, and wave functions ψ_j defined on the sites. The Fourier-representation of the wave functions is given by

$$\psi_j = \frac{1}{N} \sum_{k_n} \mathrm{e}^{\boldsymbol{i} j k_n} \psi(k_n) \ .$$

We use periodic boundary conditions $\psi_1 = \psi_{N+1} \Rightarrow \mathrm{e}^{\boldsymbol{i}(N+1)k_n} = \mathrm{e}^{\boldsymbol{i}k_n}$ which is satisfied for $\mathrm{e}^{\boldsymbol{i}Nk_n} = 1$

$$\Rightarrow N k_n = 2\pi n \Rightarrow \ k_n = \frac{2\pi n}{N} \ .$$

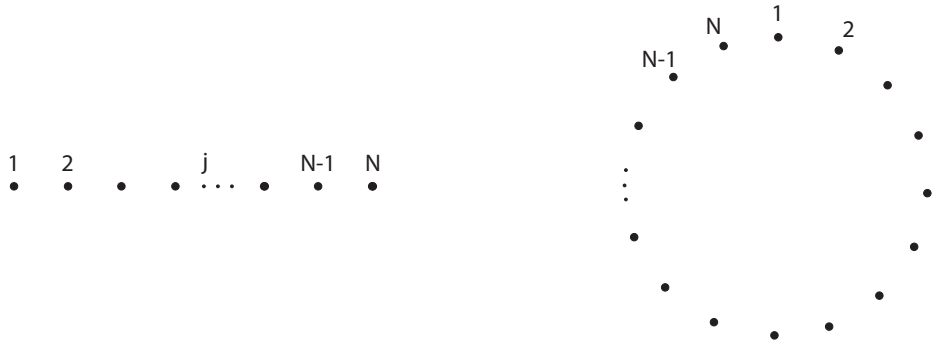

Figure 6.1: Visualization of the periodic boundary conditions, in the one dimensional case, as lattice points lying on a circle

For N lattice sites we thus have N different values of k_n, and we choose N even:

$$n = -\frac{N}{2}, -\frac{N-2}{2}, ..., \frac{N-4}{2}, \frac{N-2}{2} \quad \text{and} \quad k_n = -\pi, -\frac{N-2}{N}\pi, ..., \frac{N-4}{N}\pi, \frac{N-2}{N}\pi \ .$$

In the limit of infinite lattice sites $N \to \infty$ we have $k_n \in [-\pi, \pi)$. Changing $k_n \mapsto k_n + 2\pi$ does not change $\mathrm{e}^{\boldsymbol{i}jk_n}$. $\Rightarrow$ We identify $k = -\pi$ with $k = \pi$ and the Brillouin zone is a circle.

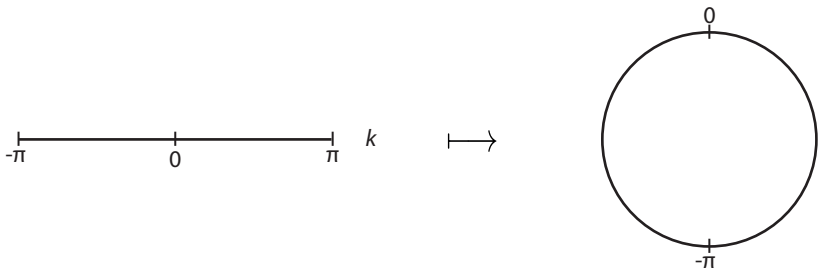

Figure 6.2: Brillouin zone for the infinite lattice with periodic boundary conditions

For infinite lattices, the Fourier sum turns into a Fourier integral $\psi_j = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{\mathit{i}jk}\psi(k)$.
For a two-dimensional lattice, we use periodic boundary conditions in both x- and y-direction.

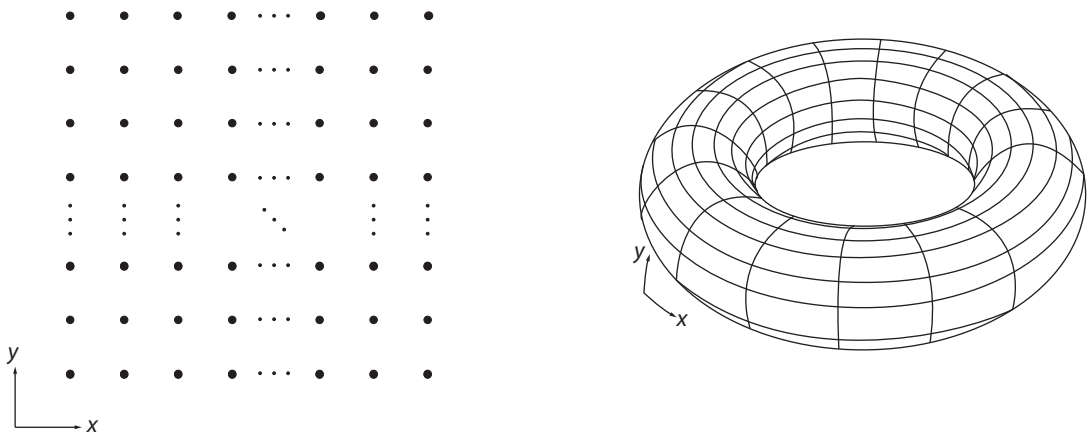

Figure 6.3: Visualization of the periodic boundary conditions in the two dimensional case as lattice points lying on a torus

There are now two momentum components k_x and k_y in a Fourier transform, defined modulo 2π, in the range $k_x = [-\pi, \pi)$, $k_y = [-\pi, \pi)$, which can be visualized as lying on a torus as well.

6.2 SSH Model

We consider a one dimensional lattice with A and B sub-lattices.

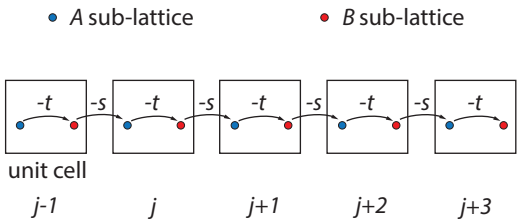

Figure 6.4: SSH Model with unit cell for translational invariance and hopping matrix elements

Now a wave function has two components $\Psi_j = (\psi_{j,A}, \psi_{j,B})$. The action of the Hamiltonian is given by

$$\hat{H} \begin{pmatrix} \psi_{j,A} \\ \psi_{j,B} \end{pmatrix} = \begin{pmatrix} -t\psi_{j,B} - s\psi_{j-1,B} \\ -t\psi_{j,A} - s\psi_{j+1,A} \end{pmatrix} .$$

We know from Bloch's theorem that the wave function has the form

$$\Psi_{k,j} = \mathrm{e}^{\mathit{i}kj} \begin{pmatrix} u_A(k) \\ u_B(k) \end{pmatrix} .$$

(We previously discussed the Bloch theorem $\psi(r) = \mathrm{e}^{\boldsymbol{i}kr} u_k(r)$ with a lattice periodic function u. Here we have two possible values in the unit cell as a two component vector.) This yields

$$\begin{aligned}\hat{H}\Psi_{k,j} &= \hat{H}\begin{pmatrix}\mathrm{e}^{\boldsymbol{i}kj}u_A(k)\\ \mathrm{e}^{\boldsymbol{i}kj}u_B(k)\end{pmatrix} = \begin{pmatrix}-t\mathrm{e}^{\boldsymbol{i}kj}u_B(k) - s\mathrm{e}^{\boldsymbol{i}k(j-1)}u_B(k)\\ -t\mathrm{e}^{\boldsymbol{i}kj}u_A(k) - s\mathrm{e}^{\boldsymbol{i}k(j+1)}u_A(k)\end{pmatrix}\\ &= \begin{pmatrix}0 & -t - s\mathrm{e}^{-\boldsymbol{i}k}\\ -t - s\mathrm{e}^{\boldsymbol{i}k} & 0\end{pmatrix}\mathrm{e}^{\boldsymbol{i}kj}\begin{pmatrix}u_A(k)\\ u_B(k)\end{pmatrix} \equiv \begin{pmatrix}0 & -\gamma(k)\\ -\gamma^*(k) & 0\end{pmatrix}\Psi_{k,j}\ .\end{aligned}$$

Dividing the eigenvalue equation $\hat{H}\Psi_{k,j} = E_k\Psi_{k,j}$ by $\mathrm{e}^{\boldsymbol{i}kj}$ leaves us with

$$\underbrace{\begin{pmatrix}0 & -t - s\mathrm{e}^{-\boldsymbol{i}k}\\ -t - s\mathrm{e}^{\boldsymbol{i}k} & 0\end{pmatrix}}_{\text{Bloch Hamiltonian}}\underbrace{\begin{pmatrix}u_A(k)\\ u_B(k)\end{pmatrix}}_{\text{Bloch wave fnc.}} = E_k\begin{pmatrix}u_A(k)\\ u_B(k)\end{pmatrix}\ .$$

For each wave vector k from the Brillouin zone, we define a two-dimensional Hilbert space of complex two-component vectors $\underline{u}(k)$, and a Hermitian 2×2 Hamiltonian $\hat{H}(k)$, and the eigenvalue problem $\hat{H}(k)\underline{u}(k) = E_k\underline{u}(k)$.
Clearly, $E_k = \pm|t + s\mathrm{e}^{\boldsymbol{i}k}|$. We now define the curce $\gamma(k) = t + s\mathrm{e}^{-\boldsymbol{i}k}\colon [-\pi,\pi) \mapsto \mathbb{C}$ with

$$\hat{H}(k) = \begin{pmatrix}0 & -\gamma(k)\\ \gamma(k) & 0\end{pmatrix}\ .$$

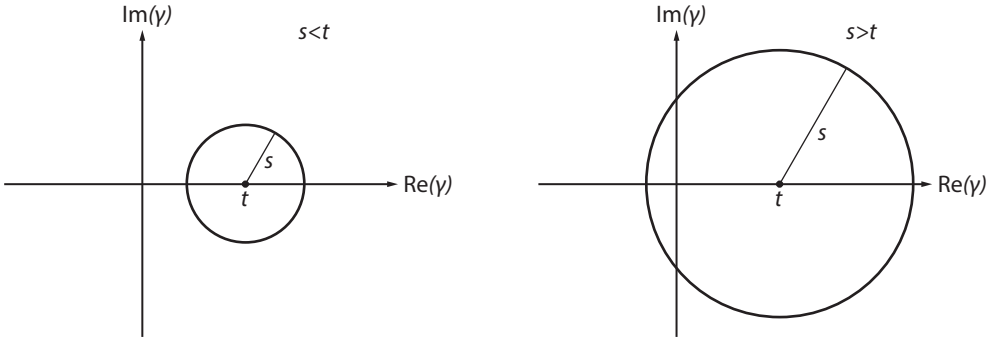

Figure 6.5: For $s > t$ the curve $\gamma(k)$ encloses the the origin, for $s < t$ it does not.

The two curves have different winding numbers

$$W \equiv \frac{1}{2\pi\boldsymbol{i}}\oint_\gamma \frac{\mathrm{d}z}{z} = \begin{cases}-1 & , s > t\\ 0 & , s < t\end{cases}\ .$$

W is undefined for the case $s = t$, which also corresponds to an eigenvalue 0 for $E_k = |\gamma_k|$ at $k = \pm\pi$.

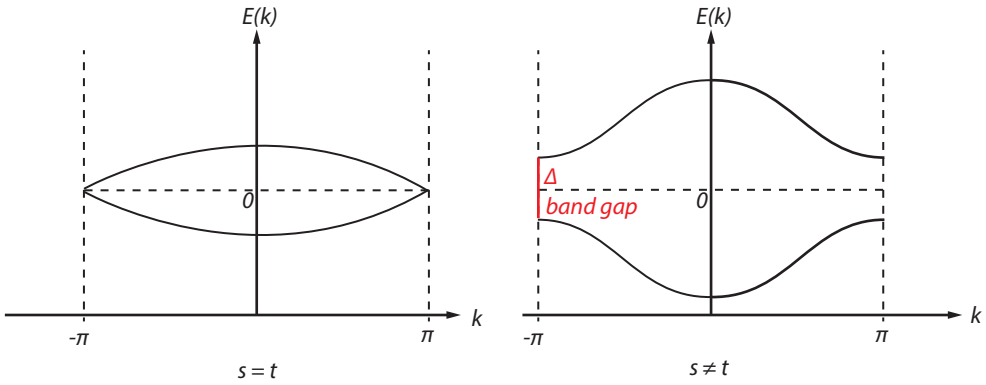

Figure 6.6: Dispersion for the different cases

A Hamiltonian is called *gapped* if there is a finite interval of energies which does not contain eigenvalues of $\hat{H}$.
Claim: If a chain is finite there exists a zero energy state localized at each end of the chain (bound state with exponentially decaying wave function; zero energy up to e^{-N} corrections) for the case $s > t$, $W = -1$.

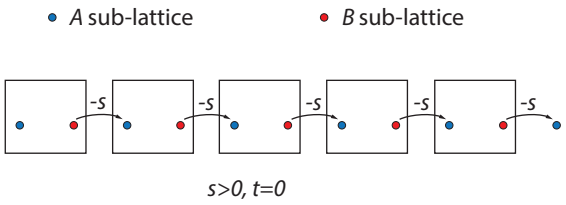

Figure 6.7: Zero energy state at the end of finite chains with $s > t$, $t = 0$

Example: In the case $s > 0, t = 0$, $\hat{H}$ has two eigenvalues $E = 0$, $\frac{N-2}{2}$ eigenvalues $E = s$, and $\frac{N-2}{2}$ eigenvalues $E = -s$.

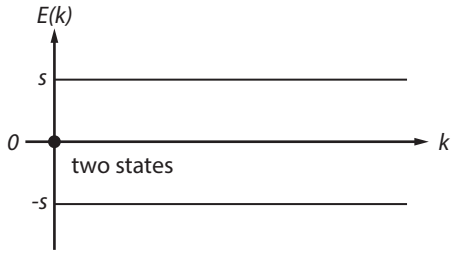

Figure 6.8: Special case of finite chain with $s > 0, t = 0$

Every $\hat{H} = \begin{pmatrix} 0 & -\gamma(k) \\ -\gamma^*(k) & 0 \end{pmatrix}$ anti-commutes with $C = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_2$ since

$$\hat{H} = -\mathrm{Re}[\gamma]\,\sigma_x + \mathrm{Im}[\gamma]\,\sigma_y \text{ where } \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } \sigma_y = \begin{pmatrix} 0 & -\boldsymbol{i} \\ \boldsymbol{i} & 0 \end{pmatrix}$$

with $\{\sigma_{x/y}\,,\,\sigma_z\} = 0 \Rightarrow \{\hat{H}\,,\,C\} = 0$.
The reversed statement is true as well: Every Hamiltonian satisfying $\{\hat{H}\,,\,C\} = 0$ has the form $\begin{pmatrix} 0 & -\gamma(k) \\ -\gamma^*(k) & 0 \end{pmatrix}$ (since $(\sigma_x, \sigma_y, \sigma_z)$ is a maximum set of anti-commuting, Hermitian 2×2 matrices) and can be characterized by its winding number.

6.3 Chern Numbers and TKNN Invariant

Consider spinless (spin-polarized) electrons on a two dimensional square lattice.

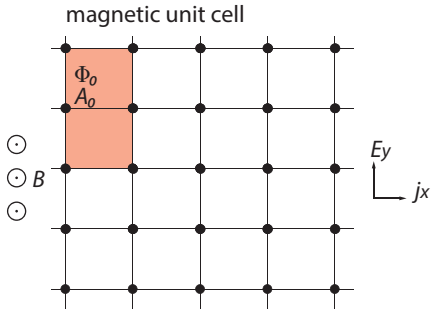

Figure 6.9: Two dimensional square lattice

In the presence of an external magnetic field perpendicular to the plane of the lattice the smallest possible unit cell encloses a flux quantum $\Phi = \Phi_0 = A_0 B = h/e$.
Consider a Hamiltonian $\hat{H}$ and a N-component wave function $\Psi_{\underline{k}}$ (where N is the number of lattice points in the unit cell) which satisfies the Schrödinger equation

$$\hat{H}(\underline{k})\Psi_{\underline{k}} = E_{\underline{k}}\Psi_{\underline{k}} \text{ with } \Psi_{\underline{k}} = \begin{pmatrix} \psi_{\underline{k},1} \\ \vdots \\ \psi_{\underline{k},N} \end{pmatrix} .$$

Application of the time-reversal Operator yields $\hat{T}\hat{H}\hat{T}^{-1} = \hat{H}^*(-\underline{k}) \neq \hat{H}(\underline{k})$.
Claim: If all bands are either completely filled or completely empty, the conductivity is given by

$$\sigma_{xy} = \frac{e^2}{\hbar}\,C \text{ with } C \in \mathbb{Z}\,.$$

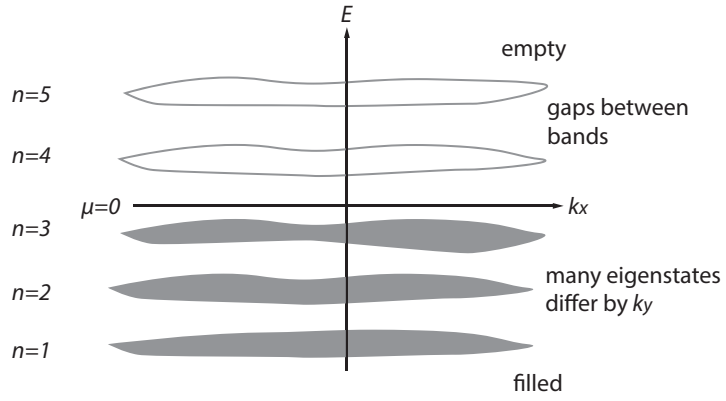

Figure 6.10: Band structure, only completely full and completely empty bands with gaps between each oter

Using the Bloch theorem $\Psi_{\underline{k}}(\underline{l}) = \mathrm{e}^{i\underline{k}\cdot\underline{l}} u_{\underline{k}}$ one can write C as

$$C = \sum_n \int_{\mathrm{BZ}} \frac{\mathrm{d}^2k}{2\pi} \left[\left(\partial_{k_x} u_j^{(n)*}(\underline{k})\right) \left(\partial_{k_y} u_j^{(n)}(\underline{k})\right) - \left(\partial_{k_y} u_j^{(n)*}(\underline{k})\right) \left(\partial_{k_x} u_j^{(n)}(\underline{k})\right) \right] .$$

Our aim is to show that C is an integer. Thouless, Kohmoto, Nightingale, Nijis (TKNN) were able to show this in 1982.
We will start from $j_x = \sigma_{xy} E_y$ where σ_{xy} is the conductivity, E_y is the electric field pointing in y-direction, and j_x is the current in x-direction.

6.3.1 Theory of Linear Response

We consider an unperturbed Hamiltonian $\hat{H}$ and eigenkets $|\psi_S(t)\rangle$ which satisfies the Schrödinger equation

$$i\hbar\partial_t |\psi_S(t)\rangle = \hat{H}|\psi_S(t)\rangle .$$

At $t = t_0$ a time-dependent external perturbation $\hat{H}_{\mathrm{ex}}$ is switched on. The new eigenstates $|\overline{\psi}_S(t)\rangle$ are solutions to the new Schrödinger equation

$$i\hbar\partial_t |\overline{\psi}_S(t)\rangle = \left[\hat{H} + \hat{H}_{\mathrm{ex}}\right] |\overline{\psi}_S(t)\rangle .$$

In the interaction picture time-dependence due to $\hat{H}_{\mathrm{ex}}$ is in the wave function, and time dependence due to $\hat{H}$ in operators

$$|\overline{\psi}_S(t)\rangle = \mathrm{e}^{-\frac{i}{\hbar}\hat{H}t} \underbrace{\hat{U}_I(t,t_0)|\overline{\psi}_S(t_0)\rangle}_{|\psi_I(t)\rangle} \qquad (*)$$

$$\Leftrightarrow |\psi_I(t)\rangle = \mathrm{e}^{\frac{i}{\hbar}\hat{H}t}|\overline{\psi}_S(t)\rangle$$

where the time evolution operator is

$$\hat{U}_I(t,t_0) = \hat{T}\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} \hat{H}_{\mathrm{ex},I}(t')\,\mathrm{d}t'\right] .$$

$$\hat{H}_{\mathrm{ex},I}(t) = \mathrm{e}^{\frac{i}{\hbar}\hat{H}t}\hat{H}_{\mathrm{ex}}(t)\mathrm{e}^{-\frac{i}{\hbar}\hat{H}t}$$

Expending (*) to lowest order yields

$$|\overline{\psi}_S(t)\rangle = \mathrm{e}^{-\frac{i}{\hbar}\hat{H}\,t}\left(\mathbb{1} - \frac{\boldsymbol{i}}{\hbar}\int\limits_{t_0}^{t}\mathrm{d}t'\;\hat{H}_{\mathrm{ex},I}(t')\right)|\psi_S(t_0)\rangle\;.$$

The expectation value of an operator $\hat{B}_S$ is given by

$$\begin{aligned}\langle\hat{B}\rangle(t) &= \langle\overline{\psi}_S(t)|\hat{B}_S|\overline{\psi}_S(t)\rangle \\ &= \langle\psi_S(t_0)|\left[\mathbb{1} - \frac{1}{\boldsymbol{i}\hbar}\int\limits_{t_0}^{t}\mathrm{d}t'\;\hat{H}_{\mathrm{ex},I}(t')\right]\underbrace{\mathrm{e}^{\frac{i}{\hbar}\hat{H}\,t}\hat{B}\mathrm{e}^{-\frac{i}{\hbar}\hat{H}\,t}}_{\hat{B}_I(t)}\left[\mathbb{1} + \frac{1}{\boldsymbol{i}\hbar}\int\limits_{t_0}^{t}\mathrm{d}t'\;\hat{H}_{\mathrm{ex},I}(t')\right]|\psi_S(t_0)\rangle + \mathcal{O}(H_{\mathrm{ex}}^2) \\ &= \langle\psi_S(t_0)|\hat{B}|\psi_S(t_0)\rangle - \frac{1}{\boldsymbol{i}\hbar}\int\limits_{t_0}^{t}\mathrm{d}t'\;\langle\psi_S(t_0)|[\hat{H}_{\mathrm{ex},I}(t')\,,\,\hat{B}_I(t)]|\psi_S(t_0)\rangle\end{aligned}$$

Taking $t_0 \to -\infty$ and denoting the initial unperturbed state as $|\psi_0\rangle$ yields

$$\delta\langle\hat{B}\rangle(t) = \frac{1}{\hbar}\int\limits_{-\infty}^{\infty}\mathrm{d}t'\;\underbrace{-\boldsymbol{i}\theta(t-t')\langle\psi_0|[\hat{B}_I(t)\,,\,\hat{H}_{\mathrm{ex},I}(t')]|\psi_0\rangle}_{\text{retarded Green function}}\;.$$

6.3.2 Conductivity Calculation

We want to calculate the current. We have

$$\begin{aligned}\hat{H} &= \frac{1}{2m}(\hat{\underline{p}} - q\hat{\underline{A}})^2 \\ \hat{j} &= \frac{\partial\hat{H}}{\partial\hat{\underline{A}}} = -q\frac{\hat{\underline{p}}}{m} = -q\hat{\underline{v}} \\ \hat{H}_{\mathrm{ex}} &= -q\frac{\hat{\underline{p}}}{m}\cdot\hat{\underline{A}} = -q\hat{\underline{v}}\cdot\hat{\underline{A}}\end{aligned}$$

and

$$\underline{E} = -\partial_t\underline{A}(t),\;\;\underline{A} = \underline{A}_0\mathrm{e}^{-\boldsymbol{i}\omega t},\;\;\underline{E} = \boldsymbol{i}\omega\underline{A}_0\mathrm{e}^{-\boldsymbol{i}\omega t},\;\;\underline{E} = \underline{E}_0\mathrm{e}^{-\boldsymbol{i}\omega t},\;\;\underline{A}(t) = \frac{\underline{E}_0}{\boldsymbol{i}\omega}\mathrm{e}^{-\boldsymbol{i}\omega t},\;\;\underline{A}_0 = \frac{\underline{E}_0}{\boldsymbol{i}\omega}\;.$$

Hence, $j_x = -qv_x$ and $\hat{H}_{\mathrm{ex}} = -q\frac{E_y}{\boldsymbol{i}\omega}\mathrm{e}^{-\boldsymbol{i}\omega t}\hat{v}_y$.
With the "volume" of the rectangular system $\Omega = L_xL_y$, we find

$$\langle j_x(0)\rangle = -\frac{\boldsymbol{i}}{\hbar}\frac{1}{\Omega}\sum_\alpha f(E_\alpha)\int\limits_{-\infty}^{0}\mathrm{d}t'\;\langle\alpha|[-q\hat{v}_x(0)\,,\,-q\frac{E_y\mathrm{e}^{-\boldsymbol{i}\omega t'}}{\boldsymbol{i}\omega}\,\hat{v}_y(t')]|\alpha\rangle$$

where $\alpha = (\underline{k}, n)$, $f(E_\alpha)$ is the Fermi-distribution, and the sum runs over all eigenstates $\hat{H}|\alpha\rangle = E_\alpha|\alpha\rangle$. We introduce a regularization η which is needed for convergence, and take $\eta \to 0$ after performing the sum:

$$\langle j_x(0)\rangle = \frac{\boldsymbol{i}e^2}{\hbar}\sum_\alpha f(E_\alpha)\int\limits_{-\infty}^{0}\mathrm{d}t'\;\frac{E_y\mathrm{e}^{-\boldsymbol{i}\omega t'+\eta t'}}{\boldsymbol{i}(\omega+\boldsymbol{i}\eta)}\langle\alpha|[\hat{v}_y(t')\,,\,\hat{v}_x(0)]|\alpha\rangle$$

We insert $\mathbb{1} = \sum_\beta |\beta\rangle\langle\beta|$ and use $\hat{v}_y(t') = \mathrm{e}^{\frac{\boldsymbol{i}}{\hbar}\hat{H}t'}\hat{v}_y(0)\mathrm{e}^{-\frac{\boldsymbol{i}}{\hbar}\hat{H}t'}$. We denote $E_\alpha = \omega_\alpha\hbar$. The integrand is given by

$$\frac{\mathrm{e}^{t'(-\boldsymbol{i}\omega+\eta)}\mathrm{e}^{\frac{t}{\hbar}(\boldsymbol{i}E_\alpha-\boldsymbol{i}E_\beta)}}{\boldsymbol{i}(\omega+\boldsymbol{i}\eta)}\left(\langle\alpha|\hat{v}_y|\beta\rangle\langle\beta|\hat{v}_x|\alpha\rangle - \langle\alpha|\hat{v}_x|\beta\rangle\langle\beta|\hat{v}_y|\alpha\rangle\right)$$

The time integration yields a factor $\frac{1}{-\boldsymbol{i}\omega+\eta+\boldsymbol{i}(E_\alpha-E_\beta)/\hbar}$. We thus find

$$\sigma_{xy} = \frac{e^2}{\boldsymbol{i}(\omega+\boldsymbol{i}\eta)}\frac{1}{\Omega}\sum_{\alpha,\beta} f(E_\alpha)\left[\frac{\langle\alpha|\hat{v}_y|\beta\rangle\langle\beta|\hat{v}_x|\alpha\rangle}{-\hbar\omega-\boldsymbol{i}\eta+E_\alpha-E_\beta} - \frac{\langle\alpha|\hat{v}_x|\beta\rangle\langle\beta|\hat{v}_y|\alpha\rangle}{-\hbar\omega-\boldsymbol{i}\eta+E_\beta-E_\alpha}\right] .$$

We use the expansion

$$\frac{1}{\pm\hbar\omega+E_\alpha-E_\beta} = \frac{1}{E_\alpha-E_\beta}\left(1\mp\frac{\hbar\omega}{E_\alpha-E_\beta}\right)+\mathcal{O}(\omega^2) .$$

Let the first-order term be denoted by σ^1 and the second-order term by σ^2.

$$\sigma^1 = \frac{e^2}{\boldsymbol{i}(\omega+\boldsymbol{i}\eta)}\sum_{\alpha,\beta} f(E_\alpha)\frac{\langle\alpha|\hat{v}_x|\beta\rangle\langle\beta|\hat{v}_y|\alpha\rangle - \langle\alpha|\hat{v}_y|\beta\rangle\langle\beta|\hat{v}_x|\alpha\rangle}{E_\alpha-E_\beta}$$

We use $\hat{v}_x = \frac{\mathrm{d}}{\mathrm{d}x}\hat{x} = \frac{\boldsymbol{i}}{\hbar}[\hat{H}_0\,,\,\hat{x}]$ to obtain

$$\langle\alpha|\hat{v}_x|\beta\rangle = \frac{\boldsymbol{i}}{\hbar}\langle\alpha|\hat{H}_0\hat{x}-\hat{x}\hat{H}_0|\beta\rangle = \frac{\boldsymbol{i}}{\hbar}(E_\alpha-E_\beta)\langle\alpha|\hat{x}|\beta\rangle$$

$$\Rightarrow \langle\alpha|\hat{v}_x|\beta\rangle\langle\beta|\hat{v}_y|\alpha\rangle + \langle\alpha|\hat{v}_y|\beta\rangle\langle\beta|\hat{v}_x|\alpha\rangle = (E_\alpha-E_\beta)\left[\langle\alpha|\hat{x}|\beta\rangle\langle\beta|\hat{v}_y|\alpha\rangle - \langle\alpha|\hat{v}_y|\beta\rangle\langle\beta|\hat{x}|\alpha\rangle\right] .$$

Since factors $E_\alpha - E_\beta$ cancel each other in numerator and denominator, we use $\sum_\beta |\beta\rangle\langle\beta| = \mathbb{1}$ and obtain

$$\sigma^1 = \frac{e^2}{\boldsymbol{i}(\omega+\boldsymbol{i}\eta)}\sum_\alpha f(E_\alpha)\,\langle\alpha|\underbrace{\hat{x}\hat{v}_y-\hat{v}_y\hat{x}}_{[\hat{x}\,,\,\hat{v}_y]=0}|\beta\rangle = 0 .$$

The second order term is

$$\sigma^2 = \frac{e^2\hbar}{\boldsymbol{i}}\sum_{\alpha,\beta} f(E_\alpha)\frac{-\langle\alpha|\hat{v}_x|\beta\rangle\langle\beta|\hat{v}_y|\alpha\rangle + \langle\alpha|\hat{v}_y|\beta\rangle\langle\beta|\hat{v}_x|\alpha\rangle}{(E_\alpha-E_\beta)^2} .$$

This is the starting point in D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs [Phys. Rev. Lett. **49**, 405 (1982)].

$\underline{v} = \nabla_{\underline{k}}\hat{H}(\underline{k})\frac{1}{\hbar}$ from $\underline{v}_g = \nabla_{\underline{k}}\omega(\underline{k}) = \frac{1}{\hbar}\nabla_{\underline{k}}E(\underline{k})$. The sums contain $\int\frac{\mathrm{d}^2k}{(2\pi)^2} \mathrel{\hat{=}} \sum_\alpha$, and

$$\langle\alpha|(\partial_{k_x}\hat{H})|\beta\rangle = \sum_{j,l}(u^*_{\alpha,j})(\partial_{k_y}\hat{H}_{jl}(\underline{k}))u_{\beta l} .$$

With integration by parts we have

$$\begin{aligned}\langle\alpha|(\partial_{k_x}\hat{H})|\beta\rangle &= -\sum_{j,l}\hat{H}_{jl}[(\partial_{k_x}u^*_{\alpha j})u_{\beta l}+u^*_{\alpha j}(\partial_{k_y}u_{\beta l})]\\ &= -\sum_{j}\left[(\partial_{k_x}u^*_{\alpha j})E_\beta u_{\beta j}+E_\alpha u^*_{\alpha j}(\partial_{k_x}u_{\beta j})\right]\ .\end{aligned}$$

Use again integration by parts to get the derivative in the second term acting on $u^*_{\alpha j}$

$$\langle\alpha|(\partial_{k_x}\hat{H})|\beta\rangle = (E_\alpha-E_\beta)\sum_j(\partial_{k_x}u^*_{\alpha j})u_{\beta j} = (E_\beta-E_\alpha)\sum_j u^*_{\alpha j}(\partial_{k_x}u_{\beta j})\ .$$

We do the same for action of ∂_{k_x} on bra and ket using integration by parts, and let only act derivatives on $|\alpha\rangle$, and $\langle\alpha|$ respectively. This yields ($\alpha=(n,\underline{k})$):

$$\sigma_{xy} = \frac{\boldsymbol{i}e^2}{\hbar}\sum_{n,E_n<0}\int\frac{\mathrm{d}^2k}{(2\pi)^2}\left[(\partial_{k_x}u^*_{\alpha j})(\partial_{k_y}u_{\alpha j})-(\partial_{k_y}u^*_{\alpha j})(\partial_{k_x}u_{\alpha j})\right]\ .$$

Rewrite this expression in terms of a Berry connection and Berry flux:
Berry connection:

$$\widetilde{A}_x = \boldsymbol{i}\langle n,\underline{k}|\partial_{k_x}|n,\underline{k}\rangle$$

Berry flux:

$$\begin{aligned}F_{xy} &= \frac{\partial\widetilde{A}_x}{\partial k_x}-\frac{\partial\widetilde{A}_x}{\partial k_y}\\ &= \boldsymbol{i}(\partial_{k_x}\langle n,\underline{k}|)(\partial_{k_y}|n,\underline{k}\rangle)-(\partial_{k_y}\langle n,\underline{k}|)(\partial_{k_x}|n,\underline{k}\rangle)\\ \Rightarrow\sigma_{xy} &= \frac{e^2}{2\pi\hbar}\sum_{n,E_n<0}\frac{1}{2\pi}\int\mathrm{d}^2k\ F_{xy}\ .\end{aligned}$$

We focus on the contribution of a single occupied band in the following.
Stokes theorem states that the integral of F_{xy} over the Brillouin zone is equal to the line integral of $\underline{\widetilde{A}}$ along the border of the BZ:

$$\frac{1}{2\pi}\int\mathrm{d}^2kF_{xy} = \frac{1}{2\pi}\oint\mathrm{d}\underline{k}\ \underline{\widetilde{A}}(\underline{k})\ .$$

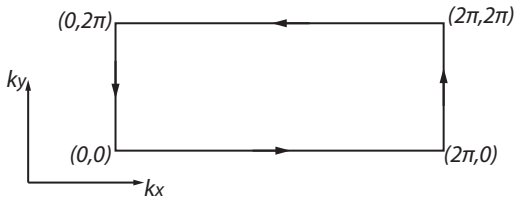

Figure 6.11: Border of the BZ for line integration

- Complex $\psi(\underline{k})$ is periodic, $\psi(\underline{k}) = \mathrm{e}^{\boldsymbol{i}\varphi}\psi_0(\underline{k})$

- $e^{i\varphi}\partial_l\psi_l(\underline{k}) \Rightarrow \underline{\widetilde{A}}(\underline{k})$ is not periodic in general.

We have reciprocal lattice vectors $G_x = (2\pi, 0)$ and $G_y = (0, 2\pi)$, and

$$\left.\begin{aligned}\psi_{\underline{k},j}(\underline{l}) &= e^{i\underline{k}\cdot\underline{l}}u_{\underline{k},j}\\ \psi_{\underline{k}+\underline{G},j}(\underline{l}) &= e^{i\phi_{\underline{k},\underline{G}}}\psi_{\underline{k},j}(\underline{l})\end{aligned}\right\} u_{\underline{k}+\underline{G}\,j} = e^{-i\underline{G}\cdot\underline{l}}e^{i\phi_{\underline{k},\underline{G}}}u_{\underline{k}j},$$

where we used $\psi_{\underline{k}+\underline{G},j} = e^{i\underline{G}\cdot\underline{l}}e^{i\underline{k}\cdot\underline{l}}u_{\underline{k}+\underline{G}\,j}$.
For the integral over the contour, we thus find

$$\begin{aligned}\oint \mathrm{d}\underline{k}\cdot\underline{\widetilde{A}} &= \int_0^{G_x}\left[\widetilde{A}_x(k_x,0) - \widetilde{A}_x(k_x,G_y)\right]\mathrm{d}k_x + \int_0^{G_y}\left[\widetilde{A}_y(G_x,k_y) - A_y(0,k_y)\right]\mathrm{d}k_y\\ &= \int_0^{G_x}(\partial_{k_x}\phi_{k_x,G_y})\mathrm{d}k_x - \int_0^{G_y}(\partial_{k_y}\phi_{k_y,G_x})\mathrm{d}k_y\\ &= \phi_{G_x,G_y} - \phi_{0,G_y} - \phi_{G_y,G_x} + \phi_{0,G_y} \equiv -2\pi C\ .\end{aligned}$$

However, by using $\psi_{\underline{k}+\underline{G},j} = e^{i\phi_{\underline{k},\underline{G}}}\psi_{\underline{k},j}$, we see that the wave functions at the corners of the BZ are related in the following way

$$\begin{aligned}\psi_{G_x+G_y} &= e^{i\phi_{G_x,G_y}}\psi_{G_x} = e^{i\phi_{G_x,G_y}}e^{i\phi_{0,G_x}}\psi_0\\ \psi_{G_x+G_y} &= e^{i\phi_{G_y,G_x}}\psi_{G_y} = e^{i\phi_{G_y,G_x}}e^{i\phi_{0,G_y}}\psi_0\\ \Rightarrow 2\pi n &= \phi_{G_x,G_y} + \phi_{0,G_x} - \phi_{0,G_y} - \phi_{G_y,G_x} \text{ with } n\in\mathbb{Z}\end{aligned}$$

$$\Rightarrow C\in\mathbb{Z} \Rightarrow \sigma_{xy} = \frac{e^2}{2\pi\hbar}\,C\ .$$

Since C is an integer, it cannot change continuously and it will not change at all if we make a small change in the Hamiltonian or its associated wave functions. C can only change when there is a degeneracy between bands. In this case, the Berry curvature becomes singular at the degeneracy point, and the integral over the Brillouin zone changes continuously.
C is called Chern number, it is a $\mathbb{Z}$ topological invariant.

6.4 Kitaev Toric Code and Anyons

We consider interacting quantum spins on a two dimensional lattice with periodic boundary conditions ("on a torus"). σ_i^x, σ_i^y are spin $\frac{1}{2}$ at each lattice site $i \Rightarrow$ 2D complex Hilbert space.

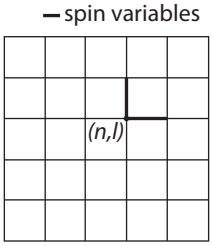

Figure 6.12: Spins are associated with links between lattice sites

Two links, a horizontal and a vertical one, are associated with each lattice site. The total Hilbert space is a direct product of the individual site spin-states. Spins are localized at specific lattice sites and are hence distinguishable. $\Rightarrow$ Spins at different links commute with each other. $\Rightarrow [\sigma_i^\alpha\,,\,\sigma_j^\beta] = 0$ if $i \neq j$, and $\{\sigma_i^\alpha\,,\,\sigma_i^\beta\} = 2\delta_{\alpha,\beta}$, where $\alpha, \beta \in \{x, y, z\}$.
We understand for $i \neq j$: $\sigma_i^\alpha \sigma_j^\alpha = \sigma_i^\alpha \otimes \sigma_j^\alpha$. In addition we have

$$[\sigma_i^\alpha \sigma_j^\alpha\,,\,\sigma_i^\beta \sigma_j^\beta] = 0 \;\; \forall i, j\;. \tag{*}$$

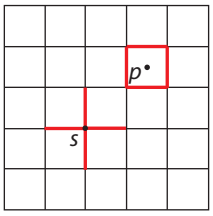

Figure 6.13: Points s lie on the lattice and the associated links are the connections to the four neighbors (star s), points p lie on the dual lattice and associated links lie around p (bound p)

We consider a Hamiltonian

$$\hat{H} = -\sum_s A_s - \sum_p B_p \text{ with } A_s = \prod_{j \in \text{star}(s)} \sigma_j^x \text{ and } B_p = \prod_{j \in \text{bound}(p)} \sigma_j^z\;.$$

Possible eigenvalues of A_s and B_p are ± 1.

$$\prod_s A_s = \prod_p B_p = +1 \tag{**}$$

for periodic boundary conditions (each link belongs to exactly two stars in this case. $\Rightarrow$ Products are one since $(\sigma_j^x)^2 = (\sigma_j^z)^2 = \mathbb{1}$). Each spin (link) occurs twice in the product. In addition we know, $[A_s\,,\,A_{s'}] = 0 = [B_p\,,\,B_{p'}]\;\; \forall s, s'; p, p'$. Consider the commutator between A_s and B_p: $[A_s\,,\,B_p] = 0\;\forall s, p$ as the A_s and B_p have either zero or two common links, and thus commute with each other due to (*). $\Rightarrow$ The A_s and B_p commute with $\hat{H}$ and can be diagonalized simultaneously with $\hat{H}$ (are good quantum numbers).
The ground state is characterized by $A_s = 1 = B_p$ (smallest energy in $\hat{H}$) with $E_0 = -2N^2$. Due to (**), any excited state must have at least two A_s or two B_p reversed. $\Rightarrow E_{\min} = 4$ is the minimum excitation energy.

Surprisingly, the ground state is four-fold degenerate. Due to the constraint (**) only $N^2 - 1$ of the A_s and $N^2 - 1$ of the B_p are independent variables. $\Rightarrow$ Two degrees of freedom are left. $\Rightarrow 2 \cdot 2 = 4$-fold degeneracy. This is a heuristic argument, and looking at $\hat{H}$ there is no freedom in choosing A_s and B_p for the ground state. We will provide a better argument in the following.

To understand the nature of the ground state degeneracy, we work in the σ^z-basis and associate with $\sigma_j^z = 1\;(-1)$ the quantity $z_j = 0\;(1)$.

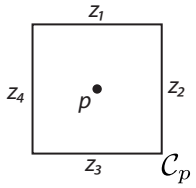

Figure 6.14: Labeling of the links around a dual lattice point

Then the ground state constraint $B_p = 1$ is equivalent to

$$\varphi_p \equiv \mathrm{mod}_2 \sum_{j \in \mathrm{bound}(\mathcal{C}(p))} z_j = 0 \, .$$

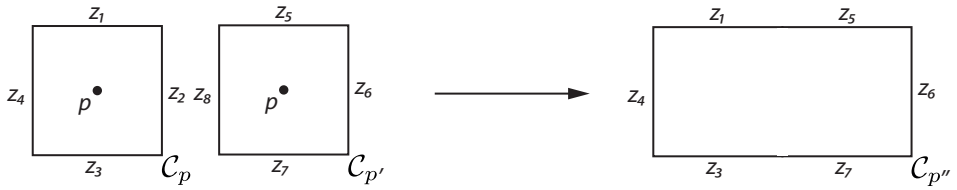

Figure 6.15: Two neighboring patches can be combined since the z of the shared links appear twice and $\mathrm{mod}_2 2 = 0 = \mathrm{mod}_2 0$

We combine two neighboring parquets and consider

$$\begin{aligned} \varphi_{\mathcal{C}''} &= \mathrm{mod}_2 \sum_{j \in \mathcal{C}''} z_j = \mathrm{mod}_2(z_1 + z_2 + z_3 + z_5 + z_6 + z_7) \\ &= \mathrm{mod}_2(z_1 + z_2 + z_3 + z_4) + \mathrm{mod}_2(z_5 + z_6 + z_7 + z_8) \\ &= \varphi_p + \varphi_{p'} = 0 \text{ in the ground state} \end{aligned}$$

$\Rightarrow \varphi_{\mathcal{C}} = 0$ for any closed path $\mathcal{C}$.

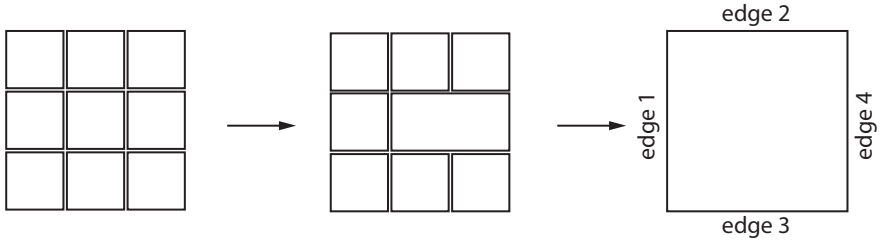

Figure 6.16: We iterate the combining procedure

Iterating the procedure, we are led to consider φ_{tot} corresponding to the whole array and have in the ground state

$$\varphi_{\mathrm{tot}} \equiv \mathrm{mod}_2 \sum_{j \in \mathcal{C}_{\mathrm{tot}}} z_j = 0 \, .$$

Due to periodic boundary conditions we have edge 1 =edge 4 and edge 2 =edge 3 . $\Rightarrow$ Each edge occurs twice in the sum. This leaves the possibility that the sum along one edge characterizes

the ground state.

$$v_1 \equiv \mathrm{mod}_2 \sum_{j\in \text{edge } 1} z_j = \begin{cases} 0 \\ 1 \end{cases} \quad , \quad v_2 \equiv \mathrm{mod}_2 \sum_{j\in \text{edge } 2} z_j = \begin{cases} 0 \\ 1 \end{cases} .$$

We define "string operators" of the type

$$Z_{\mathcal{C}} \equiv \prod_{j\in\mathcal{C}} \sigma_j^z \text{ and } X_{\mathcal{C}'} \equiv \prod_{j\in\mathcal{C}'} \sigma_j^x .$$

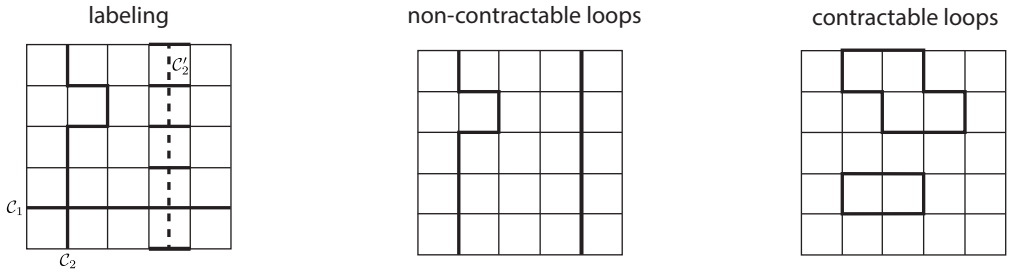

Figure 6.17: We consider paths $\mathcal{C}$ on the lattice where the associated links are along the path, and paths $\mathcal{C}'$ on the dual lattice where the associated links are the ones crossed by the path

According to the above, a contactable Z-loop yields

$$\prod_{p \text{ inside } \mathcal{C}} B_p \hat{=} \mathbb{1}$$

(here defined p are inside the loop and we can contract as before). There are two independent uncontractable Z-loops and X-loops: Z_1 and Z_2 encircling the torus in horizontal and vertical directions, respectively. The same holds for X_1 and X_2.
$\mathcal{C}_{1/2}$ and $\mathcal{C}'_{1/2}$ go in the same direction and share an even number of links (commute) whereas, $\mathcal{C}_{1/2}$ and $\mathcal{C}'_{2/1}$ go in orthogonal directions and share an odd number of links (anti-commute).

$$[X_1\,,\,Z_1] = 0 \quad , \quad [X_2\,,\,Z_2] = 0$$
$$\{X_1\,,\,Z_2\} = 0 \quad , \quad \{X_2\,,\,Z_1\} = 0$$

$\Rightarrow$ We can make correspondence $Z_1 \to \sigma_1^z$, $Z_2 \to \sigma_2^z$, $X_1 \to \sigma_2^x$, $X_2 \to \sigma_1^x$, such that the Z_i and X_i form Pauli matrices in a 2-qubit (4 dimensional) ground state manifold.
These operators are non-local, and cannot be perturbed by local perturbations.

Elementary excitations: Consider string operators associated with open contours t, t'.

$$S^z(t) \equiv \prod_{j\in t} \sigma_j^z \quad , \quad S^x(t') \equiv \prod_{j\in t'} \sigma_j^x .$$

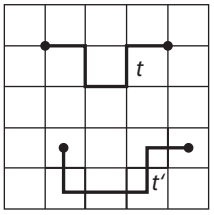

Figure 6.18: Open paths on the lattice and dual lattice, respectively

The operator $S^z(t)$ commutes with all the A_s, except for the end-point sites, where the sign of the A_s gets inverted. Similarly, $S^x(t')$ commutes with all the B_p except the end ones, which get inverted.

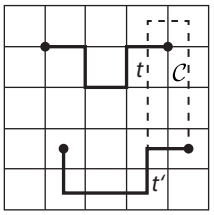

Figure 6.19: We move one end-point around another by extending the path with a closed loop $\mathcal{C}$ which adds 1 shared link.

We now consider moving an X-quasi-particle (end of a X-string) around a Z-quasi-particle (end of a Z string). This will result in a single link shared by the two strings $\Rightarrow \{S^x(\mathcal{C})\,,\, S^z(t)\} = 0$. Initial state:

$$|\psi_i\rangle = S^z(t)S^x(t')|0\rangle \equiv S^z(t)|\psi_{t'}\rangle$$

Final state:

$$\begin{aligned} |\psi_f\rangle &= S^x(\mathcal{C})S^z(t)S^x(t')|0\rangle \\ &= -S^z(t)S^x(t')S^x(\mathcal{C})|0\rangle \\ &= -S^z(t)S^x(t')|0\rangle = -|\psi_i\rangle \end{aligned}$$

Since a closed loop applied to the vacuum is the identity applied to the vacuum, $S^x(\mathcal{C})|0\rangle = |0\rangle$. As the X-loop gives rise to sign change $-1 = \mathrm{e}^{\boldsymbol{i}\pi}$, a particle exchange, which is a half loop, and a translation (translational invariant system), gives rise to $\mathrm{e}^{\boldsymbol{i}\pi/2} = \boldsymbol{i}$. $\Rightarrow$ Anyonic statistics, neither fermion (-1) nor boson (1). This particular type of anyonic statistics with phase $\boldsymbol{i}$ is called *semionic*. Such a state as considered is called a topological phase of matter. It is characterized by a energy gap, a ground state degeneracy on the torus, and fractional quasi-particles.