4 Symmetry in Quantum Mechanics

4.1 Symmetries, Conservation Laws, and Degeneracies → general (continuous)

4.2 Discrete Symmetries, Parity or Space Inversion

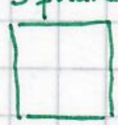
4.3 Lattice Translation as a Discrete Symmetry

4.4 The Time-Reversal Discrete Symmetry

specific symmetries

4.2, 4.3, and 4.4 talk about discrete symmetries:

square



which rotation angles give the "same" geometry"?

particular angles → discrete symmetry

Same question →

any angle → continuous symmetry

Start with 4.1: Symmetries, Conservation Laws, and Degeneracies

To set the stage: Look at classical mechanics

→ Lagrange's equations of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

$$\underbrace{q_i \text{ cyclic}} \Rightarrow p_i = \frac{\partial L}{\partial \dot{q}_i} \text{ conserved}$$

this is equivalent to saying that L has a symmetry under $q_i \to q_i + \delta q_i$

Equivalently: $\frac{dp_i}{dt} = 0 \Rightarrow \frac{\partial H}{\partial q_i} = 0$

H has a symmetry under $q_i \to q_i + \delta q_i$

Want to go to quantum case:

Consider unitary operator $\hat{\mathcal{S}}$ that differs infinitesimally from the identity transformation:

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

Hermitian generator of the "symmetry operator" $\hat{\mathcal{S}}$

e.g.: $\hat{\mathbb{1}} - i\frac{\vec{x}}{\hbar}\cdot\vec{p}$

infinitesimal translation by $\vec{x}$ generated by $\vec{p}$

Assume $\hat{H}$ is invariant under $\hat{\mathcal{S}}$, i.e., $\hat{\mathcal{S}}^+ \hat{H} \hat{\mathcal{S}} = \hat{H}$.

$$\Longrightarrow \quad [\hat{G}, \hat{H}] = 0$$

To see this, start with $\hat{\mathcal{S}}^+ \hat{H} \hat{\mathcal{S}} = \hat{H}$: plug in

$$\hat{\mathcal{S}}^+ \hat{H} \hat{\mathcal{S}} = \left(\hat{\mathbb{1}} + \frac{i\varepsilon}{\hbar}\hat{G}\right)\hat{H}\left(\hat{\mathbb{1}} - \frac{i\varepsilon}{\hbar}\hat{G}\right)$$

multiply out

$$= \hat{H} - i\frac{\varepsilon}{\hbar}\left(\hat{H}\hat{G} - \hat{G}\hat{H}\right) + O(\varepsilon^2)$$

$$= \hat{H}$$

according to $\hat{\mathcal{S}}^+ \hat{H} \hat{\mathcal{S}} = \hat{H}$

$$\Rightarrow \hat{H}\hat{G} - \hat{G}\hat{H} = 0$$

Heisenberg eq. of motion $$\frac{d\hat{G}}{dt} = \frac{1}{i\hbar}\underbrace{[\hat{G}, \hat{H}]}_{\substack{=0 \\ \text{(see above)}}} + \underbrace{\frac{\partial \hat{G}}{\partial t}}_{\substack{=0 \text{ by} \\ \text{assumption}}}$$

$$\Rightarrow \frac{d\hat{G}}{dt} = 0$$

So: $\boxed{\underbrace{\hat{\mathcal{S}}^+ \hat{H} \hat{\mathcal{S}} = \hat{H}}_{\text{symmetry}} \Rightarrow \underbrace{\hat{G} \text{ is a constant of motion}}_{\text{conservation law}}}$

e.g.: $\hat{H}$ invariant under translation $\Rightarrow$ momentum is constant of motion

$\hat{H}$ invariant under rotation $\Rightarrow$ angular momentum is constant of motion

We have a connection between "symmetry" and "conservation law".

Next, we want to bring in degeneracies.

Assume $\underbrace{[\hat{H}, \hat{\mathcal{S}}]}_{\text{sym}} = 0$ and let $|n\rangle$ be energy eigenket of $\hat{H}$ with eigenvalue E_n

$$\underbrace{\hat{H}\,\hat{\mathcal{S}}\,|n\rangle}_{\text{act on } |n\rangle} = \hat{\mathcal{S}}\,\underbrace{\hat{H}\,|n\rangle}_{E_n|n\rangle}$$

add brackets to enhance readability

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

E_n is a scalar (can be moved)

→ If $|n\rangle$ is eigenket of $\hat{H}$ and $[\hat{H}, \hat{\mathcal{S}}] = 0$, then $\hat{\mathcal{S}}|n\rangle$ is also an eigenket of $\hat{H}$ with eigen energy E_n

→ If $|n\rangle$ and $\hat{\mathcal{S}}|n\rangle$ are different states, we have a symmetry.

Specific case: $\hat{\mathcal{S}} = \underbrace{\hat{\mathcal{D}}(R)}_{\text{rotation operator}}$

(see chapter 3)

e.g.: $\hat{\mathcal{D}}_z(\phi) = \exp\left(-i\,\frac{\hat{S}_z\phi}{\hbar}\right)$

rotation by angle ϕ about the z-axis (spin-$\frac{1}{2}$ system)

$$\underbrace{\mathcal{D}^{(j)}_{m'm}(R)}_{\text{matrix elements}} = \langle j,m'|\underbrace{e^{-i\hat{\vec{J}}\cdot\hat{n}\phi/\hbar}}_{\text{rotation specified by } \hat{n} \text{ and } \phi}|j,m\rangle$$

Assume $\underbrace{[\hat{\mathcal{D}}(R), \hat{H}] = 0}_{\text{Hamiltonian is rotationally invariant}} \Rightarrow \underbrace{[\hat{\vec{J}}, \hat{H}] = 0 \;\&\; [\hat{\vec{J}}^2, \hat{H}] = 0}$

look at simultaneous eigenkets of $\hat{H}$, $\hat{\vec{J}}^2$, and $\hat{J}_z$. Call them $|n;j,m\rangle$

$\rightsquigarrow$ according to the above, the states $\hat{\mathcal{D}}(R)|n;j,m\rangle$ have the same energy as $|n;j,m\rangle$.

Since we can write

mixes the different m values

$$\hat{\mathcal{D}}(R)|n; j,m\rangle = \sum_{m'} \mathcal{D}^{(j)}_{m'm}(R)|n; j,m'\rangle,$$

the degeneracy is $2j+1$.

we know that m' can take $2j+1$ different values

e.g.: isotropic 3D HO oscillator

→ the energy levels can be labeled by n and l:

$$E_{n,l} = \left(2n + l + \tfrac{3}{2}\right)\hbar\omega$$

for each l, we have $2l+1$ different m_l levels

→ if we add an external electric or magnetic field, the symmetry is broken (preferred axis) and the energy levels get split

Very, very special case: SO(4) symmetry in the Coulomb potential

$$E_n = -\frac{E_h}{2}\frac{1}{n^2} \quad ; \quad E_h = \text{Hartree energy}$$

the fact that E_n does not depend on

l is <u>not</u> accidental!

Classically: Closed elliptical orbits $\leftrightarrow$ Runge-Lenz vector $\vec{M}$

is constant of motion.

$$\vec{M} = \frac{1}{m}\vec{p}\times\vec{L} - \frac{Ze^2}{r}\vec{r}$$

Quantum mechanically: SO(4) symmetry

Spatial dim.

Recall: Section 3.3 $\rightarrow$ SO(3)

special orthogonal (no inversion)

O(3) includes inversion

SO(4): group of rotation operators in four spatial dimensions (i.e., group of orthogonal 4×4 matrices with unit determinant)

What do we need to do to "understand" SO(4)?
We need to identify the symmetry and we need to construct generator.
This is quite a bit of work.

I will only mention a few key things.

- Need to symmetrize $\vec{M}$: $\hat{\vec{M}} = \frac{1}{2m}\left(\hat{\vec{p}} \times \hat{\vec{L}} - \hat{\vec{L}} \times \hat{\vec{p}}\right) - \frac{Ze^2}{r}\vec{r}$

use $(\hat{\vec{A}} \times \hat{\vec{B}})^+ = - \hat{\vec{B}} \times \hat{\vec{A}}$
($\hat{\vec{A}}, \hat{\vec{B}}$ Hermitian)

- One can verify $[\hat{\vec{M}}, \hat{H}] = 0 \Rightarrow \hat{\vec{M}}$ is q.m. constant of motion

- Also: $\hat{\vec{L}} \cdot \hat{\vec{M}} = \hat{\vec{M}} \cdot \hat{\vec{L}} = 0$ & $\hat{\vec{M}}^2 = \frac{2}{m}\hat{H}\left(\hat{\vec{L}}^2 + \hbar^2\right) + Z^2 e^4$

- Part of the algebra is known: $[\hat{L}_i, \hat{L}_j] = i\hbar\, \varepsilon_{ijk} \hat{L}_k$

- One can show: $[\hat{M}_i, \hat{L}_j] = i\hbar\, \varepsilon_{ijk} \hat{M}_k$
  & $[\hat{M}_i, \hat{M}_j] = -i\hbar\, \varepsilon_{ijk} \frac{2}{m} \hat{H} \hat{L}_k$

not a closed algebra

"deal" with this by restricting state space to states with negative energies: $\hat{H} \to E$

Defining $\hat{\vec{N}} = \left(-\frac{m}{2E}\right)^{1/2} \hat{\vec{M}}$, one finds a closed algebra:

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

group SO(4) ($\cong SU(2) \times SU(2)$)

It turns out (this is non-trivial!) that this algebra generates a "rotation in four spatial dimensions"

As stated earlier: the discussion given only provides a "glimpse". We will now look at a few other symmetries in a bit more detail.

4.2 Discrete Symmetries, Parity or Space Inversion

Parity operator acting on coordinate system: Right-handed coordinate system turns into left-handed coordinate system.

Throughout: looking for action of operators on state kets.

$\hat{\pi}$: parity operator (unitary)

$\hat{\pi}\,|\alpha\rangle$: space inverted state

Demand : $\underbrace{\langle\alpha|\hat{\pi}^{+}\,\hat{\vec{x}}\,\hat{\pi}|\alpha\rangle}_{\text{expectation value of } \vec{x} \text{ with respect to space inverted state should yield minus sign of } \langle\alpha|\hat{\vec{x}}|\alpha\rangle} = -\langle\alpha|\hat{\vec{x}}|\alpha\rangle$

or $\quad \hat{\pi}^\dagger \hat{\vec{x}} \hat{\pi} = -\hat{\vec{x}} \quad \Rightarrow \quad \hat{\vec{x}} \hat{\pi} = -\hat{\pi} \hat{\vec{x}}$

using that
$\hat{\pi}$ is unitary

So: we demand that $\hat{\vec{x}}$ and $\hat{\pi}$ anti-commute.

To see how $\hat{\pi}$ acts on eigenket of $\hat{\vec{x}}$, let's work out $\hat{\vec{x}} \hat{\pi} |\vec{x}'\rangle$:

$$\hat{\vec{x}} \hat{\pi} |\vec{x}'\rangle = -\hat{\pi} \underbrace{\left(\hat{\vec{x}} |\vec{x}'\rangle\right)}_{\vec{x}' |\vec{x}'\rangle} = -\vec{x}' \hat{\pi} |\vec{x}'\rangle$$

using
$\hat{\vec{x}} \hat{\pi} = -\hat{\pi} \hat{\vec{x}}$

rewrite: $\hat{\vec{x}} \left(\hat{\pi} |\vec{x}'\rangle\right) = -\vec{x}' \left(\hat{\pi} |\vec{x}'\rangle\right)$

So: $(\hat{\pi} |\vec{x}'\rangle)$ is an eigenket of $\hat{\vec{x}}$ with eigenvalue $-\vec{x}'$

$\rightsquigarrow$ $(\hat{\pi} |\vec{x}'\rangle)$ must be the same as $|-\vec{x}'\rangle$ up to a phase factor

$$\Rightarrow \quad \hat{\pi} |\vec{x}'\rangle = \underbrace{e^{i\delta}}_{} |-\vec{x}'\rangle$$

set equal to
one by convention

$$\Rightarrow \quad \hat{\pi} \left(\hat{\pi} |\vec{x}'\rangle\right) = |\vec{x}'\rangle \quad \Rightarrow \quad \hat{\pi}^2 = \hat{1}$$

$\boxed{\text{eigenvalues of } \hat{\pi} \text{ are } \pm 1}$

$\boxed{\text{Since } \hat{\pi}^{-1} = \hat{\pi}^{+} = \hat{\pi} \text{, the parity operator is Hermitian}}$

We found: $\hat{\pi}^{+} \hat{\vec{x}} \hat{\pi} = -\hat{\vec{x}} \longrightarrow \hat{\vec{x}}$ is odd under parity
(or postulated)

We can find: $\hat{\pi}^{+} \hat{\vec{p}} \hat{\pi} = -\hat{\vec{p}}$

However: $\hat{\pi}^{+} \hat{\vec{J}} \hat{\pi} = \hat{\vec{J}}$

angular momentum:

classically, think of $\underbrace{\vec{r} \times \vec{p}}_{\text{two minus signs}}$

more generally, $\hat{\vec{J}}$ generates rotation:

$$\underbrace{R^{(\text{parity})}}_{\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}} R^{(\text{rotation})} = R^{(\text{rotation})} R^{(\text{parity})}$$

this equal sign holds for 3x3 orthogonal matrices

$$\text{QM: } \hat{\pi} \underbrace{\hat{\mathcal{D}}(R)}_{e^{-i \hat{\vec{J}} \cdot \hat{n}\, \epsilon/\hbar}} = \hat{\mathcal{D}}(R) \hat{\pi}$$

$\hat{\vec{x}}, \hat{\vec{p}}$ are odd under parity ; $\hat{\vec{J}}$ is even under parity

"polar vectors" "axial vectors / pseudo vectors"

"condensed matter spin-orbit coupling"

Also: $\hat{\pi}^{-1} \; \hat{\vec{p}} \cdot \hat{\vec{S}} \; \hat{\pi} = - \hat{\vec{p}} \cdot \hat{\vec{S}}$

$\hat{\pi}^{-1} \; \hat{\vec{L}} \cdot \hat{\vec{S}} \; \hat{\pi} = + \hat{\vec{L}} \cdot \hat{\vec{S}}$

"atomic physics spin-orbit coupling"

Same name : spin-orbit coupling

But : distinct transformation properties !

We will encounter both types of spin-orbit couplings in HW / later in class.

What happens to wave function under parity?

Let $\psi(\vec{x}') = \langle \vec{x}' | \alpha \rangle$ ($|\alpha\rangle \doteq$ state ket of spinless particle)

Let $\hat{\pi} |\alpha\rangle$ be space inverted state ket.

Then : $\langle \vec{x}' | \hat{\pi} | \alpha \rangle = \langle -\vec{x}' | \alpha \rangle = \psi(-\vec{x}')$

yields $\langle -\vec{x}' |$

If $|\alpha\rangle$ eigenket of $\hat{\pi}$, then $\hat{\pi} |\alpha\rangle = \pm |\alpha\rangle \Rightarrow \langle \vec{x}' | \hat{\pi} | \alpha \rangle = \pm \langle \vec{x}' | \alpha \rangle$

even parity

$$\psi(-\vec{x}') = \pm\, \psi(\vec{x}')$$

odd parity

Examples: Parity of gr. st. 1D HO fct.? $\rightsquigarrow$ pos. parity

Parity of first exc. st. wave fct. of 1D HO? $\rightsquigarrow$ neg. parity

momentum eigenket (i.e., $e^{i\vec{k}\cdot\vec{x}}$)?
$\rightsquigarrow$ does not have definite parity

Eigen kets of H-atom? $R_{nl}(r)\, Y_l^m(\hat{r})$
$\rightsquigarrow$ parity is given by $(-1)^l$

Look at the last example in more detail:

Let's consider $\vec{x}' \xrightarrow{\text{parity}} \underbrace{-\vec{x}'}$

in Cartesian coordinates, we just have a minus sign

In spherical coordinates: $r \to r$

$\theta \to \pi - \theta$

$\phi \to \phi + \pi$

It can be shown readily:

$$Y_l^m(\hat{r}) \longrightarrow Y_l^m(-\hat{r}) = (-1)^l\, Y_l^m(\hat{r})$$

$$\hat{\pi}\,|\alpha, lm\rangle = (-1)^l\,|\alpha, lm\rangle$$

Parity properties of energy eigenstates and degeneracies?

> **Theorem 4.1:** If $[\hat{H}, \hat{\pi}] = 0$ and if $|n\rangle$ is a <ins>non-degenerate</ins> eigenket of $\hat{H}$ ($\hat{H}|n\rangle = E_n|n\rangle$), then $|n\rangle$ is also a parity eigenket.

Consider two examples:

① $\hat{H} = \frac{\hat{\vec{p}}^2}{2m}$ $\rightarrow$ energy eigenstates are $\propto \underbrace{e^{i\vec{k}\cdot\vec{x}}}$

we already said: these states do not have definite parity

Easy to check: $\hat{H}$ is invariant under parity.

But: eigenstates have indefinite parity (are not eigenstates of $\hat{\pi}$).

Our theorem cannot be applied since $|\vec{p}'\rangle$ and $|-\vec{p}'\rangle$ are degenerate!

② 1D HO Hamiltonian $\rightarrow$ all energy eigenstates are one-fold degenerate

$\rightarrow [\hat{H}, \hat{\pi}] = 0$

easy to check: $\hat{H}$ is quadratic

$\rightarrow$ theorem applies, i.e., the eigenstates of 1D HO have definite parity.

Proof of theorem 4.1:

Consider $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$.

Act with $\hat{\pi}$:

multiplying out

$$\hat{\pi}\left(\frac{1}{2}(1 \pm \hat{\pi})|n\rangle\right) = \left(\frac{1}{2}\hat{\pi} \pm \frac{1}{2}\underbrace{\hat{\pi}\hat{\pi}}_{1}\right)|n\rangle$$

reordering terms

$$= \pm\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$$

adding brackets for clarity

$$= \pm\left(\frac{1}{2}(1 \pm \hat{\pi})|n\rangle\right)$$

So: $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$ is an eigenket of $\hat{\pi}$ with eigenvalues ± 1.

Now look at $\hat{H}$ acting on $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$:

$$\hat{H}\left(\frac{1}{2}(1 \pm \hat{\pi})\right)|n\rangle = \left(\frac{1}{2}\hat{H} \pm \frac{1}{2}\underbrace{\hat{H}\hat{\pi}}_{+\hat{\pi}\hat{H}}\right)|n\rangle$$

$$= \frac{1}{2}(\hat{H} \pm \hat{\pi}\hat{H})|n\rangle$$

$$= \frac{1}{2}(1 \pm \hat{\pi})\hat{H}|n\rangle$$

$$= E_n \frac{1}{2}(1 \pm \hat{\pi})|n\rangle$$

$$= E_n\left(\frac{1}{2}(1 \pm \hat{\pi})|n\rangle\right)$$

So: $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$ is an eigenket of $\hat{H}$ with eigenvalues E_n.

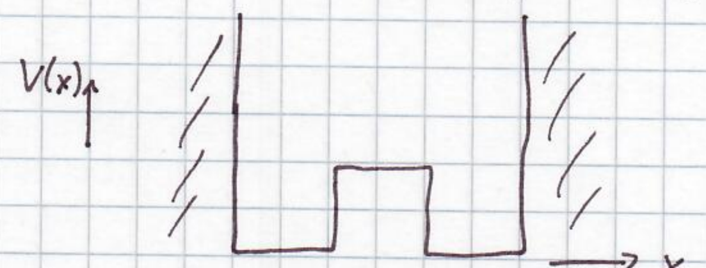
Thus: $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$ is an eigenket of $\hat{H}$ as well as an eigenket of $\hat{\pi}$.

By our assumption, the eigenstates of $\hat{H}$ are non-degenerate. Since $|n\rangle$ and $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$ are both eigenkets of $\hat{H}$, they can only differ by a phase (otherwise we would have a degeneracy, which contradicts our assumption).

Since $|n\rangle$ identical to $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$ (except for phase) and since $\frac{1}{2}(1 \pm \hat{\pi})|n\rangle$ is parity eigenket, $|n\rangle$ must also be a parity eigenket.

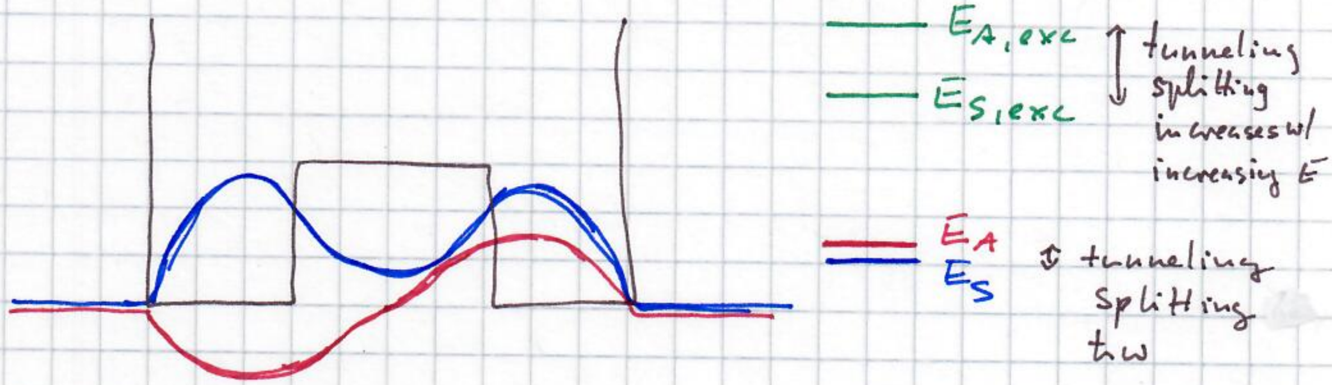
This proves the theorem.

Application: Symmetrical double-well potential (1D for simplicity)



Alternatively:

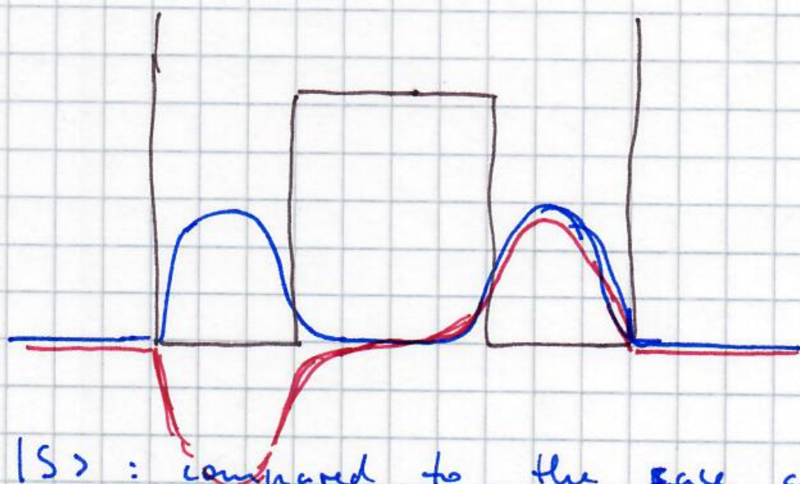
What are the eigenenergies and eigenstates?



$|S\rangle$: symmetrical (there exists "tunneling" into the classically forbidden region) → pos. parity

$|A\rangle$: anti-symmetrical → neg. parity

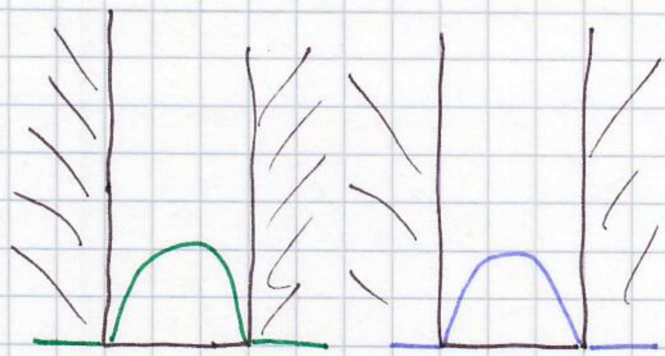
What happens when we make the barrier inside larger?



$|S\rangle$: compared to the case above, less tunneling into the classically disallowed region

$|A\rangle$: same as for $|S\rangle$; in addition, the states $|S\rangle$ and $|A\rangle$ become more similar (except for phase) in the classically allowed region ⇝ $\hbar\omega$ is smaller than above

What happens when we make the barrier infinitely large?



$|L\rangle$: state located in left well (not a parity eigenstate)

the wave fcts must be zero here

$\hbar\omega = 0$

the two wells are truly dis-connected, i.e., the Hilbert space separates into two distinct pieces.

$|R\rangle$: state located in right well (not a parity eigenstate)

$|L\rangle$ and $|R\rangle$ have the same energy $\rightarrow$ ground state has degeneracy of two

$|L\rangle$ and $|R\rangle$ are not parity eigenstates

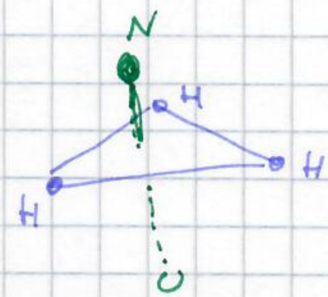
(note: this is all consistent w/ theorem 4.1)

Even though the potential is symmetric, the ground state wave functions are neither symmetric nor anti-symmetric.

Degeneracy $\longleftrightarrow$ broken symmetry!

Many examples in Nature:

e.g.: NH_3



"N wants to sit above and below the plane spanned by the three H atoms"

$\rightarrow$ oscillation frequency has wavelength of 1cm (microwave regime)

Transition matrix elements can be interpreted as parity selection rules:

$$\int \psi_0^*(x) \; x \; \underbrace{\psi_0(x)}_{\text{1d HO}} \, dx = 0$$

very easy to show

odd operator $\hat{x}$ only leads to non-zero transition probability when initial and final state have opposite parity.

Are the fundamental forces invariant under parity?

Electromagnetic? Yes (straightforward to check!)

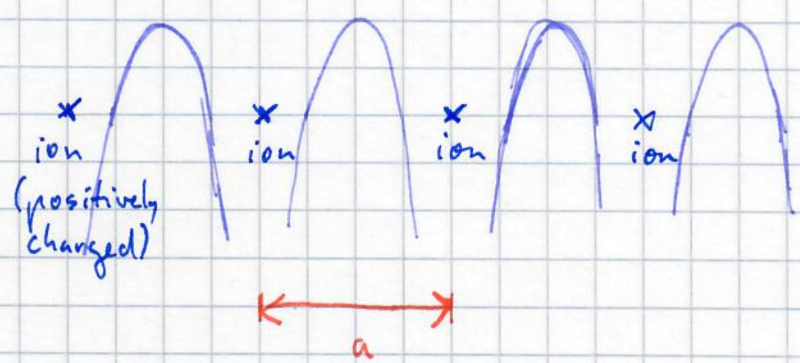
Weak interaction? No!

e.g.: $^{60}Co \to {}^{60}Ni + e^- + \bar{\nu}_e$

(see Wu et., PR <u>105</u>, 1413 (1957))

<u>4.3: Lattice translation as a discrete symmetry</u>

Let us consider an ion crystral:

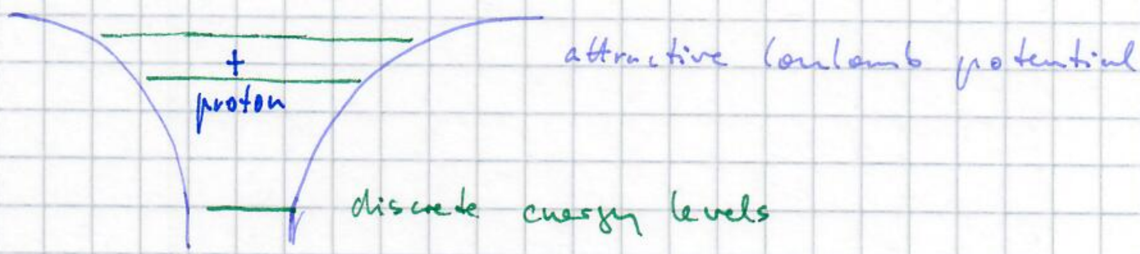


This is the potential that an electron might feel

periodicity of a

shift by a $\rightsquigarrow$ same lattice

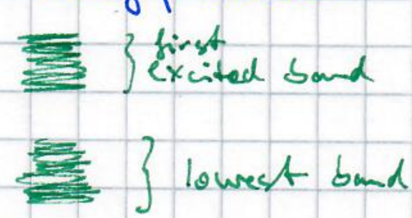
- We are very familiar w/ one electron + positive ion (= proton) $\hat{=}$ H-atom



- Two Ions / protons:

- Three ions $\rightsquigarrow$ more splitting

- Infinite number of ions (lattice) $\rightsquigarrow$ energy bands



More formally: $\hat{\tau}(l) \rightsquigarrow$ translation operator

In general: $\hat{\tau}^{+}(l)\, x\, \hat{\tau}(l) = x + l$

$$\hat{\tau}(l)\,|x'\rangle = |x' + l\rangle$$

If $l = a$: $\hat{\tau}^{+}(a)\, V(x)\, \hat{\tau}(a) = V(x+a) = V(x)$

Since kinetic energy operator is invariant under translation, it follows

$$\hat{\tau}^{+}(a)\, \hat{H}\, \hat{\tau}(a) = \hat{H}$$

$\underset{\substack{\text{using that}\\ \hat{\tau}(a) \text{ is unitary}}}{\Rightarrow}$ $\left[\hat{H}, \hat{\tau}(a)\right] = 0$

Recall: $\hat{\tau}(a)$ unitary

$\hat{\tau}(a)$ not Hermitian

$\Big\}$ expect eigenvalues to be complex number of modulus 1

Let's start with lattice with infinitely high barrier:

site $n-1$ site n site $n+1$

$\rightsquigarrow$ the sites don't talk to each other

Let: $\hat{H}\,|n\rangle = E_0\,|n\rangle$ $\rightsquigarrow$ similarly, we have $\hat{H}\,|n+1\rangle = E_0\,|n\rangle$

$\rightsquigarrow$ we have an infinite degeneracy if the number of sites is infinitely large

$$\underbrace{\hat{\tau}(a)\,|n\rangle \neq \#\,|n\rangle}$$

$|n\rangle$ is not an eigenket of $\hat{\tau}(a)$

Instead: $\hat{\tau}(a)\,|n\rangle = |n+1\rangle$

We want to construct simultaneous eigenkets of $\hat{H}$ and $\hat{\tau}(a)$.

To this end, define:

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}\,|n\rangle$$

easy to see that this is eigenket of $\hat{H}$

$$\Rightarrow \hat{\tau}(a)\,|\theta\rangle = \hat{\tau}(a) \sum_{n=-\infty}^{\infty} e^{in\theta}\,|n\rangle$$

$$= \sum_{n=-\infty}^{\infty} e^{in\theta}\,|n+1\rangle$$

$$= \sum_{n=-\infty}^{\infty} e^{-i\theta}\, e^{i(n+1)\theta}\,|n+1\rangle$$

$$= e^{-i\theta} \underbrace{\sum_{n=-\infty}^{\infty} e^{in\theta}\,|n\rangle}_{|\theta\rangle}$$

$$= e^{-i\theta}\,|\theta\rangle$$

$|\theta\rangle$ is eigenket of $\hat{H}$ and $\hat{\tau}(a)$.

$|\theta\rangle$ is parametrized by continuous variable θ.

E_0 is independent of θ.

So far: infinite barrier height $\rightarrow$ unrealistic!

Let's consider finite barrier height.

As before construct localized state $|n\rangle$ with the property

$$\hat{\tau}(a)\,|n\rangle = |n+1\rangle .$$

we demand that $|n\rangle$ has this property.

We still have $\langle n|\hat{H}|n\rangle = E_0$

However, due to "leakage", there will be off-diagonal elements:

$$\langle n'|\hat{H}|n\rangle \neq 0 \quad \text{(in general)}$$

Make the

approximation: $\langle n'|\hat{H}|n\rangle = 0 \quad \text{if } |n'-n| > 1$

this is called the tight binding approximation

idea: since the kets $|n\rangle$ are (semi-) localized, the matrix elements should become smaller w/ increasing $|n-n'|$.

Diagonal element $\langle n|\hat{H}|n\rangle = E_0$ (see above).

Nearest neighbor element $\langle n\pm 1|\hat{H}|n\rangle = -\Delta$

(this defines Δ)

Since $\hat{H}|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle$, $|n\rangle$ is not an eigen ket of $\hat{H}$.

What about $\hat{H}|\theta\rangle$?

$$\hat{H}|\theta\rangle = \hat{H}\sum_n e^{in\theta}|n\rangle$$

$$= E_0\sum_n e^{in\theta}|n\rangle - \Delta\sum_n e^{in\theta}|n+1\rangle$$

$$-\Delta\sum_n e^{in\theta}|n-1\rangle$$

$$= E_0\sum_n e^{in\theta}|n\rangle - \Delta\sum_n \underbrace{(e^{-i\theta}+e^{i\theta})}_{2\cos\theta}|n\rangle$$

$$= (E_0 - 2\Delta\cos\theta)\sum_n e^{in\theta}|n\rangle$$

$$= (E_0 - 2\Delta\cos\theta)|\theta\rangle$$

$E_0 - 2\Delta\cos\theta$ is eigenvalue of $\hat{H}$.

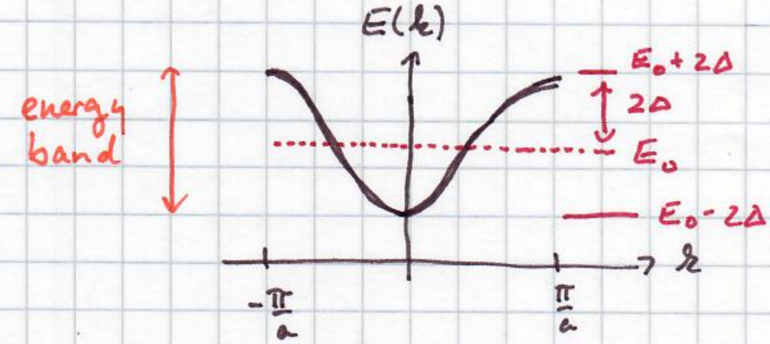
$|\theta\rangle$ is eigenket of $\hat{H}$.

What is this continuous parameter θ?

It turns out $\theta = ka$

$\rightarrow \theta \in [-\pi, \pi] \Rightarrow k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$

→ gives rise to energy band



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

$$\langle x' | \theta \rangle = e^{ikx'} \underbrace{u_k(x')}_{\text{periodic function with period } a}$$

This is the Bloch theorem:
The wave fct. of $|\theta\rangle$ ($|\theta\rangle$ is an eigenket of $\hat{\tau}(a)$) can be written as a plane wave $e^{ikx'}$ times a periodic function with periodicity a.

Note: this theorem holds even if the tight binding approximation breaks down.

4.4 The time-reversal discrete symmetry

Time reversal → should be called reversal of motion

it is <u>not</u> just $t \to -t$!!!

As a starter, let us consider the time-dependent SE:

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

Expand ψ:

$$\psi(\vec{x},t) = \sum_n c_n \underbrace{e^{-iE_n t/\hbar}\,\phi_n(t)}_{\text{complete set of states}}$$

→ If $\psi(\vec{x},t)$ is a solution to time-dep. SE, then $\psi^*(\vec{x},-t)$ is as well.

Time reversal has s.th. to do with complex conjugation!

Take a step back:

$$|\alpha\rangle \xrightarrow{\text{transf.}} |\tilde{\alpha}\rangle$$

$$|\beta\rangle \longrightarrow |\tilde{\beta}\rangle$$

If transformation is associated with unitary operator, then

$$\underbrace{\langle\tilde{\beta}|\tilde{\alpha}\rangle}_{\langle\beta|\hat{U}^{+}\hat{U}|\alpha\rangle} = \langle\beta|\alpha\rangle$$

$$\langle\beta|\underbrace{\hat{U}^{+}\hat{U}}_{\hat{1}}|\alpha\rangle = \langle\beta|\alpha\rangle$$

Rotation, translation, parity: unitary operators

$\boxed{\text{Time reversal: antiunitary}}$

Definition:

The transformation $|\alpha\rangle \to |\tilde{\alpha}\rangle = \hat{\theta}|\alpha\rangle$, $|\beta\rangle \to |\tilde{\beta}\rangle = \hat{\theta}|\beta\rangle$

is antiunitary if

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^*$$

$$\hat{\theta}\left(c_1|\alpha\rangle + c_2|\beta\rangle\right) = c_1^*\,\hat{\theta}|\alpha\rangle + c_2^*\,\hat{\theta}|\beta\rangle.$$

Antiunitary operator can be written as

$$\hat{\Theta} = \hat{U}\,\hat{K}$$

$\hat{U}$: unitary operator

$\hat{K}$: complex conjugate operator: forms the complex conjugate of any coefficient that multiplies a ket (and stands the right of $\hat{K}$

The $\hat{K}$ operator (and the time reversal operator) are a bit tricky since the effect of $\hat{K}$ changes with the basis.

What does this mean?!? To understand this, let us look at two examples:

- 1) Let $|+\rangle$ and $|-\rangle$ be eigen kets of $\hat{S}_z$. Let us use $|+\rangle$ and $|-\rangle$ as base kets and let us form new kets

$$\frac{1}{\sqrt{2}}|+\rangle \pm \frac{i}{\sqrt{2}}|-\rangle .$$

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

base kets: $\hat{K}$ takes the "prefactors" and converts them to complex conjugate

change

- 2) Let us change our basis: Let our base kets be $\frac{1}{\sqrt{2}}|+\rangle \pm \frac{i}{\sqrt{2}}|-\rangle$.

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

no change

base ket: $\hat{K}$ takes the prefactor (namely, 1) and converts the prefactor to complex conjugate ($1^* = 1$)

Let's denote time reversal operator by $\hat{\Theta}$.

We require:

$$\hat{\Theta}\, \hat{\vec{x}}\, \hat{\Theta}^{-1} = \hat{\vec{x}}$$

$$\hat{\Theta}\, \hat{\vec{p}}\, \hat{\Theta}^{-1} = -\hat{\vec{p}}$$

$$\hat{\Theta}\, \hat{\vec{J}}\, \hat{\Theta}^{-1} = -\hat{\vec{J}}$$

When we started the discussion, we noted that $\psi^*(\vec{x}, -t)$ solves the time-dep. SE, provided $\psi(\vec{x}, t)$ does.

Let's ~~look~~ look at this a bit more formally: Look at single spinless particle at time $t=0$ described by state $|\alpha\rangle$.

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

$$\Rightarrow \hat{\Theta}\, |\alpha\rangle = \int \hat{\Theta}\, \langle \vec{x}' | \alpha \rangle\, |\vec{x}'\rangle\, d^3\vec{x}'$$

$$= \int \left(\langle \vec{x}' | \alpha \rangle\right)^* \underbrace{\hat{\Theta}\, |\vec{x}'\rangle}_{|\vec{x}'\rangle}\, d^3\vec{x}'$$

$$= \int \underline{\langle \vec{x}' | \alpha \rangle^*}\, |\vec{x}'\rangle\, d^3\vec{x}'$$

So: $\psi(\vec{x}') \rightarrow \psi^*(\vec{x}')$

On the other hand:

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

$$\Rightarrow \hat{\Theta}|\alpha\rangle = \hat{\Theta}\int \langle\vec{p}\,'|\alpha\rangle\,|\vec{p}\,'\rangle\, d^3\vec{p}\,'$$

$$= \int \left(\langle\vec{p}\,'|\alpha\rangle\right)^* \underbrace{\hat{\Theta}|\vec{p}\,'\rangle}_{|-\vec{p}\,'\rangle \text{ (see below)}}\, d^3\vec{p}\,'$$

$$= \int \langle\vec{p}\,'|\alpha\rangle^*\,|-\vec{p}\,'\rangle\, d^3\vec{p}\,'$$

variable transformation $\vec{p} \to -\vec{p}\,'$ (three $\vec{p}$'s and switch of integration)

$$= \int \langle-\vec{p}\,'|\alpha\rangle^*\,|\vec{p}\,'\rangle\, d^3\vec{p}\,'$$

So: $\psi(\vec{p}) \to \psi^*(-\vec{p})$

Recall $\psi(\vec{x}) \to \psi^*(\vec{x})$

the dependence on representation is clearly visible!

What is $\hat{\Theta}|\vec{p}\rangle$?

$$\hat{\Theta}|\vec{p}\rangle = \hat{\Theta}\int \underbrace{\langle\vec{x}\,'|\vec{p}\rangle}_{\frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{x}\,'/\hbar}}\,|\vec{x}\,'\rangle\, d^3\vec{x}\,'$$

$$= \int \underbrace{\left(\hat{\Theta}\left(\frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{x}\,'/\hbar}\right)\right)}_{\frac{1}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{x}\,'/\hbar}} \underbrace{\hat{\Theta}|\vec{x}\,'\rangle}_{|\vec{x}\,'\rangle \text{ (from before)}}\, d^3\vec{x}\,' = |-\vec{p}\rangle$$

$$= \langle\vec{x}\,'|-\vec{p}\rangle$$

Theorem 4.2: If $\hat{H}$ is invariant under $\hat{\Theta}$ and the eigenket $|n\rangle$ is non-degenerate, then the corresponding energy eigenfunction is a real function times a phase factor that is independent of $\vec{x}$.

For the proof of the theorem, see the text.

So far, we looked at spinless particle. Now look at particle with spin.

For $\hat{\vec{S}}$, we demand (just as for $\hat{\vec{J}}$): $\hat{\Theta} \hat{\vec{S}} \hat{\Theta}^{-1} = -\hat{\vec{S}}$

It follows by inspection that $\hat{\Theta}$ cannot just be $\hat{K}$ (e.g., $\hat{K} \hat{S}_z \hat{K} = \hat{S}_z$).

Instead: $$\hat{\Theta} = -i \underbrace{\eta}_{\text{arbitrary phase (complex number of modulus 1)}} \frac{2\hat{S}_y}{\hbar} \hat{K} = \eta e^{-i\pi \hat{S}_y/\hbar} \hat{K}$$

(in the representation where $\hat{S}_z$ is diagonal)

for spin-$\frac{1}{2}$ particle

It follows:

$$\hat{\Theta}\left(c_+|+\rangle + c_-|-\rangle\right) = +\eta\, c_+^*|-\rangle - \eta\, c_-^*|+\rangle$$

most general spin $\frac{1}{2}$ ket ($|+\rangle$ and $|-\rangle$ are eigen kets of $\hat{S}_z$)

using: $e^{-i\pi\hat{S}_y/\hbar}|+\rangle = +|-\rangle$

& $e^{-i\pi\hat{S}_y/\hbar}|-\rangle = -|+\rangle$

$$\hat{\Theta}^2\left(c_+|+\rangle + c_-|-\rangle\right) = \hat{\Theta}\left(\eta\, c_+^*|-\rangle - \eta\, c_-^*|+\rangle\right)$$

$$= -\underbrace{\eta\eta^*}_{|\eta|^2 = 1} c_+|+\rangle - \underbrace{\eta\eta^*}_{|\eta|^2 = 1} c_-|-\rangle$$

$$= -\left(c_+|+\rangle + c_-|-\rangle\right)$$

$= -$ (the state we started with)

Kramer's degeneracy theorem

An important consequence: Any system for which $\hat{\Theta}^2|n\rangle = -|n\rangle$, such as an odd number of spin $\frac{1}{2}$ particles, has only degenerate energy levels.

assumes $\hat{H}$ and $\hat{\Theta}$ commute

$|n\rangle$ energy eigenket