Atomic Physics and Spectroscopy.

1. Why are symmetry properties so important in physics?

1. Much information can be extracted about a system if the symmetry properties of the interactions are known, even if their detailed form is not.

2. Physical symmetries lead to conservation laws and in q.m. to quantum nos.

3. The number of equations to be solved is reduced by 1 for each ignorable co-ord.

In classical mechanics,

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$-\dot{p}_i = \frac{\partial H}{\partial q_i}$$

If H is invariant under changes in q_i, then p_i = const. eg. translation, rotation.

The homogeneity and isotropy of space lead to conservation of linear and angular momentum.

- ~~Symmet~~ Symmetry is partly or wholly destroyed by applying an external field that is held fixed while system changes.

- Symmetry is even more imp. in q. m. $\Longrightarrow$ quantum nos. to classify states of system.
  - no symmetry, no q. nos.

Schrodinger eqn.

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \qquad (1)$$

Suppose U is an operator producing a symmetry transform

ie if Ψ satisfies (1) then so does $U\Psi$.

If U is a symmetry operation, then scalar products (expectation values) are left unchanged.

ie $|\langle a|b\rangle|^2 = |\langle a|U^+U|b\rangle|^2$

$= |\langle a'|b'\rangle|^2$

Then $\langle a|b\rangle = \langle a'|b'\rangle = \langle a|U^+U|b\rangle$

$U^+U = UU^+ = 1 \longleftarrow$ unitary

$U(\lambda|a\rangle) = \lambda U|a\rangle$

or

$\langle a|b\rangle = \langle a'|b'\rangle^* = \langle a|U^+U|b\rangle^*$
$= \langle b|U^+U|a\rangle$

and $U(\lambda|b\rangle) = \lambda^* U|b\rangle$

unitary antilinear.

Proof of Unitarity

- The requirement that the norm be preserved is

$$\langle\psi|U^{+}U|\psi\rangle = \langle\psi|\psi\rangle. \qquad \text{all } |\psi\rangle \text{ in } \mathcal{H}.$$

This implies the more general requirement

$$\langle\phi|U^{+}U|\chi\rangle = \langle\phi|\chi\rangle \qquad \text{all } |\phi\rangle, |\chi\rangle \text{ in } \mathcal{H}$$

as follows. First put $|\psi\rangle = |\phi\rangle + |\chi\rangle$

$$\Longrightarrow \cancel{\langle\phi|U^{+}U|\phi\rangle} + \cancel{\langle\chi|U^{+}U|\chi\rangle} + \langle\phi|U^{+}U|\chi\rangle + \langle\chi|U^{+}U|\phi\rangle$$
$$= \cancel{\langle\phi|\phi\rangle} + \cancel{\langle\chi|\chi\rangle} + \langle\phi|\chi\rangle + \langle\chi|\phi\rangle$$

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Now put $|\psi\rangle = |\phi\rangle + i|\chi\rangle$

$$\Longrightarrow i\langle\phi|U^{+}U|\chi\rangle - i\langle\chi|U^{+}U|\phi\rangle$$
$$= i\langle\phi|\chi\rangle - i\langle\chi|\phi\rangle$$

$$\therefore \quad U^{+}U = 1.$$

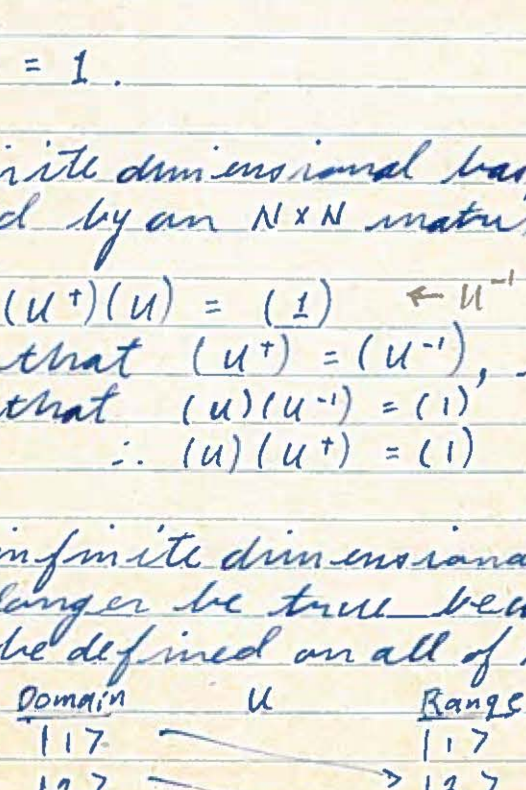
In a finite dimensional basis set, U is represented by an $N\times N$ matrix (U), and the equation

$$(U^{+})(U) = (1) \quad \leftarrow U^{-1}$$

implies that $(U^{+}) = (U^{-1})$, which in turn implies that $(U)(U^{-1}) = (1)$

$$\therefore (U)(U^{+}) = (1)$$

- In an infinite dimensional basis set, this need no longer be true because the inverse may not be defined on all of $\mathcal{H}$.



If we specify in addition that $R(U) = \mathcal{H}$,

then $$U^\dagger U = 1$$
$$\Rightarrow \quad U U^\dagger U = U$$
$$\therefore \quad U U^\dagger (U|\psi\rangle) = (U|\psi\rangle)$$

If $U|\psi\rangle$ ranges over all of $\mathcal{H}$ as $|\psi\rangle$ ranges over all of $\mathcal{H}$, then we can conclude that

$$U U^\dagger = 1 .$$

(antilinear)
Linear ~~means~~ means that ~~if~~ if

$|c\rangle = \lambda_1 |a\rangle + \lambda_2 |b\rangle$

then $U|c\rangle = \lambda_1 U|a\rangle + \lambda_2 U|b\rangle$ (linear)

$= \lambda_1^* U|a\rangle + \lambda_2^* U|b\rangle$ (antilinear)

<u>Analogy with vector space.</u>

→ $\vec{x} = \sum_{i=1}^{n} x_i \hat{e}_i$

transformations

$x_i' = \sum_k U_{ik} x_k$

- Length or norm is defined in general by

$x^2 = \sum_{i,k} g_{ik} x_i x_k$

In q.m., $g_{ik} = \delta_{i,k}$, but the vector components are in general complex.

$x^2 = (\vec{x}\cdot\vec{x}) = \sum_{i=1}^{n} x_i^* x_i$

$(\vec{x}\cdot\vec{y}) = \sum_{i=1}^{n} x_i^* y_i = (\vec{y}\cdot\vec{x})^*$

If U is a symmetry operation, then

$|(\vec{x}'\cdot\vec{y}')| = |(\vec{x}\cdot\vec{y})|$

$(\vec{x}'\cdot\vec{y}') = \sum_i x_i'^* y_i' = \sum_{ikl} (U_{ik} x_k)^* U_{il} x_l$

$$= \sum_{kl} x_k^* x_l \Big(\underbrace{\sum_i U_{ik}^* U_{il}}_{= \delta_{k,l}} \Big)$$

ie $\sum_i U_{ki}^{+} U_{il} = \delta_{k,l}$

$$U^{+} U = \underset{\sim}{1} .$$

$$U^{+} = U^{-1} \qquad \text{unitary.}$$

We said that if Ψ satisfies (1), then so does $U\Psi$. ie

$$i\hbar \frac{\partial}{\partial t} U\Psi = H U \Psi$$

If U is time independent, then

$$i\hbar \frac{\partial \Psi}{\partial t} = U^{-1} H U \Psi$$

ie $UH = HU$.

Thus symmetry operators commute with H.

- The set of all symmetry operations for a given physical system form a group. ~~ie~~

What is a group?
- a set of elements $a, b, c, \dots$ with a multiplication law and the properties

1. $a(bc) = (ab)c$ (associative law)
2. a unit element exists $\underset{\sim}{1} a = a \underset{\sim}{1} = a$