PC3130 W3L1 AY2024

Tuesday, 27 August 2024 9:46 am

Tutorial 1 — due today

Tutorial 2 — posted today

Recap Revision — Postulates of QM

(general)
· Angular momentum

· commuting observables
$[\hat{A}, \hat{B}] = 0$
$\Rightarrow \exists$ a set of common eigenstates of $\hat{A}$ & $\hat{B}$

· These common eigenstates can be labelled by their eigenvalues or quantities (eg. n, l, m) that are sufficient to tell you the eigenvalue

· Orbital angular momentum
$\vec{L} = \vec{r} \times \vec{p}$

- hydrogen atom
$|n\,l\,m\rangle$
$[H, L^2] = [L^2, L_z] = [H, L_z] = 0$
$\{H, L^2, L_z\}$ is a CSCO
ignoring spin.

· multi-electron atom
- Approximations enable us to also think about orbital angular momentum in multi-electron atoms

· Addition of angular momentum
Eg $|J^2, J_z\rangle$

$$\boxed{\begin{array}{l} \cdot\ [L_i, L_j] = i\hbar\,\varepsilon_{ijk} L_k \\ \text{defines angular momentum} \end{array}}$$

Approx - Born-Oppenheimer
- Central potential approx for multi-electron atoms
Single particle approx.

Symmetries

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$[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k$

angular momentum.
– generator of rotations

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simplify integrals ; selection rules

topological physics,
nonlinear optics,
defect physics ; group theory
(not examined)

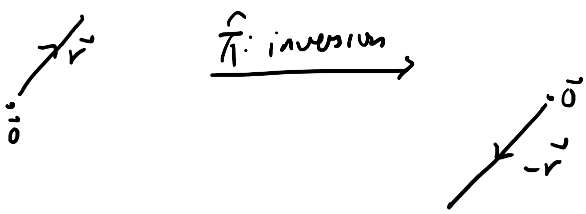
Chapter 6 Griffiths (except 6.7 - 6.8)

3 types of symmetries will be considered

1) Inversion symmetry — if a system obeys inversion sym, we can find stationary states that conserve parity.
2) Translational symmetry — —— " — translational sym., $\frac{d}{dt}\langle \vec{p} \rangle = 0$ momentum conserved
3) Rotational symmetry — —— " —— rotational " , angular momentum conserved.

Inversion symmetry

What is inversion? (spatial)



. A spatial inversion is implemented by a parity operator $\hat{\Pi}$.

$$\hat{\Pi} : \vec{r} \longrightarrow -\vec{r}$$

$\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$

$$\hat{\Pi}\, \psi(\vec{r}) = \psi(-\vec{r})$$

What are the eigenvalues of $\hat{\Pi}$?

If $\varphi(\vec{r})$ is an eigenstate of $\hat{\Pi}$, $\hat{\Pi}\varphi(\vec{r}) = p\,\varphi(\vec{r})$, p is a scalar

Note that $\hat{\Pi}(\hat{\Pi}\varphi(\vec{r})) = \hat{\Pi}(\varphi(-\vec{r})) = \varphi(\vec{r})$ for all φ.

In particular, if $\hat{\Pi}\varphi(\vec{r}) = p\,\varphi(\vec{r})$

In particular, if $\hat{\Pi}\varphi(\vec{r}) = p\,\varphi(\vec{r})$

$$\hat{\Pi}(\hat{\Pi}\varphi(\vec{r})) = \hat{\Pi}(p\varphi(\vec{r})) = p\hat{\Pi}\varphi(\vec{r}) = p(p\varphi(\vec{r})) = p^2\varphi(\vec{r})$$

But LHS $= \varphi(\vec{r})$

$\Rightarrow \quad \varphi(\vec{r}) = p^2\varphi(\vec{r})$

$\Rightarrow \quad p^2 = 1 \quad \Rightarrow \quad p = \pm 1$

Eigenstates of parity operator $\hat{\Pi}$ obey

$$\hat{\Pi}\varphi(\vec{r}) \underset{\text{definition}}{=} \varphi(-\vec{r}) = \begin{cases} +\varphi(\vec{r}) & (p=1) \quad (\varphi \text{ is an even function}) \\ -\varphi(\vec{r}) & (p=-1) \quad (\varphi \text{ is an odd function}) \end{cases}$$

(states with definite parity)

$$\hat{\Pi} = \sum_i (1)|e_i\rangle\langle e_i| + \sum_i (-1)|o_i\rangle\langle o_i|$$

What does it mean for a system to have spatial inversion symmetry?

— Look at the Hamiltonian

Eg. $\hat{H} = \frac{1}{2}m\omega^2\hat{x}^2$ $\quad$ ($x \longrightarrow -x$; $\hat{H}$ is not changed)

- has inversion symmetry.

Counter-example.

$$\hat{H} = \frac{1}{2}m\omega^2\hat{x}^2 + \underbrace{(-e)E\hat{x}}_{\substack{\text{breaks}\\ \text{inversion symmetry.}}}$$

($x \longrightarrow -x$; $\hat{H}$ will change).

Let's be more rigorous.

A system has inversion symmetry if the Hamiltonian is unchanged by a parity transformation.

Transforming an operator

An operator $\hat{Q}$ transformed under $\hat{\Pi}$ (giving $\hat{Q}'$) is defined as the operator $\hat{Q}'$ that gives the same expectation value in the untransformed state $|\psi\rangle$ as does the operator $\hat{Q}$ in the transformed state $|\hat{\Pi}\psi\rangle$.

ie. $\langle\psi|\hat{Q}'|\psi\rangle = \langle\hat{\Pi}\psi|\hat{Q}|\hat{\Pi}\psi\rangle$

$= \langle\psi|\hat{\Pi}^{\dagger}\hat{Q}\hat{\Pi}|\psi\rangle$

True for all $|\psi\rangle$.

$\Rightarrow$ $\boxed{\hat{Q}' = \hat{\Pi}^{\dagger}\hat{Q}\hat{\Pi}.}$

A system has inversion symmetry if $\hat{H}$ is unchanged by the parity transformation, ie. $\hat{H} = \hat{H}' = \hat{\Pi}^{\dagger}\hat{H}\hat{\Pi}$.

Eg. $\hat{H} = \hat{x}^2$.

Check if $\hat{H} = \hat{H}'$.

Is $\langle\psi|\hat{H}|\varphi\rangle = \langle\psi|\hat{H}'|\varphi\rangle$ for arbitrary $|\psi\rangle, |\varphi\rangle$.

$$\text{LHS} = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, x^2\, \varphi(x)$$

$$\begin{aligned}
\text{RHS} &= \langle\psi|\hat{H}'|\varphi\rangle \\
&= \langle\psi|\hat{\Pi}^{\dagger}\hat{H}\hat{\Pi}|\varphi\rangle \\
&= \langle\hat{\Pi}\psi|\hat{H}|\hat{\Pi}\varphi\rangle \\
&= \int_{-\infty}^{\infty} dx\, \psi^*(-x)\, x^2\, \varphi(-x) \\
&= \int_{+\infty}^{-\infty} (-du)\, \psi^*(u)\, (-u)^2\, \varphi(u) \\
&= \int_{-\infty}^{\infty} du\, \psi^*(u)\, u^2\, \varphi(u) = \text{LHS}
\end{aligned}$$

$u = -x$
$du = -dx$

$$= \int_{-\infty} du\, \psi^*(u)\, u^2\, \psi(u)$$

So $\hat{H} = \hat{x}^2$ obeys $\hat{H} = \hat{\Pi}^{\dagger} \hat{H} \hat{\Pi}$ //

<u>Claim</u>: If $\hat{H} = \hat{\Pi}^{\dagger} \hat{H} \hat{\Pi}$ (has inversion symmetry),

then $[\hat{\Pi}, \hat{H}] = 0$

and $\exists$ a set of common eigenstates of $\hat{\Pi}$ and $\hat{H}$.

ie. $\exists$ a set of eigenstates of $\hat{H}$ that are $\underbrace{\text{either even or odd}}_{\text{(definite parity)}}$.

— If these eigenstates are non-degenerate, then they <u>must</u> have definite parity.

(eg $\hat{H} = \frac{1}{2} m\omega^2 \hat{x}^2$ —— system has inversion symmetry (see above)

—— Eigenstates are non-degenerate.

$\Rightarrow$ Eigenstates of $\hat{H}$ have definite parity.)

(see slides)

<u>Claim</u> $\hat{H} = \hat{\Pi}^{\dagger} \hat{H} \hat{\Pi} \Rightarrow [\hat{\Pi}, \hat{H}] = 0$.

Thinking about this...

We need to show $[\hat{\Pi}, \hat{H}] = 0$

$\hat{\Pi}\hat{H} = \hat{H}\hat{\Pi}$ —(1)

We have $\hat{H} = \hat{\Pi}^{\dagger} \hat{H} \hat{\Pi}$ (inversion sym)

LHS of (1): $\hat{\Pi}\hat{H} = \hat{\Pi}(\hat{\Pi}^{\dagger}\hat{H}\hat{\Pi}) = \hat{\Pi}\hat{\Pi}^{\dagger}\hat{H}\hat{\Pi}$

RHS of (1): $\hat{H}\hat{\Pi}$

So for LHS = RHS we need $\hat{\Pi}\hat{\Pi}^{\dagger} = \mathbb{1}$

We know $\hat{\Pi}^2 = \mathbb{1}$

so it is sufficient to show $\hat{\Pi} = \hat{\Pi}^{\dagger}$.

We will show that $\hat{\Pi} = \hat{\Pi}^{\dagger}$.

We will show that $\hat{\pi} = \hat{\pi}^\dagger$.

i.e. $\langle \psi | \hat{\pi} | \varphi \rangle = \langle \psi | \hat{\pi}^\dagger | \varphi \rangle$ for general $|\psi\rangle, |\varphi\rangle$.

$$= \langle \hat{\pi} \psi | \varphi \rangle$$

$$\text{RHS} = \langle \hat{\pi}\psi | \varphi \rangle = \int_{-\infty}^{\infty} dx\, \psi^*(-x)\, \varphi(x)$$

$u = -x$
$du = -dx$

$$= \int_{\infty}^{-\infty} (-du)\, \psi^*(u)\, \varphi(-u)$$

$$= \int_{-\infty}^{\infty} du\, \psi^*(u)\, \varphi(-u)$$

$$= \langle \psi | \hat{\pi} \varphi \rangle$$

$$= \langle \psi | \hat{\pi} | \varphi \rangle = \text{LHS}. \quad //$$

So $\hat{\pi} = \hat{\pi}^\dagger$.

$$\hat{\pi}\hat{H} \underset{\substack{\text{inv.}\\ \text{sym}}}{=} \hat{\pi}(\hat{\pi}^\dagger \hat{H} \hat{\pi}) \underset{\hat{\pi}\text{ Hermitian}}{=} \hat{\pi}(\hat{\pi}\hat{H}\hat{\pi}) = \hat{\pi}^2 \hat{H}\hat{\pi} \underset{\substack{\text{definitions}\\ \text{of } \hat{\pi}}}{=} \mathbb{1}\hat{H}\hat{\pi} = \hat{H}\hat{\pi}$$

$$\Rightarrow [\hat{\pi}, \hat{H}] = 0 \text{ for } \hat{H} = \hat{\pi}^\dagger \hat{H} \hat{\pi}. \quad //$$

<u>Summary</u>

- defined inversion/parity transformation $\hat{\pi}$
- explained what it means for a system to have inversion symmetry
- showed that $[\hat{\pi}, \hat{H}] = 0$ for systems with inversion symmetry.

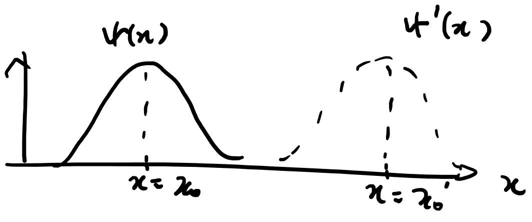
$\Rightarrow$ If $\hat{H}$ has non-degenerate eigenvalues, the eigenstates of $\hat{H}$ are either odd or even.

eg Harmonic oscillator.

<u>Translation symmetry</u>

Translation symmetry

- What is translation?



$\longmapsto$

translation τ

$$x_0' = \tau x_0$$

$$\psi'(x) = \psi(\tau^{-1} x)$$

$y = x^2$ $\qquad$ $y = (x-1)^2$

$y = f(x)$

$\tau : x \longrightarrow x+1$

$\tau^{-1} : x \longrightarrow x-1$

$f'(x+1) = f(x)$

$$f'(x) = f(x-1) = (x-1)^2.$$