PHYS 487: Lecture # 3

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Recap

1. Symmetry: suppose $\hat{A}$ is a transformation that leaves $\hat{H}$ unchanged, then $[A, H] = 0$
2. $\langle O \rangle = \langle \psi | O | \psi \rangle = \langle \psi | AOA | \psi \rangle$. (interpret as active or passive transformation)
3. Translation in space:
$$T(a)\psi(x) = \psi(x - a) \tag{1}$$
Here,
$$T(a) = \exp(-ia\hat{p}/\hbar) \tag{2}$$
Where $T(a)$ is unitary, or in other words, $T^{-1} = T^\dagger$. You can also consider a passive transformation:
$$T^\dagger(a)\hat{x}T(a) = \hat{x} + a \tag{3}$$
4. Bloch's theorem: SS: $\psi(x)\exp(iqx)u(x)$ where $u(x)$ is periodic in a.

Lecture Span

- Symmetries

Conservation of Momentum

We expect momentum to be conserved if there is a constant potential. In other words, $[H, T(a)] = 0$ for all a. We consider an infinitesimal translation $a = \delta$. Then

$$T(\delta) = e^{-i\delta\hat{p}/\hbar} \approx 1 - i\frac{\delta}{\hbar}\hat{p} \implies [\hat{H}, \hat{p}] = 0 \tag{4}$$

$$\frac{d}{dt}\langle p \rangle = \frac{i}{\hbar}\langle [H, p] \rangle = 0 \tag{5}$$

Generally: symmetry implies conserved quantities. Say $\hat{O}$ with

$$|\psi(t)\rangle = \sum_k c_k(t) |\varphi_k\rangle$$

with

$$\hat{O} |\varphi_k\rangle = \lambda_k |\varphi_k\rangle$$

Say $[O, H] = 0$, then $\partial_t \langle O \rangle = 0$ (Ehrenfest theorem). Then cofficients

$$P(\lambda_k) = |\langle \varphi_k | \psi(t) \rangle|^2 \tag{6}$$

Then

$$|\psi\rangle = \sum_m a_m \exp(-iE_m t/\hbar) |\psi_m\rangle \tag{7}$$

$$P(\lambda_k) = |\sum_m a_m \exp(-iE_m t/\hbar) \langle \varphi_k | \psi_m \rangle |^2 \tag{8}$$

Then, because φ_k and ψ_m have the same eigenbasis, then let $\varphi_k = \psi_m$, then we get

$$= |\sum_m a_m \exp(-iE_m t/\hbar) \langle \varphi_k | \varphi_m \rangle |^2 = |a_k|^2 \tag{9}$$

Parity

Parity is defined as:

$$\hat{\Pi}\psi(x) = \psi(-x) \tag{10}$$

1. $\hat{\Pi}$ is an observable. Therefore, it is Hermitian and unitary.
2. Eigenvalues of $\hat{\Pi}$ are ± 1.
3. In inversion-symmetric potentials: $V(x) = V(-x)$. Then $[H, \Pi] = 0$.
4. For the case of inversion-symmetric potentials, $\hat{\Pi}\psi_n(x) = \psi_n(-x) = \pm\psi(x)$
5. Operator transformations: $Q' = \Pi^\dagger Q \Pi$. Consider

$$\Pi^\dagger \hat{x} \Pi = -\hat{x} \tag{11}$$

$$\Pi^\dagger \hat{p} \Pi = -\hat{p} \tag{12}$$

In general, $Q'(x,p) = Q(-x,-p)$.

Selection Rule

Recall: $\langle i|Q|j\rangle = 0$. Selection rule: Matrix elements must be equal to 0 due to a symmetry. (assume i and k are orthogonal)

Consider the electric dipole $\vec{p}_e = q \cdot \vec{r}$. We can apply this parity study to Hydrogen-like atoms, since their potentials are centro-symmetric or parity symmetric. Then consider

$$\langle n'l'm'|\hat{p}_e|nlm\rangle = -\langle n'l'm'|\hat{\Pi}^\dagger \hat{p}_e \hat{\Pi}|nlm\rangle \tag{13}$$

If this matrix element is not zero, then a transition can occur. The magnitude of this matrix element shows how "hard" it is to enforce a transition from $|nlm\rangle$ to $|n'l'm'\rangle$.

Meaning of n,l,m

$$\text{SS: } \psi_{nlm}(r,\theta,\phi) = R_{nl}(r) Y_l^m(\theta,\phi) \tag{14}$$

Important: l is the only one changed by parity.

$$\hat{\Pi}\psi_{nlm}(r,\theta,\phi) = (-1)^l \psi_{nlm}(r,\theta,\phi) \tag{15}$$

Then

$$\langle n'l'm'|\hat{p}_e|nlm\rangle = -\langle n'l'm'|(-1)^{l'} p_e (-1)^l|nlm\rangle \tag{16}$$

$$= (-1)^{l+l'+1}\langle n'l'm'|p_e|nlm\rangle \tag{17}$$

If $l + l'$ is even, then this matrix element must be 0. (Laporte's Rule). Generally,

$$\langle \psi_f|\hat{\mu}|\psi_i\rangle = 0 \quad \text{if } \psi_f \mu \psi_i \text{ is odd} \tag{18}$$

Where μ is the transition moment operator.

Rotational Symmetry

1. Generator is probably angular momentum
2. If rotational symmetry is conserved, then so is angular momentum probably

Generating rotations: we can start at the z axis.

$$R_z(\varphi)\psi(r,\theta,\phi) = \psi'(r,\theta,\phi) = \psi(r,\theta,\phi-\varphi) \tag{19}$$

Expect:

$$R_z(\varphi) = e^{-i\varphi\hat{L_z}/\hbar} \tag{20}$$

Where $L_z = xp_y - yp_x$. We can study this formula infinitesimally: $\hat{x} \to \delta y$ and $y \to y + \delta x$ (remember, rotation around z axis). Then

$$R_z(\delta) \sim 1 - \frac{i\delta}{\hbar}L_z \tag{21}$$

Sanity check:

$$R_z^\dagger \hat{x} R_z = x + \frac{i\delta}{\hbar}[L_z, x] = x - \delta y \tag{22}$$

Similarly:

$$R_z^\dagger \hat{y} R_z = y + \delta x \tag{23}$$

Going to finite:

$$R_z(\varphi+\delta) = R_z(\varphi)R_z(\delta) = R_z(\delta)R_z(\varphi) \tag{24}$$

Then we get

$$R_z(\varphi+\delta) - R_z(\varphi) = R_z(\varphi)R_z(\delta) - R_z(\varphi) \tag{25}$$

$$= R_z(\varphi)\left(-\frac{i\delta}{\hbar}L_z\right) \tag{26}$$

Write as a differential equation:

$$\frac{\partial R}{\partial \varphi} = -\frac{i}{\hbar}RL_z \tag{27}$$

Rotational Symmetries

Analogous to translational symmetry with momentum conservation, this means that

$$[\hat{H}, \hat{L}] = 0 \tag{28}$$

Also

$$\frac{d}{dt}\langle L\rangle = \frac{i}{\hbar}\langle[\hat{H}, \hat{L}]\rangle = 0 \tag{29}$$

This means that we have a common basis between $\hat{H}$, $\hat{L^2}$, and $\hat{L}_z$.

$$H\psi_{nlm} = E_n\psi_{nlm} \tag{30}$$

$$L_z\psi_{nlm} = m\hbar\psi_{nlm} \tag{31}$$

$$L^2\psi_{nlm} = l(l+1)\hbar^2\psi_{nlm} \tag{32}$$