Lecture 12

$e_1 = \{|\psi_i\rangle\}$ 1D

$e_1 = \{|\varphi_a\rangle\}$

k

$$\begin{pmatrix} \langle\psi|H|\psi\rangle & \langle\psi|H|\varphi\rangle \\ \langle\varphi|H|\psi\rangle & \langle\varphi|H|\varphi\rangle \end{pmatrix}$$

Two last ingredients to study electronic structure

1. Spin
2. Time-reversal symmetry

1. So far $G \subset \mathbb{R}^3 \rtimes O(3)$

electrons have spin-$\frac{1}{2}$

In the absence of spin-orbit coupling (SOC)

$$H_{e^-} = H_0 \otimes \sigma_0$$

completely spin-independent

2x2 identity matrix in the space of electron spin

If we have SOC, we need to use representations of $SU(2)$ to describe how rotations act on spin

Reminder: $SU(2)$ - group of 2x2 unitary matrices w/

determinant 1

$g \in SU(2)$ $\quad e^{-i\theta\hat{n}\cdot\sigma/2}$ $\quad$ spin $\frac{1}{2}$ representation

$\theta \in [0, 2\pi)$

$\hat{n}$ is a 3d unit vector

$\theta = 2\pi \quad g = -\sigma_0$

To encode this, we can extend the Euclidean group by a new element $\bar{E}$

$$\bar{E}^2 = E$$

$\rho(\bar{E}) =$ identity matrix $\quad \ell \in \mathbb{Z}$

$\rho(\bar{E}) = -$ identity matrix $\quad \ell$ half-integer

Example: In $SO(3) \supset D_2 = \{C_{2x}, C_{2y}, C_{2z}\}$

$$C_{2x} C_{2y} = C_{2z}$$

In $SU(2)$ Defining representation $\rho_{\frac{1}{2}}$

$$\rho_{\frac{1}{2}}(C_{2x}) = e^{-i\pi\sigma_x/2} = -i\sigma_x$$

$$\rho_{\frac{1}{2}}(C_{2y}) = e^{-i\pi/2\,\sigma_y} = -i\sigma_y$$

$$\rho_{\frac{1}{2}}(C_{2z}) = -i\sigma_z$$

$$\rho_{\frac{1}{2}}(C_{2x})\rho_{\frac{1}{2}}(C_{2y}) = (-i\sigma_x)(-i\sigma_y)$$

$$= -(i\sigma_z) = \rho_{\frac{1}{2}}(C_{2z})$$

$$\rho_{\frac{1}{2}}(C_{2y})\rho_{\frac{1}{2}}(C_{2x}) = (-i\sigma_y)(-i\sigma_x)$$

$$= +i\sigma_z$$

$$= \rho_{\frac{1}{2}}(\bar{E})\rho_{\frac{1}{2}}(C_{2z})$$

so in $SU(2)$

$$C_{2x} C_{2y} = \bar{E} C_{2y} C_{2x}$$

Double group of D_2

$$\{ E, C_{2x}, C_{2y}, C_{2z}, \bar{E}, \bar{E} C_{2x}, \bar{E} C_{2y}, \bar{E} C_{2z} \}$$

$$C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = \bar{E} \quad - Q$$

$H = \{ E, \bar{E} \} \triangleleft SU(2)$

$$SU(2)/H \cong SO(3)$$

1st isomorphism theorem

$SU(2)$ is a double cover of $SO(3)$

For rotations: View (double) point groups as subgroups of $SU(2) \cong Spin(3)$

$$Spin(3)/\{E, \bar{E}\} = SO(3)$$

$$\mathrm{Pin}(3)/\{E,\bar{E}\} \cong O(3)$$

Two possibilities: $I^2 = \begin{cases} E \leftarrow \mathrm{Pin}_-(3) \\ \bar{E} \leftarrow \mathrm{Pin}_+(3) \end{cases}$

$\mathrm{Pin}_-(3)$ is the physical choice spin-$\frac{1}{2}$s tranform like magnetic field

$$\mathrm{Pin}_-(3) = SU(2) \times \{E, I\}$$
$$= \{g, gI \mid g \in SU(2)\ gI = Ig\}$$

For spin-$\frac{1}{2}$ particles, symmetry groups of Hamiltonians will be subgroups

$$\mathbb{R}^3 \rtimes Pin_-(3) \supset G \quad \text{double space groups}$$

If η is a representation of a double group

1) $\eta(E) = \eta(\bar{E}) \Rightarrow \eta$ is a single-valued representation
$\Rightarrow \eta$ is also a representation of "ordinary" space groups

② $\eta(E) = -\eta(\bar{E}) \to \eta$ is a double valued representation.

Ex: double group Q, 222^d ← double groups

$Q = \{E, C_{2x}, C_{2y}, C_{2z}, \bar{E}, \bar{E}C_{2x}, \bar{E}C_{2y}, \bar{E}C_{2z}\}$

$C_{2x}C_{2y} = C_{2z}$

$C_{2y}C_{2x} = \bar{E}C_{2z}$

$C_{2i}^{-1} = \bar{E}C_{2i}$

$$C_{2x}^2 = C_{2y}^2 = C_{2z}^2 = \bar{E}$$

$$C_{2x} C_{2y} C_{2x}^{-1} = \bar{E} C_{2y} C_{2x} C_{2x}^{-1} = \bar{E} C_{2y}$$

5 conjugacy classes: $\{E\}$

$\rightarrow$ 5 irreducible representations $\{\bar{E}\}$

$\{C_{2x}, \bar{E} C_{2x}\}$

$\{C_{2y}, \bar{E} C_{2y}\}$

$\{C_{2z}, \bar{E} C_{2z}\}$

	E	$\bar{E}$	C_{2x}	C_{2y}	C_{2z}
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	1	1	-1	1	-1
Γ_4	1	1	-1	-1	1

$\bar{\Gamma}_5 \,|\, 2 \quad -2 \quad 0 \quad 0 \quad 0$

$\Gamma_1, \Gamma_2, \Gamma_3, \Gamma_4$ are irreps of D_2 if we forget about $\bar{E}$

$\bar{\Gamma}_5(E) = \sigma_0$

$\bar{\Gamma}_5(\bar{E}) = -\sigma_0$

$\bar{\Gamma}_5(C_{2i}) = -i\sigma_i$

② Time-reversal symmetry T

On Hilbert space

$$T\vec{x}T^{-1} = \vec{x}$$

$$T\vec{p}T^{-1} = -\vec{p}$$

But time-reversal <u>cannot</u> be unitary

$$[x_i, p_j] = i\hbar\delta_{ij}$$

$$T[x_i, p_j]T^{-1} = [Tx_iT^{-1}, Tp_jT^{-1}]$$

$$= [x_i, -p_j]$$

$= -i\hbar$

Resolution: T is an antiunitary operator

Definition of an antiunitary operator:

Let $\{|v_i\rangle\}$ be a set of basis vectors

T is an antiunitary operator if:

① $T(\alpha|v_i\rangle + \beta|v_j\rangle) = \alpha^* T|v_i\rangle + \beta^* T|v_j\rangle$

② $\langle T v_j | T v_i \rangle = \langle v_j | v_i \rangle^*$

$= \langle v_i | v_j \rangle$

we can introduce a matrix

$$U_T^{ij} = \langle v_i | T v_j \rangle$$

to see how T acts on a state

$$|v\rangle = \sum_i a_i |v_i\rangle$$

$$T|v\rangle = \sum_i T(a_i|v_i\rangle)$$

$$= \sum_i a_i^* T|v_i\rangle$$

$$= \sum_{ij} a_i^* |v_j\rangle\langle v_j|Tv_i\rangle$$

$$= \sum_i C_T^{ji} a_i^* |v_j\rangle$$

we can say that T is represented

by $U_T \mathcal{K}$ ← complex conjugation of scalars

$$\mathcal{K}|v_i\rangle = |v_i\rangle$$

$$\mathcal{K}\alpha = \alpha^* \mathcal{K}$$

Given two vectors $|v\rangle = \sum_i a_i |v_i\rangle$

$|w\rangle = \sum_j b_j |v_j\rangle$

$$\langle Tv | Tw \rangle = \langle w | v \rangle = \vec{b}^* \cdot \vec{a}$$

$$\parallel$$

$$\left(a^T \cdot U_T^\dagger\right)\left(U_T \vec{b}^*\right) \qquad U_T^\dagger = U_T^{-1}$$

Antiunitary operators T can be represented as $U_T \mathcal{K}$ w/ U_T a unitary matrix

Ex: spin-$\frac{1}{2}$ particles

$|\uparrow\rangle$, $|\downarrow\rangle$ basis states

$$T|\uparrow\rangle = -|\downarrow\rangle$$

$$T|\downarrow\rangle = +|\uparrow\rangle$$

$$\text{"} T = i\sigma_y K \text{"}$$

$$i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$\langle\uparrow|T\uparrow\rangle = 0$$

$$\langle\downarrow|T\downarrow\rangle = 0$$

$$\langle\uparrow|T\downarrow\rangle = 1$$

$$\langle\downarrow|T\uparrow\rangle = -1$$

$$T\left(\alpha|\uparrow\rangle + \beta|\downarrow\rangle\right)$$
$$= -\alpha^*|\downarrow\rangle + \beta^*|\uparrow\rangle$$

Let T be antiunitary $\rightarrow$ T^2 is a unitary operator

$$T^2 = U_T K U_T K$$
$$= U_T U_T^*$$

$$T^2(\alpha|v_i\rangle + \beta|v_j\rangle)$$

$$\alpha \quad T^2|v_i\rangle + \beta \, T^2|v_j\rangle$$

$$\langle T^2 v | T^2 w\rangle = \langle Tw | Tv\rangle = \langle v | w\rangle$$

Also . $T\vec{x}T^{-1} = \vec{x}$ $\rightarrow$ we want

T to commute w/ all spatial symmetries

Schur's lemma $T^2 = \lambda$ Identity

$$\lambda = \pm 1$$

$$T^2 = U_T U_T^* = \lambda$$

$$U_T = \lambda U_T^T = \lambda^2 U$$

spin-statistics theorem: $\lambda = +1$ for integer spin - single-valued representations

$\lambda = -1$ for double-valued reps (half-integer spin)