Z_2 Class

時間反転演算子 $\hat{T}$

$\hat{K}$ を波動関数の共役をとる演算子とする. $\frac{1}{2}$ スピン系で

$$\hat{T} = -i\sigma_2\hat{K} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \hat{K} \tag{1}$$

$$\hat{T}^2 = -1 \tag{2}$$

$$\left\langle \hat{T}\psi \middle| \hat{T}\phi \right\rangle = \langle \phi | \psi \rangle \tag{3}$$

$$\left\langle \psi \middle| \hat{T}\phi \right\rangle = -\left\langle \phi \middle| \hat{T}\psi \right\rangle \tag{4}$$

$$\begin{aligned} \left\langle \hat{T}\psi \middle| \hat{T}\hat{A}\hat{T}^{-1} \middle| \hat{T}\phi \right\rangle &= \left\langle \hat{T}\psi \middle| \hat{T}\hat{A}\phi \right\rangle \\ &= \left\langle \hat{A}\phi \middle| \psi \right\rangle = \langle \phi | \hat{A}^\dagger | \psi \rangle \end{aligned} \tag{5}$$

時間反転対称な系

$$\hat{T}^{-1}\hat{H}(k)\hat{T} = \hat{H}(-k) \tag{6}$$

$T|u_n(k)\rangle$ は $\hat{H}(-k)$ の固有状態である

$$\hat{H}(-k)\hat{T}|u_n(k)\rangle = \hat{T}\hat{H}(k)|u_n(k)\rangle = E_n(k)\Big(\hat{T}|u_n(k)\rangle\Big) \tag{7}$$

w 行列

$$w_{\alpha\beta}(k) = \langle u_\alpha(-k)| \hat{T} |u_\beta(k)\rangle \tag{8}$$

と定める．

$$\hat{T} |u_\beta(k)\rangle = w_{\alpha\beta}(k) |u_\alpha(-k)\rangle \tag{9}$$

$$|u_\alpha(-k)\rangle = w^*_{\alpha\beta}(k)\hat{T} |u_\beta(k)\rangle \tag{10}$$

w 行列の性質

Unitary

$$\begin{aligned}
\left(w(k)^\dagger w(k)\right)_{\alpha\beta} &= w^*_{\gamma\alpha}(k) w_{\gamma\beta}(k) \\
&= \left(\langle u_\gamma(-k)| \hat{T} |u_\alpha(k)\rangle\right)^* \left(\langle u_\gamma(-k)| \hat{T} |u_\beta(k)\rangle\right) \\
&= \left\langle \hat{T} u_\alpha(k) \middle| u_\gamma(-k) \right\rangle \left\langle u_\gamma(-k) \middle| \hat{T} u_\beta(k) \right\rangle \\
&= \left\langle \hat{T} u_\alpha(k) \middle| \hat{T} u_\beta(k) \right\rangle \\
&= \langle u_\beta(k)|u_\alpha(k)\rangle = \delta_{\alpha\beta}
\end{aligned} \tag{11}$$

$w(-k)w(k) = -1$

$$\begin{aligned}
\hat{T}^2 |u_\alpha(k)\rangle &= - |u_\alpha(k)\rangle \\
&= w_{\beta\alpha}(k)\hat{T} |u_\beta(-k)\rangle \\
&= w_{\beta\alpha}(k) w_{\gamma\beta}(-k) |u_\gamma(k)\rangle
\end{aligned} \tag{12}$$

$$\text{よって} w_{\gamma\beta}(-k) w_{\beta\alpha}(k) = -\delta_{\alpha\gamma}$$

$w(k) = -w(-k)^\intercal$

$$\begin{aligned}
w_{\alpha\beta}(k) &= \langle u_\alpha(-k)| \hat{T} |u_\beta(k)\rangle \\
&= - \langle u_\beta(k)| \hat{T} |u_\alpha(-k)\rangle \\
&= -w_{\beta\alpha}(-k)
\end{aligned} \tag{13}$$

TRIM Λ では $w(\Lambda)$ は反対称行列

Berry 接続行列

$$a_{i,\alpha\beta}(k) = -i \langle u_\alpha(k)| \partial_i |u_\beta(k)\rangle \tag{14}$$

ここで $i = 1, 2, 3$ であり, i それぞれに行列 $a_i(k)$ が対応する.
$a_i(k)$ は Hermite 行列である

$$a_{i,\alpha\beta}(k) = a^*_{i,\beta\alpha}(k) \tag{15}$$

w 行列と Berry 接続行列の関係

$$a_i(-k) = w(k)a^*_i(k)w^\dagger(k) + iw(k)\partial_i w^\dagger(k) \tag{16}$$

上式を変形すると

$$\mathrm{tr}[a_i(k)] = \mathrm{tr}[a_i(-k)] + i\,\mathrm{tr}\Big[w^\dagger(k)\partial_i w(k)\Big] \tag{17}$$

証明

$$|u_\alpha(-k)\rangle = w^*_{\alpha\beta}(k)\left|\hat{T}u_\beta(k)\right\rangle$$

を用いると

$$\begin{aligned}
a_{i,\alpha\beta}(-k) &= -i \langle u_\alpha(-k)| (-\partial_i) |u_\beta(-k)\rangle \\
&= iw_{\alpha\gamma}(k)\left\langle \hat{T}u_\gamma(k)\right| \partial_i\Big(w^*_{\beta\lambda}(k)\left|\hat{T}u_\lambda(k)\right\rangle\Big) \\
&= iw_{\alpha\gamma}(k)\left\langle \hat{T}u_\gamma(k)\right| \Big(\partial_i w^*_{\beta\lambda}(k)\Big)\left|\hat{T}u_\lambda(k)\right\rangle \\
&+ iw_{\alpha\gamma}(k)\left\langle \hat{T}u_\gamma(k)\right| w^*_{\beta\lambda}(k)\partial_i\left|\hat{T}u_\lambda(k)\right\rangle
\end{aligned} \tag{18}$$

$$\begin{aligned}
(\text{上式}) &= iw_{\alpha\gamma}(k)\Big(\partial_i w^*_{\beta\lambda}(k)\Big)\left\langle \hat{T}u_\gamma(k)\middle|\hat{T}u_\lambda(k)\right\rangle \\
&= iw_{\alpha\gamma}(k)\Big(\partial_i w^*_{\beta\lambda}(k)\Big)\delta_{\gamma\lambda} \\
&= iw_{\alpha\gamma}(k)\partial_i w^*_{\beta\gamma}(k) \\
&= i\Big(w(k)\partial_i w^\dagger(k)\Big)_{\alpha\beta}
\end{aligned} \tag{19}$$

$$
\begin{aligned}
(\text{下式}) &= i w_{\alpha\gamma}(k) w^*_{\beta\lambda}(k) \left\langle \hat{T} u_\gamma(k) \right| \partial_i \left| \hat{T} u_\lambda(k) \right\rangle \\
&= i w_{\alpha\gamma}(k) w^*_{\beta\lambda}(k) \left\langle \hat{T} u_\gamma(k) \middle| \hat{T} \partial_i u_\lambda(k) \right\rangle \\
&= i w_{\alpha\gamma}(k) w^*_{\beta\lambda}(k) \left\langle \partial_i u_\lambda(k) \middle| u_\gamma(k) \right\rangle \\
&= w_{\alpha\gamma}(k) w^*_{\beta\lambda}(k) (-i \left\langle u_\gamma(k) \middle| \partial_i u_\lambda(k) \right\rangle)^* \\
&= w_{\alpha\gamma}(k) w^*_{\beta\lambda}(k) a^*_{i,\gamma\lambda} \\
&= \left(w(k) a_i^*(k) w^\dagger(k) \right)_{\alpha\beta}
\end{aligned}
\tag{20}
$$

よって

$$
a_i(-k) = w(k) a_i^*(k) w^\dagger(k) + i w(k) \partial_i w^\dagger(k) \tag{21}
$$

これをトレースを取る. $w^\dagger(k) w(k) = 1$ を用いると

$$
\begin{aligned}
\mathrm{tr}[a_i(-k)] &= \mathrm{tr}\left[w(k) a_i^*(k) w^\dagger(k) \right] + i\, \mathrm{tr}\left[w(k) \partial_i w^\dagger(k) \right] \\
&= \mathrm{tr}[a_i^*(k)] - i\, \mathrm{tr}\left[(\partial_i w(k)) w^\dagger(k) \right] \\
&= \mathrm{tr}[a_i(k)] - i\, \mathrm{tr}\left[w^\dagger(k) \partial_i w(k) \right]
\end{aligned}
\tag{22}
$$

□

空間反転対称性を持つ系での Z_2 分類

空間反転対称性を持つ系では

$$
\hat{P}^{-1} \hat{H}(k) \hat{P} = \hat{H}(-k) \tag{23}
$$

TRIMΛ では

$$
\hat{P}^{-1} \hat{H}(\Lambda) \hat{P} = \hat{H}(\Lambda) \tag{24}
$$

より, パリティ ν はよい量子数となる.