

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

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

$$\hat{T}^2 = -1 \quad (2)$$

$$\langle \hat{T}\psi | \hat{T}\phi \rangle = \langle \phi | \psi \rangle \quad (3)$$

$$\langle \psi | \hat{T}\phi \rangle = -\langle \phi | \hat{T}\psi \rangle \quad (4)$$

$$\begin{aligned} \langle \hat{T}\psi | \hat{T}\hat{A}\hat{T}^{-1} | \hat{T}\phi \rangle &= \langle \hat{T}\psi | \hat{T}\hat{A}\phi \rangle \\ &= \langle \hat{A}\phi | \psi \rangle = \langle \phi | \hat{A}^\dagger | \psi \rangle \end{aligned} \quad (5)$$

時間反転対称な系

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

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

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

w 行列

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

と定める。

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

$$| u_\alpha(-k) \rangle = w_{\alpha\beta}^*(k) \hat{T} | u_\beta(k) \rangle \quad (10)$$

w 行列の性質

Unitary

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

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

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

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

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

TRIM Λ では $w(\Lambda)$ は反対称行列

Berry 接続行列

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

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

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

w 行列と Berry 接続行列の関係

$$a_i(-k) = w(k) a_i^*(k) w^\dagger(k) + i w(k) \partial_i w^\dagger(k) \quad (16)$$

上式を変形すると

$$\text{tr}[a_i(k)] = \text{tr}[a_i(-k)] + i \text{tr}[w^\dagger(k) \partial_i w(k)] \quad (17)$$

証明

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

を用いると

$$\begin{aligned} a_{i,\alpha\beta}(-k) &= -i \langle u_\alpha(-k) | (-\partial_i) | u_\beta(-k) \rangle \\ &= i w_{\alpha\gamma}(k) \langle \hat{T}u_\gamma(k) | \partial_i (w_{\beta\lambda}^*(k)) | \hat{T}u_\lambda(k) \rangle \\ &= i w_{\alpha\gamma}(k) \langle \hat{T}u_\gamma(k) | (\partial_i w_{\beta\lambda}^*(k)) | \hat{T}u_\lambda(k) \rangle \\ &\quad + i w_{\alpha\gamma}(k) \langle \hat{T}u_\gamma(k) | w_{\beta\lambda}^*(k) \partial_i | \hat{T}u_\lambda(k) \rangle \end{aligned} \quad (18)$$

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

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

よって

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

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

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

□