熱統計力学 2 レポート No.2

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問 1

$\langle x_1 x_2 \rangle_C$ は $n_1 = n_2 = 1$ なので

$$\begin{aligned} 1 &= \sum_j k_j m_{j1} = k_1 m_{11} + k_2 m_{21} \\ 1 &= \sum_j k_j m_{j2} = k_1 m_{12} + k_2 m_{22} \end{aligned} \tag{1}$$

$\sum_j k_j = k_1 + k_2 = 1$ に対しては

$$\begin{aligned} (k_1, k_2) &= (1, 0) \\ \boldsymbol{m}_1 = (m_{11}, m_{12}) &= (1, 1) \end{aligned} \tag{2}$$

$\sum_j k_j = k_1 + k_2 = 2$ に対しては

$$\begin{aligned} (k_1, k_2) &= (1, 1) \\ \boldsymbol{m}_1 = (m_{11}, m_{12}) &= (1, 0) \\ \boldsymbol{m}_2 = (m_{21}, m_{22}) &= (0, 1) \end{aligned} \tag{3}$$

したがって

$$\begin{aligned} \langle x_1 x_2 \rangle_C &= (-1)^0 (0)! \frac{1}{1!} \frac{\langle x_1^1 x_2^1 \rangle}{1! \cdot 1!} + (-1)^1 (1)! \frac{1}{1!} \frac{\langle x_1^1 x_2^0 \rangle}{1! \cdot 0!} \frac{1}{1!} \frac{\langle x_1^0 x_2^1 \rangle}{0! \cdot 1!} \\ &= \langle x_1 x_2 \rangle - \langle x_1 \rangle \langle x_2 \rangle \end{aligned} \tag{4}$$

問 2

$\langle x_1 x_2 x_3 \rangle_C$ は $n_1 = n_2 = n_3 = 1$ なので

$$\begin{aligned} 1 &= \sum_j k_j m_{j1} = k_1 m_{11} + k_2 m_{21} + k_2 m_{31} \\ 1 &= \sum_j k_j m_{j2} = k_1 m_{12} + k_2 m_{22} + k_2 m_{32} \\ 1 &= \sum_j k_j m_{j3} = k_1 m_{13} + k_2 m_{23} + k_2 m_{33} \end{aligned} \tag{5}$$

$\sum_j k_j = k_1 + k_2 + k_3 = 1$ に対しては

$$
\begin{aligned}
(k_1, k_2, k_3) &= (1, 0, 0) \\
\boldsymbol{m}_1 = (m_{11}, m_{12}, m_{13}) &= (1, 1, 1)
\end{aligned} \tag{6}
$$

$\sum_j k_j = k_1 + k_2 + k_3 = 2$ に対しては

$$
\begin{cases}
(k_1, k_2, k_3) = (1, 1, 0) \\
\qquad \boldsymbol{m}_1 = (1, 1, 0) \\
\qquad \boldsymbol{m}_2 = (0, 0, 1)
\end{cases} \tag{7}
$$

$$
\begin{cases}
(k_1, k_2, k_3) = (1, 0, 1) \\
\qquad \boldsymbol{m}_3 = (1, 0, 1) \\
\qquad \boldsymbol{m}_4 = (0, 1, 0)
\end{cases} \tag{8}
$$

$$
\begin{cases}
(k_1, k_2, k_3) = (0, 1, 1) \\
\qquad \boldsymbol{m}_5 = (0, 1, 1) \\
\qquad \boldsymbol{m}_6 = (1, 0, 0)
\end{cases} \tag{9}
$$

また $\sum_j k_j = k_1 + k_2 + k_3 = 3$ に対しては

$$
\begin{aligned}
(k_1, k_2, k_3) &= (1, 1, 1) \\
\boldsymbol{m}_1 &= (1, 0, 0) \\
\boldsymbol{m}_2 &= (0, 1, 0) \\
\boldsymbol{m}_3 &= (0, 0, 1)
\end{aligned} \tag{10}
$$

以上から

$$
\begin{aligned}
\langle x_1 x_2 x_3 \rangle_C = &(-1)^0 (0)! \frac{1}{1!} \frac{\langle x_1 x_2 x_3 \rangle}{1! \cdot 1! \cdot 1!} \\
&+ (-1)^1 (1)! \frac{1}{1!} \frac{\langle x_1^1 x_2^1 x_3^0 \rangle}{1! \cdot 1! \cdot 0!} \frac{1}{1!} \frac{\langle x_1^0 x_2^0 x_3^1 \rangle}{0! \cdot 0! \cdot 1!} \\
&+ (-1)^1 (1)! \frac{1}{1!} \frac{\langle x_1^1 x_2^0 x_3^1 \rangle}{1! \cdot 0! \cdot 1!} \frac{1}{1!} \frac{\langle x_1^0 x_2^1 x_3^0 \rangle}{0! \cdot 1! \cdot 0!} \\
&+ (-1)^1 (1)! \frac{1}{1!} \frac{\langle x_1^0 x_2^1 x_3^1 \rangle}{0! \cdot 1! \cdot 1!} \frac{1}{1!} \frac{\langle x_1^1 x_2^0 x_3^0 \rangle}{1! \cdot 0! \cdot 0!} \\
&+ (-1)^2 (2)! \frac{1}{1!} \frac{\langle x_1^1 x_2^0 x_3^0 \rangle}{1! \cdot 0! \cdot 0!} \frac{1}{1!} \frac{\langle x_1^0 x_2^1 x_3^0 \rangle}{0! \cdot 1! \cdot 0!} \frac{1}{1!} \frac{\langle x_1^0 x_2^0 x_3^1 \rangle}{0! \cdot 0! \cdot 1!}
\end{aligned} \tag{11}
$$

$$
\begin{aligned}
\therefore \ \langle x_1 x_2 x_3 \rangle_C = &\langle x_1 x_2 x_3 \rangle - \langle x_1 x_2 \rangle \langle x_3 \rangle - \langle x_1 x_3 \rangle \langle x_2 \rangle \\
&- \langle x_2 x_3 \rangle \langle x_1 \rangle + 2 \langle x_1 \rangle \langle x_2 \rangle \langle x_3 \rangle
\end{aligned} \tag{12}
$$

問 3

$U(\beta)$ を展開した際の 3 次項は

$$
\begin{aligned}
T_\tau\left(-\frac{1}{3!}\int_0^\beta \mathrm{d}\tau\int_0^\beta \mathrm{d}\tau'\int_0^\beta \mathrm{d}\tau'' V(\tau)V(\tau')V(\tau'')\right) =& -\frac{1}{6}\int_0^\beta \mathrm{d}\tau\int_0^\tau \mathrm{d}\tau'\int_0^{\tau'} \mathrm{d}\tau'' V(\tau)V(\tau')V(\tau'') \\
&-\frac{1}{6}\int_0^\beta \mathrm{d}\tau\int_0^\tau \mathrm{d}\tau''\int_0^{\tau''} \mathrm{d}\tau' V(\tau)V(\tau'')V(\tau') \\
&-\frac{1}{6}\int_0^\beta \mathrm{d}\tau'\int_0^{\tau'} \mathrm{d}\tau\int_0^{\tau} \mathrm{d}\tau'' V(\tau')V(\tau)V(\tau'') \\
&-\frac{1}{6}\int_0^\beta \mathrm{d}\tau'\int_0^{\tau'} \mathrm{d}\tau''\int_0^{\tau''} \mathrm{d}\tau V(\tau')V(\tau'')V(\tau) \\
&-\frac{1}{6}\int_0^\beta \mathrm{d}\tau''\int_0^{\tau''} \mathrm{d}\tau\int_0^{\tau} \mathrm{d}\tau' V(\tau'')V(\tau)V(\tau') \\
&-\frac{1}{6}\int_0^\beta \mathrm{d}\tau''\int_0^{\tau''} \mathrm{d}\tau'\int_0^{\tau'} \mathrm{d}\tau V(\tau'')V(\tau')V(\tau)
\end{aligned}
\tag{13}
$$

積分の仮変数は任意なので

$$
T_\tau\left(-\frac{1}{3!}\int_0^\beta \mathrm{d}\tau\int_0^\beta \mathrm{d}\tau'\int_0^\beta \mathrm{d}\tau'' V(\tau)V(\tau')V(\tau'')\right) = -\int_0^\beta \mathrm{d}\tau\int_0^\tau \mathrm{d}\tau'\int_0^{\tau'} \mathrm{d}\tau'' V(\tau)V(\tau')V(\tau'')
\tag{14}
$$