熱・統計力学演習〈第1回〉

$\boxed{1}$ (a)

$$\bar{x} = \sum_{k=0}^{\infty} k \cdot \frac{\mu^k}{k!} e^{-\mu}$$

$$= \sum_{k=1}^{\infty} \frac{\mu^{k-1}}{(k-1)!} e^{-\mu} \cdot \mu$$

$$= \sum_{k=0}^{\infty} \frac{\mu^k}{k!} \cdot e^{-\mu} \cdot \mu$$

$$= e^{\mu} \cdot e^{-\mu} \cdot \mu = \mu$$

$$\boxed{\sum_{i=0}^{\infty} \frac{\mu^i}{i!} = e^{\mu}}$$

$$\overline{x^2} = \sum_{k=0}^{\infty} k^2 \cdot \frac{\mu^k}{k!} e^{-\mu}$$

$$= \sum_{k=1}^{\infty} \frac{k\mu^{k-1}}{(k-1)!} e^{-\mu} \cdot \mu$$

$$= \sum_{k=0}^{\infty} (k+1) \cdot \frac{\mu^k}{k!} \cdot e^{-\mu} \cdot \mu$$

$$= \sum_{k=0}^{\infty} k \cdot \frac{\mu^k}{k!} e^{-\mu} \cdot \mu + \sum_{k=0}^{\infty} 1 \cdot \frac{\mu^k}{k!} \cdot e^{-\mu} \cdot \mu$$

$$= (\mu+1) e^{\mu} \cdot e^{-\mu} \cdot \mu = \mu^2 + \mu.$$

$$\sigma^2 = \overline{x^2} - (\bar{x})^2 = \mu^2 + \mu - \mu^2 = \mu$$

平均値：

$\int$ (期待値) × (確率).　　$\langle x \rangle = \int x \cdot P(x)\, dx$.

分散：

(2乗平均) − (平均)^2

$\cancel{\boxed{2}\ (a)}$

$\boxed{1}$ (b)

$$\overline{X} = \int_0^\infty dx\ \alpha e^{-\alpha x}\ dx$$

$$= \alpha \frac{d}{d\alpha} \int_0^\infty dx\ (-e^{-\alpha x})$$

$$= \alpha \cdot \frac{d}{d\alpha} \left[+ \frac{1}{\alpha} e^{-\alpha x} \right]_0^\infty$$

$$= -\alpha \cdot \frac{d}{d\alpha} \left(\frac{1}{\alpha} \right) = \frac{1}{\alpha}$$

$$\overline{x^2} = \int_0^\infty dx\ \alpha x^2\ e^{-\alpha x}\ dx$$

$$= \alpha \frac{d^2}{d\alpha^2} \int_0^\infty dx \cdot e^{-\alpha x}$$

$$= \alpha \cdot \frac{d^2}{d\alpha^2} \cdot \left[- \frac{1}{\alpha} e^{-\alpha x} \right]_0^\infty$$

$$= \alpha \frac{d^2}{d\alpha^2} \cdot \left(+ \frac{1}{\alpha} \right)$$

$$= -\alpha \frac{d}{d\alpha} \cdot \left(\frac{1}{\alpha^2} \right) = \frac{2}{\alpha^2}$$

$$\sigma^2 = \frac{2}{\alpha^2} - \left(\frac{1}{\alpha} \right)^2 = \frac{1}{\alpha^2}$$

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$\boxed{2}$ (a) $P_r = {}_nC_r \, p^r \cdot (1-p)^{N-r}$

$$= \frac{N!}{r!(N-r)!} p^r \cdot (1-p)^{N-r}$$

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(b) $$\bar{r} = \sum_{r=0}^{N} r \cdot \underbrace{\frac{N!}{r!(N-r)!} p^r \cdot (1-p)^{N-r}}_{=P_r}$$

$$= \sum_{r=1}^{N} \frac{N!}{(r-1)!(N-r)!} p^r \cdot (1-p)^{N-r}$$

$$= \sum_{r=0}^{N-1} \frac{N!}{r!(N-r-1)!} p^{r+1} \cdot (1-p)^{N-r-1}.$$

$$= Np \cdot \left[\sum_{r=0}^{N-1} \frac{(N-1)!}{r!\underbrace{(N-r-1)}_{(N-1)-r.}!} p^r \cdot (1-p)^{\underbrace{N-r-1}_{(N-1)-r}} \right]$$

$$= Np$$

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$$\overline{r^2} = \sum_{r=0}^{N} r^2 \cdot \frac{N!}{r!(N-r)!} p^r \cdot (1-p)^{N-r}$$

$$= \sum_{r=1}^{N} r \cdot \frac{N!}{(r-1)!(N-r)!} p^r \cdot (1-p)^{N-r}$$

$$= \sum_{r=0}^{N-1} (r+1) \frac{N!}{r!(N-r-1)!} p^r \cdot (1-p)^{N-r}$$

$$= \sum_{r=0}^{N-1} r \cdot \frac{N!}{r!(N-r-1)!} p^r (1-p)^{N-r} + \sum_{r=0}^{N-1} \frac{N!}{r!(N-r-1)!} p^r (1-p)^{N-r}$$

$$= Np \{ (N-1)p + 1 \}$$

$$\sigma^2 = \overline{r^2} - (\bar{r})^2 = NpQ$$

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$\boxed{3}$ (a) $\Gamma(t+1) = \int_0^{+\infty} dx\ x^t e^{-x}$

$= \int_0^{\infty} dx \cdot x^t \cdot \{-(e^{-x})'\}$

$= -\underbrace{[x^t \cdot e^{-x}]_0^{\infty}}_{=0} + \int_0^{\infty} dx \cdot t x^{t-1} \cdot e^{-x}$

$= t \cdot \Gamma(t)$ //

$\left(\begin{aligned} \Gamma(1) &= \int_0^{\infty} e^{x} dx \\ &= e^{x}\Big|_0^{\infty} = 1. \end{aligned} \right)$

$\Gamma(n+1) = n \cdot \Gamma(n) = \cdots = n!\,\Gamma(1) = n!$ //

(b)'

$\Gamma(n+1) = \int_0^{\infty} dx\ x^n e^{-x}$ $\quad x = ny,\ dx = n dy.$

$= \int_0^{\infty} n dy \cdot n^n y^n e^{-ny}$

$= n^{n+1} \int_0^{\infty} dy\ y^n e^{-ny}$ $\quad y^n = e^{n \log y}.$

$= n^{n+1} \int_0^{\infty} dy\ e^{-n(y - \log y)}$

$f(y) = y - \log y.$

Taylor 展開: $f(y) = f(y_0) + f'(y_0)(y-y_0) + \frac{1}{2} f''(y_0)(y-y_0)^2 + \cdots$

$y = y_0$ で.

鞍部点法 $\quad f'(y) = 1 - \frac{1}{y} = 0. \rightarrow \therefore y_0 = 1.$

$f(y) = 1 + \frac{1}{2} f''(1)(y-1)^2 + \cancel{\cdots}$

$f''(1) = \frac{1}{y^2}\Big|_{y=1} = 1.$

$\therefore f(y) \approx 1 + \frac{1}{2}(y-1)^2$

鞍部点法: 積分関数の漸近~~■~~展開を求める重要な方法の1つ.

$$n! = \Gamma(n+1)$$
$$= n^{n+1}\int_0^\infty dy\, e^{-n\{1+\frac{1}{2}(y-1)^2\}}$$

(変数変換： $z = \sqrt{n/2}\,(y-y_0)$
$z = \sqrt{n/2}\,(y-1)$, $dz = \sqrt{\frac{n}{2}}\,dy$.)

$$= n^{n+1}\int_{-\sqrt{n/2}}^{\infty} \sqrt{\frac{2}{n}}\,dz\cdot e^{-n-z^2}$$
$$= n^{n+1}\cdot 2^{1/2}\cdot n^{-1/2}\cdot e^{-n}\int_{-\sqrt{n/2}}^{\infty} e^{-z^2}\,dz.$$
n(大) $\to -\infty$.

$$\approx n^{n+1/2}\cdot 2^{1/2}\cdot e^{-n}\cdot\sqrt{\pi} = \sqrt{2\pi n}\cdot n^n\cdot e^{-n}$$
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2項分布 $\xrightarrow[N\to\infty]{}$ Gauss分布 を求める：

~~N, N-r~~ n(大)のとき.

$$\boxed{\log n! \approx n\log n - n}$$

$\boxed{4}$ (a). $P_r = \dfrac{N!}{r!(N-r)!}\,p^r q^{N-r}.$

$$\log P_r = \log\left(\frac{N!}{r!(N-r)!}\,p^r q^{N-r}\right)$$
$$= \log N! - \log r! - \log(N-r)! + \log p^r + \log q^{N-r}$$
$$= N\log N - \cancel{N} - r\log r + \cancel{r} - (N-r)\log(N-r) + \cancel{(N-r)}$$
$$+ r\log p + (N-r)\log q.$$

$$= N\log N - r\log r - (N-r)\log(N-r) + r\log p + (N-r)\log q$$

$r = Ns \to$
$$= N\log N - Ns\log Ns - N(1-s)\log N(1-s)$$
$$+ \underline{Ns\log p} + \underline{N(1-s)\log q}.$$

$$= \cancel{N\log N} - \cancel{Ns\log N} - \cancel{N\log N} - N\log(1-s) + \cancel{Ns\log N} + Ns\log(1-s)$$
$$-Ns\log s \qquad + \cdots$$

$$= -Ns\log s - N(1-s)\log(1-s) +$$
$$Ns\log p + N(1-s)\log q$$
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(a)より。

4 (b) $\phi(s) = -Ns\log s - N(1-s)\log(1-s) + Ns\log p + N(1-s)\log q.$

$$\phi'(s) = -N\log s - \cancel{N} + N\log(1-s) + \cancel{N} + N\log p - N\log q.$$

$$= -N\{\log s - \log(1-s) - \log p + \log q\}$$

$$\phi''(s) = -N\left(\frac{1}{s} + \frac{1}{1-s}\right).$$

$$\phi(p) = -Np\log p - N(1-p)\log(1-p) + Np\log p + N(1-p)\log(1-p)$$

$$= 0$$

$$\phi'(p) = -N\{\log p - \log(1-p) - \log p + \log(1-p)\} = 0$$

$$\phi''(p) = -N\cdot\left(\frac{1}{p} + \frac{1}{q}\right) = -N/pq \qquad (p+q=1).$$

(c) $\phi(s) = \phi(p) + \phi'(p)(s-p) + \frac{1}{2}\phi''(p)(s-p)^2.$

$$= 0 + 0 + \frac{1}{2}\cdot\left(-\frac{N}{pq}\right)\cdot(s-p)^2$$

$$= -\frac{N}{2pq}(s-p)^2$$

(d) (a)-(c)より。

$s = r/N.$

$$\log P_r \approx -\frac{N}{2pq}(s-p)^2 = -\frac{N}{2pq}\left(\frac{r}{N} - p\right)^2$$

$$= -\frac{1}{2Npq}(r-Np)^2$$

$$\therefore P_r = \exp\left(-\frac{1}{2Npq}(r-Np)^2\right)$$

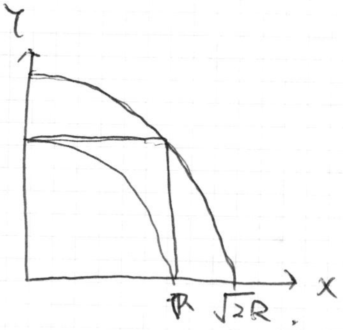
規格化定数を考えて、

$\int P_r dr$ A. $= \sqrt{2\pi Npq}$ $\qquad \therefore P_r = \frac{1}{\sqrt{2\pi Npq}}\exp\left(-\frac{(r-Np)^2}{2Npq}\right)$

5 (a) $\int_{-\infty}^{\infty} e^{-ax^2} dx$

$ax^2 \to t^2$, $dt = \sqrt{a}\, dx$.

$\int_0^{\infty} e^{-t^2} dt \to \int_0^{\infty}\int_0^{\infty} e^{-x^2-y^2} dxdy$



$\frac{1}{4} \int_0^r \int_0^\theta f(r)\, r\sin\theta\, dr d\theta = \frac{1}{4} \cdot 2\pi \int_0^r r f(r)\, dr$

$\frac{\pi}{2} \int_0^R r e^{-r^2} dr < \int_0^R \int_0^R e^{-x^2-y^2} dxdy < \frac{\pi}{2} \int_0^{\sqrt{2}R} r e^{-r^2} dr$.

$\frac{\pi}{2} \cdot -\frac{1}{2} e^{-r^2} \Big|_0^R < \left\{ \int_0^R e^{-x^2} dx \right\}^2 < \frac{\pi}{2} \cdot -\frac{1}{2} e^{-r^2} \Big|_0^{\sqrt{2}R}$.

$\downarrow R \to \infty$ $\qquad$ $\downarrow R \to \infty$

$\pi/4$ $\qquad$ $\pi/4$.

$\therefore \int_0^{\infty} e^{-x^2} dx = \sqrt{\frac{\pi}{4}} = \frac{\sqrt{\pi}}{2}$.

$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$.

$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$.

$\int_0^{\infty} e^{-ax^2} dx = \frac{\sqrt{\pi}}{2\sqrt{a}}$

N