密度行列

$$\psi(r,t)=\sum_n C_n(t)\phi_n(r)$$

2準位系 $\psi(r,t)=C_1(t)\phi_1(r)+C_2(t)\phi_2(r)$

$$\rho=\begin{pmatrix}\rho_{11} & \rho_{12}\\ \rho_{21} & \rho_{22}\end{pmatrix}=\begin{pmatrix}C_1C_1^* & C_1C_2^*\\ C_2C_1^* & C_2C_2^*\end{pmatrix}=\begin{pmatrix}C_1\\ C_2\end{pmatrix}\begin{pmatrix}C_1^* & C_2^*\end{pmatrix}=\psi\psi^*=|\psi\rangle\langle\psi|$$

ρ_{11}：下の準位にいる確率

ρ_{12}：複素双極子モーメント（遷移双極子モーメント）に比例

$\rho_{21}=\rho_{12}^*$

ρ_{22}：上の準位にいる確率

演算子Aの期待値

$$\begin{aligned}\langle\psi|A|\psi\rangle&=\langle C_1\phi_1+C_2\phi_2|A|C_1\phi_1+C_2\phi_2\rangle\\ &=C_1^*C_1A_{11}+C_2^*C_1A_{21}+C_1^*C_2A_{12}+C_2^*C_2A_{22}\\ &=\rho_{11}A_{11}+\rho_{12}A_{21}+\rho_{21}A_{12}+\rho_{22}A_{22}\\ &=\mathrm{Tr}(\rho A)\end{aligned}$$

$$\because\ \rho A=\begin{pmatrix}\rho_{11} & \rho_{12}\\ \rho_{21} & \rho_{22}\end{pmatrix}\begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}=\begin{pmatrix}\boxed{\rho_{11}A_{11}+\rho_{12}A_{21}} & \rho_{11}A_{12}+\rho_{12}A_{22}\\ \rho_{21}A_{11}+\rho_{22}A_{21} & \boxed{\rho_{21}A_{12}+\rho_{22}A_{22}}\end{pmatrix}$$

波動関数がわかっている量子力学系：純粋状態

　　状態ベクトル$\begin{pmatrix}C_1\\ C_2\end{pmatrix}$が確定

波動関数（状態ベクトル）が完全にはわかっていない：混合状態

　　情報が完全ではないー全系のうち一部分のみの情報

多粒子系では統計的性質のみ（状態nにいる確率）がわかっている場合が多い

一般化した密度演算子$\rho=\sum_\psi P_\psi|\psi\rangle\langle\psi|$　P_ψ：系が状態ベクトル$|\psi\rangle$をとる比率

$|\psi\rangle=\sum_n C_n|n\rangle$のとき$\rho=\sum_\psi P_\psi\sum_n\sum_m C_nC_m^*|n\rangle\langle m|=\sum_\psi P_\psi\sum_n\sum_m\rho_{nm}|n\rangle\langle m|$

$$\left|\psi_j\right\rangle = C_{1j}(t)\left|1\right\rangle + C_{2j}(t)\left|2\right\rangle$$

$$\rho = \sum_j P_j \left|\psi_j\right\rangle\left\langle\psi_j\right| = \sum_j P_j \begin{pmatrix} |C_{1j}|^2 & C_{1j}C_{2j}^* \\ C_{2j}C_{1j}^* & |C_{2j}|^2 \end{pmatrix}$$

$\left|\psi_j\right\rangle = C_1\left|1\right\rangle + e^{i\phi_j}C_2\left|2\right\rangle$　$\left|1\right\rangle$と$\left|2\right\rangle$の振幅の位相差ϕ_jが一様分布

N個の量子力学系　j番目の系に対する確率$P_j = \dfrac{1}{N}$とする

$$\begin{aligned}
\rho_{12} &= \sum_j P_j C_{1j}C_{2j}^* \\
&= C_1C_2^* \frac{1}{N}\sum_{j=1}^{N} e^{i\phi_j} \\
&= C_1C_2^* \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{i\phi} \\
&= 0
\end{aligned}$$

$=0$　コヒーレンスが0

単一モード（単色）の熱輻射(熱的光源をフィルターで単色化)

$$P_\psi = P_n = \frac{e^{-n\hbar\omega/k_BT}}{\sum_j e^{-j\hbar\omega/k_BT}} = e^{-n\hbar\omega/k_BT}(1-e^{-\hbar\omega/k_BT})$$

$\rho = (1-e^{-\hbar\omega/k_BT})\sum_n e^{-n\hbar\omega/k_BT}\left|n\right\rangle\left\langle n\right|$　対角項のみ

1 つの自由度あたり配分されている光子数の期待値

$$\left\langle n\right\rangle = \sum_n nP_n = (1-e^{-\hbar\omega/k_BT})\sum_n ne^{-n\hbar\omega/k_BT} = -(1-e^{-\hbar\omega/k_BT})\frac{\partial}{\partial(\hbar\omega/k_BT)}\sum_n e^{-n\hbar\omega/k_BT}$$

$$= -(1-e^{-\hbar\omega/k_BT})\frac{\partial}{\partial(\hbar\omega/k_BT)}\left[\frac{1}{(1-e^{-\hbar\omega/k_BT})}\right] = \frac{e^{-\hbar\omega/k_BT}}{1-e^{-\hbar\omega/k_BT}} = \frac{1}{e^{\hbar\omega/k_BT}-1}$$

Planck分布

問：混合状態の演算子Aの期待値$< A >= \mathrm{Tr}(\rho A)$を示せ

$\rho(t_0) = \left|\psi\right\rangle\left\langle\psi\right|$　$\left|\psi\right\rangle = \dfrac{1}{\sqrt{2}}\left(\left|\phi_1\right\rangle + \left|\phi_2\right\rangle\right)$　$\rho = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$

$\left|\psi\right\rangle = \dfrac{1}{\sqrt{2}}\left(\left|\phi_1\right\rangle - \left|\phi_2\right\rangle\right)$　$\rho = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}$

} **純粋状態**

$\rho(t_0) = \dfrac{1}{2}\left|\phi_1\right\rangle\left\langle\phi_1\right| + \dfrac{1}{2}\left|\phi_2\right\rangle\left\langle\phi_2\right|$　$\rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$　**混合状態**

光における混合状態の例　無偏光の光、部分偏光の光、インコヒーレント光

$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$: x方向に偏光した状態の波動関数

$|\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$: y方向に偏光した状態の波動関数

任意の純粋状態

$$\begin{pmatrix} a \\ b \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad |a|^2 + |b|^2 = 1$$

この純粋状態の密度行列は

$$\rho = \begin{pmatrix} aa^* & ab^* \\ ba^* & bb^* \end{pmatrix}$$

x偏光状態　$a = 1, \quad b = 0$

$$\rho_x = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

y偏光状態　$a = 0, \quad b = 1$

$$\rho_x = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

45°偏光　$a = 1/\sqrt{2}, \quad b = 1/\sqrt{2}$

$$\rho_{45^\circ} = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

135°偏光　$a = -1/\sqrt{2}, \quad b = 1/\sqrt{2}$

$$\rho_{135^\circ} = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}$$

x偏光状態50%とy偏光状態50%の混合状態

$$\rho = \frac{1}{2}\rho_x + \frac{1}{2}\rho_y = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

45°偏光状態50%と135°偏光状態50%の混合状態

$$\rho = \frac{1}{2}\rho_{45^\circ} + \frac{1}{2}\rho_{135^\circ} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

密度行列の満たす運動方程式

$$\dot{\rho} = \sum_{\psi} P_{\psi}(|\dot{\psi}\rangle\langle\psi| + |\psi\rangle\langle\dot{\psi}|) = -\frac{i}{\hbar}\sum_{\psi} P_{\psi}(H|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|H)$$

$$= -\frac{i}{\hbar}[H, \rho]$$

$$[H, \rho] = H\rho - \rho H$$

$$H\rho = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}\begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \begin{pmatrix} H_{11}\rho_{11} + H_{12}\rho_{21} & H_{11}\rho_{12} + H_{12}\rho_{22} \\ H_{21}\rho_{11} + H_{22}\rho_{21} & H_{21}\rho_{12} + H_{22}\rho_{22} \end{pmatrix}$$

$$H = H_0 + H' = \begin{pmatrix} E_1 & -\mu_{12}E_0\cos\omega t \\ -\mu_{21}E_0\cos\omega t & E_2 \end{pmatrix}$$

$$\frac{d\rho_{11}}{dt} = -\frac{i}{\hbar}(H\rho - \rho H)_{11} = -\frac{i}{\hbar}(H_{11}\rho_{11} + H_{12}\rho_{21} - \rho_{11}H_{11} - \rho_{12}H_{21}) = -\frac{i}{\hbar}(H_{12}\rho_{21} - \rho_{12}H_{21})$$

$$\frac{d\rho_{22}}{dt} = -\frac{i}{\hbar}(H\rho - \rho H)_{22} = -\frac{i}{\hbar}(H_{21}\rho_{12} + H_{22}\rho_{22} - \rho_{21}H_{12} - \rho_{22}H_{22}) = -\frac{i}{\hbar}(H_{21}\rho_{12} - \rho_{21}H_{12})$$

$$= -\frac{i}{\hbar}[(-\mu_{21}E_0\cos\omega t)\rho_{12} - \rho_{21}(-\mu_{12}E_0\cos\omega t)] = -i(\eta\rho_{21} - \eta^*\rho_{12})$$

$$\frac{d\rho_{12}}{dt} = -\frac{i}{\hbar}(H\rho - \rho H)_{12} = -\frac{i}{\hbar}(H_{11}\rho_{12} + H_{12}\rho_{22} - \rho_{11}H_{12} - \rho_{12}H_{22})$$

$$= -\frac{i}{\hbar}[(H_{11} - H_{22})\rho_{12} + (\rho_{22} - \rho_{11})H_{12}]$$

$$= -\frac{i}{\hbar}[(E_1 - E_2)\rho_{12} - \mu_{12}E_0\cos\omega t(\rho_{22} - \rho_{11})]$$

$$= i\omega_0\rho_{12} + i\frac{\mu_{12}E_0}{\hbar}\cos\omega t(\rho_{22} - \rho_{11})$$

$$= i\omega_0\rho_{12} + i\eta(\rho_{22} - \rho_{11})$$