# Pravegael Education 

CSIR NET-JRF, GATE, IIT-JAM, JEST, TIFR and GRE for Physics H.N. 28 A/1, Jia Sarai, Near IIT-Delhi, Hauz Khas, New Delhi-110016

Contact: +91-89207-59559, 8076563184
Website: www.pravegaa.com I Email: pravegaaeducation@gmail.com

## Chapter 8 Canonical Ensemble ( $E, V, N)$

## 3. Microcanonical ensemble of the combined system

Since the combined system $A$ is isolated, the distribution function in the combined phase space is given by the microcanonical distribution function $\rho(q, p)$,

$$
\begin{gather*}
\rho(q, p)=\frac{\delta(E-H(q, p))}{\int d q d p \delta(E-H(q, p))}, \quad \int d q d p \delta(E-H)=\Omega(E)  \tag{1}\\
\rho(q, p)=\frac{\delta(E-H)}{\Omega(E)}
\end{gather*}
$$

where $\Omega(E)$ is the density of phase space.
Calculation of $A_{2}$. It is not the distribution function $\rho(q, p)$ of the total system $A$ that we are interested in, but the distribution function $\rho_{1}$ of the small system $A_{1}$. One hence needs to trace out $A_{2}$ :

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$$
\begin{align*}
& \rho_{1}(q(1), p(1))=\int d q(2) d p(2) \rho \\
& =\frac{\int d q(2) d p(2) \delta\left(E-\left(H_{1}+H_{2}\right)\right)}{\Omega(E)}=\frac{\Omega_{2}\left(E-H_{1}\right)}{\Omega(E)} \tag{2}
\end{align*}
$$

where $\Omega_{2}\left(E_{2}\right)=\Omega_{2}\left(E-H_{1}\right)$ is the phase space density of $A_{2}$.
Small $E_{1}$ expansion. Now, we make use of the fact that $A_{1}$ is a much smaller system than $A_{2}$ and therefore the energy $E_{1}$ given by $H_{1}$ is much smaller than the energy of the combined system:

$$
E_{1} \ll E
$$

In this case, we can approximate (2) by expanding the slowly varying logarithm of $\Omega_{2}\left(E_{2}\right)=\Omega_{2}\left(E-H_{1}\right)$ around the $E_{2}=E$ as

$$
\begin{equation*}
\ln \Omega_{2}\left(E_{2}\right)=\ln \Omega_{2}\left(E-H_{1}\right) \simeq \ln \Omega_{2}(E)-\left[\frac{\partial \ln \Omega_{2}}{\partial E_{2}}\right]_{E_{2}=E} H_{1}+\ldots \tag{3}
\end{equation*}
$$

and neglect the higher-order terms since $H_{1}=E_{1} \ll E$.
Derivatives of the entropy. Using,

$$
\begin{equation*}
S=k_{B} \ln \left(\frac{\Gamma(E, V, N)}{\Gamma_{0}}\right)=k_{B} \ln \left(\frac{\Omega(E) \Delta}{\Gamma_{0}}\right) \tag{4}
\end{equation*}
$$

where $\Delta$ is the width of the energy shell, we find that derivatives of the entropy like

$$
\begin{equation*}
\frac{1}{T}=\frac{\partial S}{\partial E}=k_{B} \frac{\partial \ln \Omega(E)}{\partial E} \tag{5}
\end{equation*}
$$

can be taken with respect to the logarithm of the phase space density $\Omega(E)$.

## Boltzmann Factor

Using (5) for the larger system $A_{2}$ we may rewrite (3) as

$$
\begin{aligned}
\Omega_{2}\left(E-H_{1}\right) & =\exp \left[\ln \Omega_{2}(E)-\left.\frac{\partial \ln \Omega_{2}\left(E_{2}\right)}{\partial E_{2}}\right|_{E_{2}=E} H_{1}+\ldots .\right] \\
& =\Omega_{2}(E) \exp \left[-\frac{H_{1}}{k_{B} T_{2}}\right]
\end{aligned}
$$

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The temperature $T_{2}$ of the heat reservoir $A_{2}$ by whatever small amount of energy the large system $A_{2}$ gives to the small system $A_{1}$. Both systems are thermally coupled, such that $T_{1}=T_{2}=T$. We hence find with (2).

$$
\begin{equation*}
\rho_{1}(q(1), p(1))=\frac{\Omega_{2}}{\Omega(E)} e^{-\frac{H_{1}}{k_{B} T}} \propto e^{-\frac{H_{1}}{k_{B} T}} \tag{6}
\end{equation*}
$$

The factor $\exp \left[-H_{1} /\left(k_{B} T\right)\right]$ is called the Boltzmann factor.

