

Project for the exam: AMS (DSE)

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Theoretical Framework

"Ludwig Boltzmann, who spent much of his life studying statistical mechanics, died in 1906, by his own hand. Paul Ehrenfest, carrying on the work, died similarly in 1933. Now it is our turn to study statistical mechanics." States of Matter (1975), by David L. Goodstein

Ising model

Concepts of statistical mechanics: entropy [1]

- Fundamental postulate of statistical mechanics $S = k_b \ln |\Gamma|$
- Where S is the thermodynamic entropy, k_b is Boltzmann constant and $|\Gamma|$ the volume in the phase space

$$S(X_{0},...,X_{r}) = k_{b} \ln \int_{\Gamma} dx = k_{b} \int dx \prod_{i=0}^{r} \left[\theta(X_{i}(x) - (X_{i} - \Delta X_{i})) \theta(X_{i} - X_{i}(x)) \right]$$
(1)

- $(X_0, ..., X_r)$ are the extensive variables
- The θ functions assures that the integrand is not null only in the interval $X_i \Delta X_i \leq X_i(x) \leq X_i$

Concepts of statistical mechanics: micro-canonical ensamble

Lets focus on a particular observable A (extensive)

$$S(X; a) = k_b \ln \int_{\Gamma} dx \delta(A(x) - a)$$
 (2)

$$S(X) = S(X; a*) \ge S(X; a) \tag{3}$$

$$\frac{|\Gamma(a)|}{|\Gamma|} = \frac{1}{|\Gamma|} \int_{\Gamma} dx \delta(A(x) - a)$$

$$= \exp\left\{\frac{1}{k_b} \left[S(X; a) - S(X; a^*)\right]\right\}$$

$$\simeq \exp\left\{\frac{1}{k_b} \left[\frac{\partial^2 S}{\partial A^2}|_{a^*} (a - a^*)^2\right]\right\}$$

$$a^* = \langle A(x) \rangle = \frac{1}{|\Gamma|} \int_{\Gamma} dx A(x)$$
(5)

(5)

Concepts of statistical mechanics: canonical ensemble

$$a^* = \frac{1}{|\Gamma|} \int_{\Gamma} dx_s dx_R A(x_s) \tag{6}$$

$$\langle A(x) \rangle = \int dx_s dx_r A(x_S) \delta(H^{(s)})$$
 (7)

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_s dx_r A(x_s) \delta(H^S(x_s) + H^R(x_R) - H^S(x_S))$$
 (8)

$$\langle A(x) \rangle = \frac{1}{|\Gamma|} \int dx_s A(x_s) \times \int dx_r \delta(H^R(x_R) - (E - H^{(S)}(x_s)))$$
 (9)

$$\int dx_r \delta(H^R(x_R) - (E - H^{(S)}(x_s))) \simeq \exp\left\{\frac{1}{k_b} S^R(E - H^S)\right\}$$
(10)

Concepts of statistical mechanics: canonical ensemble

$$\exp\left\{\frac{1}{k_b}S^R(E-H^S)\right\} \simeq \exp\left[\frac{1}{k_b}S^R(E)\right] \exp\left[-\frac{1}{k_b}\frac{\partial S^{(R)}}{\partial E}|_E H^{(S)}(x_S)\right]$$
(11)

$$\langle A(x) \rangle = \frac{1}{Z} \int dx_s A(x_s) exp \left[-\frac{H^{(S)}(x_s)}{k_b T} \right]$$
 (12)

$$Z = \int dx_s \exp\left[-\frac{H^S(x_s)}{k_b T}\right]$$
 (13)

$$\langle A(x) \rangle = \frac{1}{Z} \int dE \int dx \delta(H(x) - E) A(x) \exp(-\frac{E}{k_b T})$$
 (14)

$$\langle A(x)\rangle = \frac{1}{Z} \int dE' a^*(E') exp \left[-\frac{E' - TS(E')}{k_b T} \right]$$
 (15)



Bibliography I



Luca Peliti. *Statistical mechanics in a nutshell*. Princeton University Press, 2011.

ROC and ϕ factor