RIGOROUS LOWER BOUND ON THE COMPRESSIBILITY OF A CLASSICAL SYSTEM

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A simple inequality is proved, from which a rigorous lower bound on the compressibility of a classical system with purely repulsive or hard core interaction follows immediately.

In this note we prove the following simple inequality: let p be a probability measure on the positive integers. Let $p_n = P_n/n!$ be the probability of integer n. Suppose that the second moment of p exists and that for all $n \geqslant 0$:

$$(P_{n+2}/P_{n+1}) \geqslant (P_{n+1}/P_n) - A, \quad \text{where } A > -1. \qquad \text{(a)}$$

If some $P_n = 0$, it is to be understood that $P_m = 0$ for all $m \geqslant n$. Then:

$$\frac{\langle (n - \langle n \rangle)^2 \rangle}{\langle n \rangle} \geqslant \frac{1}{1+A} . \qquad (1)$$

Equality in (1) is obtained:

if $A > 0$, for $P_n = \dfrac{N!}{(N-n)!} \dfrac{A^n}{(1+A)^N}$ for $n \leqslant N$,

(N arbitrary integer $\geqslant 1$) and zero otherwise.

if $A = 0$, for $P_n = \alpha^n e^{-\alpha}$ with α real, $\alpha > 0$.

if $-1 < A < 0$, for $P_n =$

$= (-A)^n (1+A)^{\alpha} \alpha(\alpha+1)\dots(\alpha+n-1)$ with α real, $\alpha > 0$.

Proof: From Schwarz' inequality:

$$\{\langle n \rangle (1+A)\}^2 = \left\{\sum_0^\infty \frac{1}{n!} P_n\left(\frac{P_{n+1}}{P_n} + nA\right)\right\}^2 \leqslant$$

$$\leqslant \sum_0^\infty \frac{1}{n!} P_n\left(\frac{P_{n+1}}{P_n} + nA\right)^2 . \qquad (2)$$

expanding the right hand side and using (a), one gets (1). The cases of equality in (1) are obtained easily.

As an application, consider a system of classical particles, enclosed in a box of volume V, interacting through a 2 body potential φ; the system is described in the grand canonical formalism. Let z be the fugacity, Z the grand partition function, T the absolute temperature, and $\beta = (kT)^{-1}$. This defines a probability p on the integers by:

$$P_n = Z^{-1} z^n \int dx_1 \dots dx_n \exp[-\beta \sum_{i<j} \varphi(x_i - x_j)]. \qquad (3)$$

For purely repulsive potentials and for hard core potentials, i.e. potentials such that (1): $\varphi(x-y) = +\infty$ for $|x-y| < a$, (2): for any finite sequence of $n+1$ points $x_0, \dots, x_n$ such that $|x_i - x_j| \geqslant a$ for all i and j,

$$\sum_{i=1}^{n} \varphi(x_0 - x_i) \geqslant -B,$$

where B is a real (positive) constant, one can prove easily [1,2] under the additional assumption

$$\int (1 - \exp[-\beta\varphi_+(x)])\, dx < \infty, \qquad \text{(b)}$$

where $\varphi_+(x) = \max(\varphi(x), 0)$, that condition (a) is satisfied, with:

$$A = zD = z\, e^{\beta B} \int (1 - \exp[-\beta\varphi_+(x)])\, dx \qquad (4)$$

(For repulsive potentials, $B = 0$ and $\varphi_+ = \varphi$.) Therefore, for all positive z and V:

$$\chi = \frac{1}{\rho}\frac{d\rho}{dP} = \frac{\beta}{\rho} \frac{\langle (n - \langle n \rangle)^2 \rangle}{\langle n \rangle} \geqslant \frac{\beta}{\rho} \frac{1}{1+zD}$$

where $P = \ln Z/V$ is the pressure, $\rho = \langle n \rangle / V$ the

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density, and χ the compressibility. For repulsive or hard core potentials satisfying a weak tempering condition which is closely related to (b) and slightly stronger, the thermodynamic limit exists [3]. Inequality (5) still holds in the limit as a Lipschitz condition on the pressure. This proves directly in the grand canonical formalism the continuity of the pressure as a function of the density (proofs have already been given in the canonical formalism under various assumptions [1,2,4]) and gives a lower bound on the compressibility.

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