THE CRITICAL STATE OF A FLUID AND
HEISENBERG UNCERTAINTY PRINCIPLE

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Abstract: For a well-established microscopic model of a fluid the critical dispersion of its micro-constituents is motivated, introduced and explained as a standardization of the so-called thermodynamic dispersion. The visualization of the critical dispersion for different substances suggests its isotonic statistical dependence on the mass of the micro-constituents of fluids. The estimate of the coefficient of the linear regression reveals a connection between a microscopic aspect of the critical state and the Heisenberg uncertainty principle.

1. Introduction

From the atomistic viewpoint a fluid consists of interacting micro-constituents which are subject to thermal motion. According to the Maxwell hypothesis (cf. Moeschlin, Grycko [3], Section 1.5) the momentary momenta of the micro-constituents can be viewed as realizations of normally distributed random vectors whose covariance matrix is interrelated with the temperature.

A single component $U_i^{(j)}$ of a momentum random vector $U^{(j)}$ is a random variable to which the variance and therefore also the dispersion $(\mathrm{var}(U_i^{(j)}))^{1/2}$ can be attributed. Analogously, if the fluid is confined to a container, the so-

called configurational dispersion can be derived from the position data of the micro-constituents. The idea of availability of such micro-data is inspired by computer experimental insights into thermodynamic systems (cf. Moeschlin, Grycko [3]).

In the present contribution Section 2 has got a preparatory function; the so-called thermodynamic dispersion is motivated and introduced in Section 3. A standardization of the thermodynamic dispersion turns out (Section 4) to be statistically interrelated with the Planck constant.

2. The Uniform Distribution on a Ball and the Variance of its Projections

Let $R > 0$ be the radius of the ball $B_R(0)$,

$$B_R(0) := \{(x_1, x_2, x_3) \in \mathbb{R}^3 | x_1^2 + x_2^2 + x_3^2 \leq R^2\}.$$

Put

$$\Omega := [0; 2\pi] \times [-\pi/2; +\pi/2] \times [0; R].$$

Let us endow the topological space Ω with its Borel σ-field $\mathcal{A}$. The Lebesgue density

$$f : \Omega \to \mathbb{R}_+, \qquad f(\varphi, \vartheta, r) := \frac{3}{4\pi R^3} \cdot r^2 \cdot \cos \vartheta,$$

induces a probability measure $P := f\lambda^3$ on $(\Omega, \mathcal{A})$. Let us define the random vector $X := (X_1, X_2, X_3) : \Omega \to B_R(0)$ by

$$X_1(\varphi, \vartheta, r) := r \cos(\varphi) \cos(\vartheta),$$

$$X_2(\varphi, \vartheta, r) := r \sin(\varphi) \cos(\vartheta),$$

$$X_3(\varphi, \vartheta, r) := r \sin(\vartheta).$$

The random vector is obviously centered and uniformly distributed on $B_R(0)$. Performing standard integrations we obtain:

$$\mathrm{var}(X_i) = \frac{1}{5} \cdot R^2 \qquad (i = 1, 2, 3) \tag{1}$$

for the variances of the components X_1, X_2, X_3 of the random vector X.

3. The Thermodynamic Dispersion

Let us suppose that a fluid consisting of N micro-constituents of mass $m > 0$ has attained a thermal equilibrium at the (absolute) temperature $T > 0$. If the fluid is confined to a container $B \subset \mathbb{R}^3$ of volume

$$V := \lambda^3(B)$$

(where λ^3 denotes the 3-dimensional Lebesgue measure), then the particle density ϱ is obviously given by

$$\varrho = \frac{N}{V}. \tag{2}$$

A momentary micro-state of the fluid is described by the $6N$-tuple

$$(x; v) := (x^{(1)}, \ldots, x^{(N)}; v^{(1)}, \ldots, v^{(N)}) \in B^N \times \mathbb{R}^{3N}; \tag{3}$$

$x^{(j)}$ denotes the position and $v^{(j)}$ the velocity of the j-th micro-constituent of the fluid, $j = 1, \ldots, N$.

The description (3) can be equivalently expressed as

$$(x; u) := (x^{(1)}, \ldots, x^{(N)}; u^{(1)}, \ldots, u^{(N)}) \in B^N \times \mathbb{R}^{3N}; \tag{4}$$

whereby

$$u^{(j)} := m \cdot v^{(j)} \qquad (j = 1, \ldots, N)$$

denotes the momentum of the j-th micro-constituent.

Definition 3.1. The segments $(x^{(1)}, \ldots, x^{(N)})$ and $(u^{(1)}, \ldots, u^{(N)})$ in (4) are called the configurational segment and the dynamical segment, respectively.

According to the Maxwell hypothesis (cf. Moeschlin, Grycko [3], Section 1.5) the momentary momenta $u^{(1)}, \ldots, u^{(N)}$ can be interpreted as realizations of stochastically independent random vectors $U^{(1)}, \ldots, U^{(N)}$ distributed according to the 3-dimensional centered normal distribution

$$N(0, \sigma_u^2 \cdot I_3) = N(0, \sigma_u^2) \otimes N(0, \sigma_u^2) \otimes N(0, \sigma_u^2) \tag{5}$$

with the covariance matrix $\sigma_u^2 \cdot I_3, I_3$ being the 3×3-identity matrix. The variance σ_u^2 has the physical interpretation

$$\sigma_u^2 = m \cdot k_B \cdot T; \tag{6}$$

m denotes here the mass of a micro-constituent, $k_B = 1.38 \cdot 10^{-23}$ J/K the Boltzmann constant and T the temperature of the fluid.

Definition 3.2. The parameter σ_u in (5) and (6) is called the dynamical dispersion (of the micro-constituents of the fluid).

Remark 3.3. Formula (6) implies that

$$\sigma_u = (m \cdot k_B \cdot T)^{1/2}.$$

It follows that the dynamical dispersion is an intensive parameter, i.e. it does not alter if the volume of the container and the quantity of the fluid are increased by the same factor.

In order to introduce a configurational pendant of the dynamical dispersion as an intensive thermodynamic parameter we consider the following abstract experiment.

Suppose we are able to isolate exactly one micro-constituent of the fluid in a container maintaining a prescribed particle density ϱ (cf. (2)); a natural choice of the container is the ball

$$B_R(0) := \{(x_1, x_2, x_3) \in \mathbb{R}^3 | x_1^2 + x_2^2 + x_3^2 \leq R^2\},$$

whose radius R fulfills the condition

$$\varrho = \frac{1}{V} = \frac{3}{4\pi R^3};$$

we obtain

$$R = \left(\frac{3}{4\pi\varrho}\right)^{1/3}. \tag{7}$$

A momentary position $x^{(1)} \in B_R(0)$ of the single micro-constituent can now be interpreted as a realization of a random vector $X^{(1)} = (X_1^{(1)}, X_2^{(1)}, X_3^{(1)})$ which is uniformly distributed on $B_R(0)$.

Definition 3.4. The configurational dispersion (of the micro-constituents of the fluid) σ_x is defined by

$$\sigma_x := (\text{var}(X_i^{(1)}))^{1/2} \qquad (i = 1, 2, 3), \tag{8}$$

i.e. as the square root of the variance of the random variables $X_1^{(1)}, X_2^{(1)}, X_3^{(1)}$ modelling the Cartesian coordinates of the momentary position of the single micro-constituent of the "fluid" in the container $B_R(0)$.

Remark 3.5. According to (1) of Section 2 we have

$$\sigma_x^2 = \frac{1}{5}R^2. \tag{9}$$

Combining (7), (8) and (9) we obtain

$$\sigma_x = \frac{1}{5^{1/2}} \cdot \left(\frac{3}{4\pi\varrho} \right)^{1/3} \tag{10}$$

for the configurational dispersion σ_x.

Remark 3.6. Formula (10) indicates that the configurational dispersion is a function of the particle density ϱ; σ_x can be interpreted as an intensive parameter describing the thermodynamic state of the fluid.

Definition 3.7. Let a fluid consisting of N micro-constituents of mass $m > 0$ confined to a container $B \subset \mathbb{R}^3$ of volume V be given at the temperature T. Recall Definition 3.2 and Definition 3.4. The product

$$D := \sigma_x \cdot \sigma_u$$

is called the thermodynamic dispersion (of the micro-constituents of the fluid).

Remark 3.3 and formula (10) imply the following expression for the thermodynamic dispersion:

$$D = \frac{1}{5^{1/2}} \cdot \left(\frac{3}{4\pi\varrho} \right)^{1/3} \cdot (m \cdot k_B \cdot T)^{1/2}. \tag{11}$$

Remark 3.8. The thermodynamic dispersion is an intensive parameter carrying the physical unit Js (Joule times second).

Remark 3.9. In (11) the mass m of a micro-constituent is expressed in kg. In order to rewrite (11) in terms of the relative molecular mass m_r we remind the reader that m_r can be defined by:

$$m_r := m \cdot N_A, \tag{12}$$

where N_A denotes the (modified) Avogadro number,

$$N_A = 6.02 \cdot 10^{26} \, \text{kg}^{-1}.$$

We obtain

$$D = \frac{1}{5^{1/2}} \cdot \left(\frac{3}{4\pi\varrho} \right)^{1/3} \cdot (m_r \cdot k_B \cdot T/N_A)^{1/2}. \tag{13}$$

4. The Critical Dispersion and its Statistical Dependence on the Relative Molecular Mass

The thermodynamic dispersion D as introduced in Definition 3.7 and expressed in formula (13) of Section 3 depends not only on the substance (material) but also on the thermodynamic state of the fluid.

In order to motivate a standardization of the thermodynamic dispersion we remind the reader of the so-called critical state that can be attributed to quite a lot of substances. The critical state of a substance is described in particular by the critical temperature T_c and the critical density ϱ_c; T_c and ϱ_c carry important information about the fluid; from the critical data the parameters of the van der Waals equation of state can be computed (for a detailed description of the critical state of a fluid cf. Bergmann, Schaefer [1]). For our context we stress the fact that T_c and ϱ_c are material properties.

Definition 4.1. Let a substance S with the relative molecular mass m_r of its micro-constituents be considered. Suppose that the critical temperature T_c and the critical density ϱ_c of substance S are determined. The critical dispersion D_c (of the micro-constituents) of S is defined by (cf. (13) of Section 3):

$$D_c = \frac{1}{5^{1/2}} \cdot \left(\frac{3}{4\pi\varrho_c}\right)^{1/3} \cdot (m_r \cdot k_B \cdot T_c/N_A)^{1/2}; \tag{14}$$

k_B denotes here the Boltzmann constant and $N_A = 6.02 \cdot 10^{26} \mathrm{kg}^{-1}$ the modified Avogadro number.

Remark 4.2. According to formula (13) of Section 3 and formula (14) of the present section the critical dispersion may be viewed as the thermodynamic dispersion in the critical state of the fluid. Since m_r, T_c and ϱ_c are material properties, so is also the critical dispersion.

For the following analysis of the critical dispersion the critical data of seventeen substances $(H_2, He, Ne, Ar, Kr, Xe, Ra, F_2, Cl_2, Br_2, J_2, O_2, F_2O,$ $HCl, Cl_2, N_2, H_2O)$ are utilized. In Figure 1 the values of the critical dispersion are depicted versus the relative molecular masses of the seventeen substances. The visual impression suggests that the critical dispersion tends to increase with increasing relative molecular mass whereby statistically the data can be explained by a linear dependence. The least squares coefficient γ of linear regression attains the value

$$\gamma = 4.45 \cdot 10^{-35} \,\mathrm{Js}, \tag{15}$$

which approximates the value $\hbar/2$ of Heisenberg position-momentum uncertainty bound (cf. Greiner [2], p. 65) where $\hbar = 1.05 \cdot 10^{-34} \mathrm{Js}$ denotes the

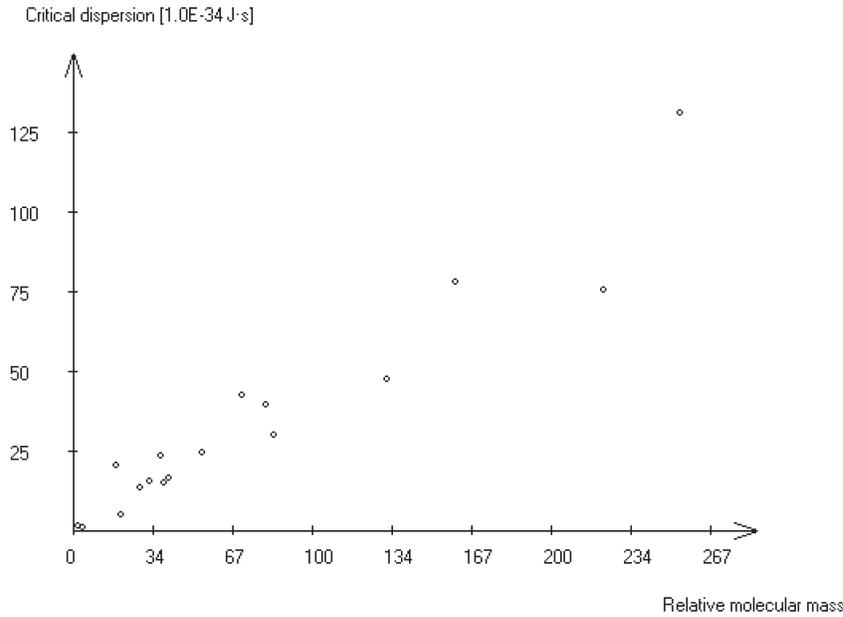Critical dispersion [1.0E-34 J·s]

Figure 1: Critical dispersion versus relative molecular mass

Planck constant. The relative approximation error is less than 20%.

Remark 4.3. The result has the following interpretation: Consider a model substance, i.e. a substance whose relative molecular mass m_r has the value $m_r = 1$. The critical dispersion of the micro-constituents of this model substance approximates Heisenberg position-momentum uncertainty bound.

Remark 4.4. The statistical result can be expressed by the approximatively valid equation (cf. (14) and (15)):

$$\frac{1}{5^{1/2}} \cdot \left(\frac{3}{4\pi \varrho_c} \right)^{1/3} \cdot \left(\frac{k_B \cdot T_c}{m_r \cdot N_A} \right)^{1/2} = \frac{\hbar}{2} \tag{16}$$

interrelating the critical data ϱ_c and T_c of substances with their relative molecular mass m_r.

A physical explanation of the discussed statistical result would probably shed new light on the connection between the microscopic aspects of critical phenomena and Heisenberg uncertainty principle.

Acknowledgments

References

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