The generalized variable for kinetic temperature

1992 J. Phys. A: Math. Gen. 25 4517

(http://iopscience.iop.org/0305-4470/25/17/013)

J. Phys. A: Math. Gen. 25 (1992) 4517-4520. Printed in the UK

The generalized variable for kinetic temperature

V J Menon† and D C Agrawal‡

† Department of Physics, Banaras Hindu University, Varanasi 221005, India
‡ Department of Farm Engineering, Banaras Hindu University, Varanasi 221005, India

Received 9 December 1991, in final form 20 April 1992

Abstract. A very general formula is obtained for the variable representing the kinetic temperature of a system of particles moving in any dimension and having arbitrary mean-field interaction, speeds and statistics. Interesting consequences emerge in the case of the Bose and Fermi distributions.

1. Introduction

For an equilibrium statistical mechanical system the concept of the kinetic temperature is considered to be well understood [1], [2, pp 77, 138], [3-6], i.e. one supposedly knows how to find a one-body dynamical variable θ in the system's rest frame such that

$$\langle\theta\rangle = kT. \tag{1}$$

Here the expectation value is computed with respect to an underlying distribution function f, k is the Boltzmann constant and T denotes the thermodynamic temperature. Indeed, for *classical* systems (labelled by the subscript Cl) and obeying Maxwell-Boltzmann statistics one has the celebrated equipartition formula due to Tolman as reported by Landsberg [4]

$$\theta_{\mathrm{Cl}} = p_x \partial E / \partial p_x \tag{2}$$

where p_x is the x-component of the molecule's momentum and E is the single-particle energy (Hamiltonian) written as a function of coordinates and momenta. It is trivial to verify that θ_{Cl} reduces to p_x^2/m or to $c^2 p_x^2/E$ according to whether the classical gas is non-relativistic [1-3] or relativistic [5, 6] provided the potential is velocity-independent. A corresponding formula of θ applicable to the Bose–Einstein and Fermi–Dirac systems is, however, not known in the literature [2, p 183].

A very important question arises at this juncture namely, what is the most general, one-shot, expression of the equilibrium kinetic temperature θ of a system of particles placed in an arbitrary-dimensional space, moving freely or under a mean-field, non-relativistic or relativistic in character, and obeying either classical or quantum statistics? The aim of the present paper is to derive such an expression for θ and to summarize its main consequences.

0305-4470/92/174517+04\$04.50

2. Formulation

Let D be the dimensionality of the position space, E the energy of a typical molecule, $\boldsymbol{p}$ its momentum vector with Cartesian components p_j, and $\boldsymbol{v} = \partial E/\partial \boldsymbol{p}$ its velocity vector with components v_j ($j = 1, 2, \ldots, D$). The most probable one-body distribution function f can be written in the compact form [2, p 183]

$$f = gF \qquad F = \{z^{-1}\exp(\beta E) + \sigma\}^{-1} \tag{3a}$$

where g is the spin degeneracy factor, z the fugacity, $\beta = (kT)^{-1}$ the inverse thermodynamic temperature and σ a signature number with permitted values

$$\sigma = 0, -1, +1 \tag{3b}$$

according to whether the statistics is Maxwell, Bose or Fermi. We note the identity

$$(1 - \sigma F)Fv_j = -\partial F/\partial p_j \qquad 1 \leqslant j \leqslant D. \tag{4}$$

Multiplying both sides of (4) by p_j and integrating over p_j yields

$$\int_{-\infty}^{\infty} \mathrm{d}p_j\, p_j \beta(1 - \sigma F)Fv_j = \int_{-\infty}^{\infty} \mathrm{d}p_j\, F. \tag{5}$$

In going from (4) to (5) a partial integration has been performed on the right-hand side, remembering that $p_j F$ vanishes at both the limits $p_j = \pm\infty$ (because F vanishes exponentially at $E = +\infty$ as seen from the definition (3a)).

Integrating (5) further over the remaining momentum components $\mathrm{d}p_1 \ldots \mathrm{d}p_{j-1}, \mathrm{d}p_{j+1} \ldots \mathrm{d}p_D$ and summing over j from 1 to D we obtain

$$\frac{1}{kT}\int \mathrm{d}^D p \sum_{j=1}^{D} p_j v_j (1 - \sigma F) f = D \int \mathrm{d}^D p\, f. \tag{6}$$

Comparison of (6) with (1) leads directly to the identification of the desired variable for the kinetic temperature as

$$\theta = \frac{\boldsymbol{p} \cdot \boldsymbol{v}}{D}(1 - \sigma F) = \frac{\theta_{\mathrm{M}}}{1 + \sigma \exp[(\mu - E)/kT]} \tag{7a}$$

where we have introduced the symbols

$$\theta_{\mathrm{M}} = \frac{\boldsymbol{p} \cdot \boldsymbol{v}}{D} = \frac{\boldsymbol{p}}{D} \cdot \nabla_p E \qquad \mu = kT \ln z. \tag{7b}$$

3. Discussion

Equations (7a and b) are the main results of the present paper and their interesting algebraic consequences are displayed in table 1 for the sake of ready reference. The following points deserve special mention, assuming the energy E to be always measured with respect to the ground level:

(i) Perhaps the most important message of (7) is that the general variable θ (whose expectation value equals the thermodynamic temperature kT) is not only a function of the coordinates and momenta but also depends on the numerical value of T in the *quantum* case. This fact may be explained by remembering that the process of temperature equilibration [3, 6] proceeds via a sequence of two-body collisions which

Table 1. Algebraic consequences of the general formula (7).

Distribution	Parameters	Dynamical variable	At lower energies (T fixed)	At higher energies (T fixed)
Maxwell	$\sigma=0$	$\theta_M=\frac{p\cdot v}{D}$	$\theta_M\to 0$ if $\lvert p\rvert\to 0$	$\theta_M\to\frac{\lvert p\rvert\lvert v\rvert}{D}$ if $\lvert p\rvert\to\infty$
Bose	$\sigma=-1, \mu<0$	$\theta_B=\frac{\theta_M}{1-\exp[-(\lvert\mu\rvert+E)/kT)]}$	$\theta_B\to\frac{kT\theta_M}{\lvert\mu\rvert+E}$ if $\lvert\mu\rvert+E\ll kT$	$\theta_B\to\theta_M$ if $\lvert\mu\rvert+E\gg kT$
Fermi	$\sigma=+1, \mu>0$	$\theta_F=\frac{\theta_M}{1+\exp[(\mu-E)/kT]}$	$\theta_F\to\frac{\theta_M}{\exp[(\mu-E)/kT]}$ if $\mu-E\gg kT$	$\theta_F\to\theta_M$ if $E-\mu\gg kT$

atoms of a gas undergo against the atoms in the walls of the containing vessel. The density of states available to a scattered gas atom of momentum p contains an extra factor $1\pm F$ where the plus sign corresponds to a Bose enhancement and minus sign to a Fermi suppression. Therefore, in a quantum gas the factor $1\pm F$ multiplies the usual dynamical variable θ_M.

(ii) For the *Maxwell* distribution having $\sigma=0$ the kinetic temperature variable is just θ_M of (7*b*) in agreement with the existing treatments [1-6]. The fact that θ_M depends only on the canonical Hamilton variables and not on the numerical value of T is a reflection of the classical nature of the system.

(iii) In the case of the Bose distribution having $\sigma=-1$, $z<1$ and $\mu<0$, we find from table 1 that at any momentum

$$\theta_B\geqslant\theta_M \qquad \text{for } T\geqslant 0. \tag{8}$$

The fact that θ_B depends not only on the canonical variables but also on the numerical value of T is a reflection of the quantum nature of the system.

(iv) As regards the Fermi distribution characterized by $\sigma=+1, z>1, \mu>0$, table 1 shows that at all positive T and at any momentum we have $\theta_F<\theta_M$. As T tends towards absolute zero the Fermi distribution f tends to become more and more degenerate in the sense that the particles tend to occupy levels lying below the chemical potential μ. Hence assuming $E<\mu$ and the system to be cool, we find

$$\theta_F\approx\theta_M\exp[(E-\mu)/kT]\to 0 \qquad \text{as } T\to 0. \tag{9}$$

This result has the nice physical interpretation that although the particles below the Fermi level have substantial momentum (i.e. sizeable value of θ_M) yet their kinetic temperature variable θ_F is vanishingly small when the Fermi system becomes cold. To our knowledge such a result has not been reported before.

(v) Equations (7*a* and *b*) may be used to estimate directly the mean kinetic energy of a particle at the specified temperature. We shall illustrate this point for a free *non-relativistic ideal* gas kept in a box so that $E=p^2/2m$ where m is the mass. Then the mean kinetic energy per particle is estimated by E^* which satisfies (7*a*) with θ replaced by kT itself, i.e.

$$1+\sigma\exp[(\mu-E^*)/kT]=2E^*/DkT. \tag{10}$$

Clearly E^* equals $DkT/2$ in classical statistics ($\sigma=0$) but not so in quantum statistics ($\sigma=\pm 1$).

(vi) Before finishing, it may be added that our central formula ($7a$) has been derived in the barycentric frame of the system. The question of performing Galilean/Lorentz transformations leading to a moving frame does not concern us here as this aspect has been dealt with elsewhere [5] in the literature.

Acknowledgments

VJM and DCA are grateful to the University Grants Commission, new Delhi, for the award of a Research Scientist A position and a Minor Research Project, respectively.

References

[1] Zemansky M W and Dittman R H 1981 *Heat and Thermodynamics* (New York: McGraw-Hill) p 291
[2] Huang K 1987 *Statistical Mechanics* (Singapore: Wiley)
[3] Crawford F S 1987 *Am. J. Phys.* **55** 180
[4] Landsberg P T 1978 *Thermodynamics and Statistical Mechanics* (London: Oxford University Press; reprinted by Dover, 1990) pp 190, 193
[5] Landsberg P T 1970 Contribution in *A Critical Review of Thermodynamics* ed E H Stuart, B Gal-Or and A J Brainard (Baltimore, MD: Mono Book) p 253
ter Haar D and Wergeland H 1971 *Phys. Rep.* C **1** 31
[6] Menon V J and Agrawal D C 1991 *Am. J. Phys.* **59** 258