Developments in Normal and Gravitational Thermodynamics

by Geoffrey L. Sewell*

Department of Physics, Queen Mary and Westfield College
Mile End Road, London E1 4NS, U.K.

Abstract

We review developments in three areas of thermodynamics, resulting from advances in statistical mechanics and relativity theory. These concern (a) the resolution of some basic questions, concerning the thermodynamic variables and the phase structure of normal matter, (b) thermodynamical instabilities in non-relativistic gravitational systems, and (c) Black Hole thermodynamics, as formulated in terms of strictly observable quantities, and thus not involving any BH entropy concept.

1. Introduction

The object of this article is to discuss advances in three areas of thermodynamics, that have stemmed from progress in quantum statistical mechanics and general relativity. I shall keep the mathematics here very simple, even though the advances that I am going to discuss depend largely on results obtained by rather abstract arguments.

The three areas of thermodynamics I shall discuss are those of normal systems, i.e. ones whose energies are extensive variables; non-relativistic gravitational systems, whose energies are not extensive, because of the long range of the Newtonian interactions; and Black Holes, which arise as a consequence of relativistic gravitational collapse of stars.

I shall start, in §2, with an expose' of developments in the statistical thermodynamics of normal systems, that have been achieved within the framework in which a macroscopic system is represented as an infinitely extended one of finite density [1-3]. This amounts to an idealisation, which serves to reveal intrinsic bulk properties of macro-systems, that are otherwise masked by boundary and other finite-size effects. In particular, by contrast with the traditional statistical mechanics of finite systems, it accommodates the *phase structure* of matter, as manifested not only by the singularities in thermodynamic potentials, but also by the coexistence of equilibrium states with different microstructures. Here, I shall sketch two basic and relatively new results, obtained within this framework [3, Ch.4], that go beyond those of traditional statistical, as well as classical, thermodynamics. The first provides an answer to the fundamental question of what comprises a complete set of macroscopic observables, corresponding to the thermodynamic variables of a system.

* Partially supported by European Capital and Mobility Contract No. CHRX- Ct.92-0007

The second establishes a statistical mechanical basis for the empirically known connection between two *a priori* distinct characteristics of phase transitions, namely thermodynamic singularities and phase coexistence.

I shall then provide a brief note, in §2, on the thermodynamics of non-relativistic gravitational systems, consisting of fermions of a single species that interact via Newtonian forces. Here, the main result [4] is that these systems have negative *microcanonical* specific heat in a certain regime, and consequently are unstable there with respect to energy exchanges with thermal reservoirs.

In §3, I shall pass to the thermodynamics of Black Holes. This poses rather special conceptual problems because, by its very nature, a Black Hole has no observable microstructure. Hence, the standard concept of entropy as a structural property of an operationally determinable microstate [5, Ch.5] is inapplicable to it; and therefore the proposed extension [6,7] of this concept to non-observable objects has a subjective component. In order to restore objectivity to the theory, I have made a different approach to the thermodynamics of processes involving the exchange of matter with Black Holes [8]. This is based exclusively on observable quantities and thus involves no BH entropy concept. Here, I shall provide a simple and, I believe, improved treatment of the argument of [8], which leads to Bekenstein's formula [6] for a generalised second law of thermodynamics, but now interpreted within a framework built on the observables of the exterior region of the Black Hole.

2. Normal Systems

A normal system is one whose energy is an extensive variable. At the quantum mechanical level, this means that the potential energy of interaction between the particles in two disjoint regions is a 'surface effect': for precise mathematical specifications of this, see [3, Ch.4]. In fact, the extensivity condition is fulfilled by systems with suitably short-range interactions or even by electrically neutral Coulomb systems, because of Debye screening [9].

As is well known, the extensivity property permits one to represent normal macroscopic systems in the so-called thermodynamical limit, where they are idealised as infinitely extended assemblies of particles [1-3]. This is the model we shall employ, since it is needed for the mathematically sharp characterisation of macroscopic phenomena such as thermodynamic singularities, phase coexistence and irreversibilty.

Thermodynamic Variables. In Classical Thermodynamics (CT), the macrostate of a system is represented by a set $q = (q_1, .. , q_n)$ of intensive variables, that are global densites of extensive conserved quantities, such as energy, magnetic moment, etc. The entropy density is then a function, s, of q, whose form governs the thermodynamics of the system. We note here that, for any given system, *CT provides no specification of the variables, q, or even of their number, n.* For that, as well as for the form of s, we need to pass to the statistical mechanical model, Σ, of the system.

There, we introduce the concept of *thermodynamic completeness*, as applied to a set

$\hat{Q} = (\hat{Q}_1, .. , \hat{Q}_n)$, of extensive conserved observables of Σ, in the following way [3, Ch.4]. Denoting by $\hat{q} = (\hat{q}_1, .. , \hat{q}_n)$ the intensive observables, given by the global densities of $\hat{Q}$, we term $\hat{Q}$ thermodynamically complete if

(C.1) $\hat{Q}_1$ *is the energy;*

(C.2) $(\hat{Q}_1, .. , \hat{Q}_n)$ *are linearly independent; and*

(C.3) *if* $\hat{s}(\rho)$ *is the entropy density* of a mixed state* ρ *of* Σ, *then*

(a) for any given expectation value q *of* $\hat{q}$, *there is precisely one state,* ρ_q, *that maximises* $\hat{s}$, *and*

(b) the same is not true for any proper subset of $(\hat{q}_1, .. , \hat{q}_n)$.

In other words, $\hat{Q}$ is thermodynamically complete if the value of its density, $\hat{q}$, determines the equilibrium microstate, without redundancy. For example, in the case of a ferromagnetic system, such as the Ising model, $\hat{q}$ comprises the energy density and the polarisation.

We assume, as the condition for Σ to support a thermodynamics, that it possesses a complete set of extensive conserved observables, $\hat{Q}$, that is unique, up to linear combinations. The intensive thermodynamical variables of the system are then the expectation values, q, of the global densities, $\hat{q}$, of $\hat{Q}$.

Thermodynamic Potentials. The equilibrium entropy density of Σ, as a function of the thermodynamical variables q may be seen from the condition (C.3a) to be

$$s(q) \equiv \hat{s}(\rho_q) \tag{2.1}$$

In fact, this is a generalisation of the standard definition of microcanonical entropy [10], and reduces to that in the case where $\hat{Q}$ consists of the energy only.

We can also represent the thermodynamics of the system in the canonical description, by the Legendre transform, p, of s : this is just the pressure, in units of $k_B T$. Thus, denoting by $\theta = (\theta_1, .. , \theta_n)$ the thermodynamic conjugates of q,

$$p(\theta) = \max_q (s(q) - \theta.q); \ \theta.q \equiv \sum_{j=1}^{n} \theta_j q_j \tag{2.2}$$

Note. The maximisation of $s - \theta.q$ corresponds to the minimisation of the Gibbs free energy and thus occurs precisely when q takes an equilibrium value, $\overline{q}$. By the completeness condition (C3), this determines the corresponding equilibrium microstate $\rho_{\overline{q}}$. Thus, the condition for *phase coexistence*, for given θ, is that $s - \theta.q$ attains its maximum at more than one value of q.

The above definitions of s and p imply [3, Ch.4]) that the former is concave and the latter convex, i.e., for $0 < \lambda < 1$,

$$s(\lambda\theta + (1 - \lambda)\theta') \geq \lambda s(\theta) + (1 - \lambda) s(\theta') \tag{2.3}$$

* This is defined [1, Ch.7] as a natural generalisation, to infinite systems, of the density of the Von Neumann entropy, $-kTr(\rho \log \rho)$, of a microstate whose density matrix is ρ.

and

$$p(\lambda\theta + (1-\lambda)\theta') \le \lambda p(\theta) + (1-\lambda)p(\theta') \tag{2.4}$$

These are thermodynamic stability properties. They imply [11] that the functions s and p are continuous, except possibly at the boundaries of their domains of definition. On the other hand, they do not guarantee differentiability; and, in fact, p can support singularities, as given by points, θ, where it is not differentiable [1,3]. Such points correspond, of course, to phase transitions.

Equilibrium States and Phase Structure. This last observation brings us to the point that, in Classical Thermodynamics, there are two characterisations of phase transitions, namely,

(a) singularities in thermodynamic potentials; and

(b) coexistence of different equilibrium states.

Here, we define phase coexistence as in the Note following equn. (2.2).

In fact, although (a) and (b) are *a priori* distinct from one another, it is generally assumed, on empirical grounds, that they always arise together. It is therefore natural to ask whether there is any *neccessary* connection, imposed by the underlying quantum statistical structure, between these characterisations. The answer to this question is provided by the following Proposition, which was proved [3, Ch.4] on the basis of the concavity/convexity properties (2.3) and (2.4).

Proposition. *Under the above definitions and assumptions, phase coexistence occurs at precisely those values of θ where the potential p is not differentiable.*

In other words, the structures imposed by the quantum statistical model render the characterisations (a) and (b) equivalent.

3. Non-relativistic Gravitational Systems

We consider now a system, Σ_N, of N electrically neutral, massive fermions of one species, interacting via Newtonian forces. This is a model of a neutron star, and its Hamiltonian takes the form

$$H_N = -\frac{\hbar^2}{2m}\sum\nolimits_{j=1}^{N}\Delta_j \; - \kappa m^2 \sum\nolimits_{j,k(\neq j)=1}^{N} r_{jk}^{-1} \tag{3.1}$$

where κ is the gravitational constant, Δ_j is the Laplacian for the j'th particle, and r_{jk} is the distance between the j'th and k'th particles.

Because of the long range of the interactions, the energy of the system is *not* an extensive variable, and so the theory of §2 is inapplicable to this model. In fact [4], for a sequence of systems Σ_N, occupying geometrically similar spatial regions, the volume now scales as N^{-1}, instead of N : this results from the competition between the Newtonian attraction, which favours implosion, and the Fermi pressure. Correspondingly, the energy,

E_N, and the microcanonical entropy, S_N, scale as $N^{7/3}$ and N, respectively, and the system enjoys the following thermodynamic properties [4].

(G1) *If* $N^{-7/3}E_N$, NV_N *converge to* e, v, *respectively, as* $N\rightarrow\infty$, *then the microcanonical specific entropy* $N^{-1}S_N$ *converges to a function,* s, *of* (e,v).

(G2) *There is a regime in which* s *is convex w.r.t.* e, *i.e. where the system is unstable against energy exchanges with a thermal reservoir.*

(G3) *The system undergoes a phase transition, of the Van der Waals type, when* s *changes from concave to convex w.r.t.* e.

For further properties of the model, see Refs. [2, Section 4.2] and [12-14]. In particular, when N becomes sufficiently large, $\approx 10^{60}$, the non-relativistic model becomes unphysical, since it implies that the mean particle velocities are comparable with the speed of light.

4. Black Hole Thermodynamics

According to Classical General Relativity, the collapse of a star, due to gravitational implosion, results in the formation of a Black Hole [15, Pt.7], i.e. a bounded spatial region, from which no light can escape. Thus, the only observables of the BH that can be perceived from the outside are its mass, electric charge and angular momentum, these being the ones that are registered by the external gravitational and electromagnetic fields [15, P.876]. This is Wheeler's famous principle that "Black Holes have no Hair", the word 'hair' here meaning 'microstructure observable from outside'. It has dramatic consequences for thermodynamics, since it implies that a BH has no operationally determinable microstate. The concepts of statistical mechanics, including that of entropy, are therefore inapplicable to it, and, consequently, the standard form of the Second law of Thermodynamics has no predictive value for processes in which observable systems discharge matter into the Hole.*

On the other hand, the relativistic mechanics of Black Holes [16] exhibits remarkable analogies with classical thermodynamics, with the surface area of a Hole playing the role of entropy. Bekenstein [6] argued that these analogies carried physical content by showing that, in certain Gedankenexperiments, in which matter was dropped into a Black Hole, the sum of the entropy, S, of the exterior region and the area, A, of the BH, multiplied by a certain constant, λ, never decreased, i.e.,

$$\Delta S + \lambda \Delta A \geq 0, \tag{4.1}$$

On this basis, he proposed that the BH had entropy λA, and that processes involving BH's conformed to a Generalised Second Law (GSL), represented by equn. (4.1). This proposal was supported [7,17] by Hawking's subsequent argument that Black Holes act as sources of thermal radiation, of quantum mechanical origin, with temperature corresponding to the assumed form, λA, of the BH entropy. At the quantum statistical level, Bekenstein introduced a *subjective* element into the theory, suggesting that this entropy

---

* This remark was credited to J. A. Wheeler by Bekenstein [6].

was an information-theoretic quantity, that represented the external observer's ignorance of the state of the BH.

In order to recast the theory in purely objective terms, that retain the standard connections between thermodynamic variables and underlying microstructures, we have provided a different treatment of processes involving Black Holes [8]. This is based on the statistical thermodynamics of the exterior, observable region, and does not involve any concept of a BH entropy. As we shall see, it leads to a version of the GSL (4.1), as adapted to open systems, but with the last term there representing mechanical work on the BH, not entropy.

We formulate the theory on the basis of a thermodynamics of a test-body, Σ, which is placed in the Hawking radiation of a Black Hole, B, and exchanges mass, electric charge and angular momentum with both B and the radiation. Σ is thus an *open system.* Accordingly, we base our treatment on the following general principles.

(I) *The Second Law of Thermodynamics, which tells us that the Gibbs potential, Φ, of an open system cannot spontaneously increase. Equivalently [18, Ch.2], if mechanical work, W, is done on the system, then*

$$W \geq \Delta\Phi \tag{4.2}$$

(II) *The laws of Black Hole Mechanics [16], which ensue from General Relativity. These are that*

(BH1) the total energy, electric charge and angular momentum of the BH and the exterior system are conserved in any process;

(BH2) the surface gravity, σ, i.e. the (proper) acceleration of a freely infalling body at the surface of B, is uniform over that surface;

(BH3) the surface area, A, of B is a function of its energy, E_B, charge, Q_B, and angular momentum, J_B, and satisfies the differential relation

$$\sigma c^2 dA/8\pi\kappa = dE_B - \phi dQ_B - \omega.dJ_B \tag{4.3}$$

where ϕ is the electric potential and ω the angular velocity of B; and

(BH4) A increases in irreversible processes, and remains constant in reversible ones. Here, it is the the origination of the BH from the collapse of a star that is the source of the irreversibility.

(III) *The Hawking thermal radiation phenomenon [17], which we have shown [19] to be a general, model-independent consequence of the basic principles of quantum theory, relativity and statistical thermodynamics. The temperature of this radiation is*

$$T = \hbar\sigma/2\pi kc \tag{4.4}$$

and its electric potential and angular velocity are those of B, namely ϕ and ω, respectively.

Note. The laws of Black Hole Mechanics, (BH1-4), have an obvious analogy with classical thermodynamics, with σ and A playing the roles of temperature and entropy, respectively. However, we do *not* interpret A as an entropy, for the following reasons.

(1) In the case of a normal physical system, a microstate corresponds to a density matrix, ρ, whose explicit form may be operationally determined, and the entropy is a function, $-kTr(\rho\log\rho)$, of this state, which provides a measure of its disorder [2, P.57]. Thus, its essential significance is not merely that it has an information-theoretic form, but that it represents a *structural property* of the microstate. In the case of a Black Hole, however, no similar quantity could exist, since the BH has no observable microstructure.

(2) One sees immediately from (4.3) that the last term in (4.1) l.h.s. corresponds to the mechanical work required to effect changes $\Delta E_B,\ \Delta Q_B,\ \Delta J_B$ in $E_B,\ Q_B,\ J_B$, respectively. Hence, apart from the considerations of (1), there is no call for it to be regarded as an entropy.

(3) Whereas thermodynamic irreversibility arises as a result of 'phase mixing', there is no such mechanism operating in (BH4).

Derivation of the GSL. We now pass to the thermodynamics of a body, Σ, placed in the Hawking radiation of a Black Hole, B. Thus, by (III), Σ is immersed in a heat bath of temperature T, electric potential ϕ and angular velocity ω. Its Gibbs potential is therefore

$$\Phi = E - TS - \phi Q - \omega.J \tag{4.5}$$

where $E,\ S,\ Q$ and J are its energy, entropy, charge and angular momentum, respectively.

Suppose now that Σ is placed just outside B and that it then discharges some of its matter into this Black Hole. Then it follows from (I) and equn. (4.5) that

$$\Delta S \geq T^{-1}(\Delta E - \phi\Delta Q - \omega.\Delta J) \tag{4.6}$$

$$= -T^{-1}((\Delta E_B - \phi\Delta Q_B - \omega.\Delta J_B),\ by\ (IIa) \tag{4.6a}$$

$$\geq -T^{-1}\sigma c^2 dA/8\pi\kappa,\ by\ (IIc,d) \tag{4.6b}$$

Hence, by (4.4),

$$\Delta S + \lambda\Delta A \geq 0;\ with\ \lambda = kc^3/4\kappa\hbar \tag{4.7}$$

This is precisely the GSL proposed by Bekenstein, though now we interpret the area term as representing mechanical work, rather than entropy.

We can easily extend our treatment to cover the situation where Σ is transported by some machine $\mathcal{M}$ from an exterior position to the boundary of B, then discharges matter into this BH, and is finally brought back by $\mathcal{M}$ to its starting point. Thus, denoting the increments in an arbitrary thermodynamic variable, V, of Σ for the first, second and third phase of this operation by $\Delta_1 V, \Delta_2 V$ and $\Delta_3 V$, respectively, it follows from (4.2) that the total work, W, done on the system by $\mathcal{M}$ satisfies the inequality

$$W \geq \Delta_1\Phi + \Delta_3\Phi; \tag{4.8}$$

while it follows from (4.5)-(4.7) that

$$\Delta_2\Phi + \Delta E_B - T\lambda\Delta A - \phi\Delta Q_B - \omega.\Delta J_B \leq 0 \tag{4.9}$$

Hence, denoting by ΔV the change in a variable V over the whole operation, we infer from (4.4), (4.8) and (4.9) the following extended form of the GSL.

Proposition. *In any operation involving the exchange of matter between a system, Σ, and a Black Hole, B, the total mechanical work done on Σ by external agencies satisfies the inequality*

$$W \geq \Delta\Psi \tag{4.10}$$

where

$$\Psi = E + E_B - T(S + \lambda A) - \phi(Q + Q_B) - \omega.(J + J_B) \tag{4.11}$$

Comment. This is a generalised version of the Second Law, as represented by (4.2). Here, Ψ is evidently the relevant thermodynamic potential for the system composed of Σ and B.

References

1. D. Ruelle: "Statistical Mechanics", W. A. Benjamin, Inc., New York, 1969

2. W. Thirring: "Quantum Mechanics of Large Systems", Springer, New York, Vienna, 1980

3. G. L. Sewell: "Quantum Theory of Collective Phenomena", Oxford University Press, Oxford, New York, 1989

4. P. Hertel and W. Thirring: Pp. 310-323 of "Quanten und Felder", Ed. H. P. Durr, Vieweg, Braunschweig, 1971

5. J. Von Neumann: "Mathematical Foundations of Quantum Mechanics", Princeton University Press, 1955

6. J. Bekenstein: Phys. Rev. D **7**, 2333 (1973); and Pp. 42- 62 of "Jerusalem Einstein Centenary Conference", Ed. Y. Neeman, Addison-Wesley, Reading, MA, 1981

7. S. W. Hawking: Phys. Rev. D **13**, 2188 (1976)

8. G. L. Sewell: Phys. Lett. A **122**, 309 (1987); Erratum, Phys. Lett. A **123**, 499 (1987)

9. J. L. Lebowitz and E. H. Lieb: Adv. Math. **9**, 316 (1972)

10. R. B. Griffiths: J. Math. Phys. **1447**, (1965)

11. R. T. Rockafellar: "Convex Analysis", Princeton University Press, 1970

12. P. Hertel, H. Narnhofer and W. Thirring: Commun. Math. Phys. **28**, 159, (1972)

13. H. Narnhofer and G. L. Sewell: Commun. Math. Phys. **71**, 1, (1980)

14. J. Messer: J. Math. Phys. **22**, 2910, (1981)

15. C. W. Misner, K. Thorne and J. A. Wheeler: "Gravitation", W. H. Freeman, San Francisco, 1973

16. J. M. Bardeen, B. Carter and S. W. Hawking: Commun. Math. Phys. **31**, 161, (1973)

17. S. W. Hawking: Commun. Math. Phys. **43**, 199, (1975)

18. L. D. Landau and E. M. Lifschitz: "Statistical Physics", Pergamon Press, Oxford, 1959

19 G. L. Sewell: Ann. Phys. **41**, 201, (1982)