LETTERS TO PROGRESS IN PHYSICS

Is Classical Statistical Mechanics Self-Consistent?

(A paper in honour of C. F. von Weizsäcker, 1912–2007)

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In addition to his outstanding achievements in physics and activities in policy, C.-F. von Weizsäcker is famous for his talks, given as a member of the Academy Leopoldina. Due to the latter, I could learn quite a lot from his methodological writings. In particular, he is the only modern thinker I'm aware of who has pointed to the difference between Newton's and Laplace's notions of state. But this difference is essential for the relationship between classical and quantum physics. Moreover it is the clue to overcoming Gibbs' paradox within classical statistical mechanics itself.

1 Introduction

With Carl-Friedrich Freiherr von Weizsäcker (1912–2007) an outstanding physicist, philosopher and human being passed away. Born into a family with long traditions of widespread interests, activities and education — his father was a highly ranked diplomat, his younger brother Richard was President of Western Germany — he showed from the very beginning a strong interest in both physics and philosophy. His talks as a member of the German Academy of Sciences Leopoldina are famous not only by their original content, but also by his humour. His books on methodological and historical issues display his broad scope, and are full of wise insights. As a master, he acknowledged the masters of the past; one can learn from him how to learn from the masters, then and now. Notably, I remember his reference to Euler's (1707–1783) reasoning on the equivalence of causal (differential equations) and teleological descriptions (minimum principles), and his pointing to the difference between the notions of state as used by Newton (1643–1727), and today, respectively [1]. As the latter has profound implications even for modern physics, I would like to honour von Weizsäcker through outlining its relevance for statistical and quantum physics.

2 State and motion

2.1 Conservation laws vs laws of motion

Descartes (1596–1650), Huygens (1629–1695), Newton and Euler started their exposition of the basic laws with the conservation of (stationary) state. This is followed by the change of state and eventually by the change of location (equation of motion). The location of a body is not a state variable, because it changes even without the action of an external force, i.e., without reason. The latter kind of reasoning was abandoned at the end of 18th century as part of scholastics ([1], p. 235). The centre of the Lagrange (1736–1813) formalism is occupied by the Lagrangian equation of motion, i.e., equations for the non-state variable location (represented by the generalized coordinates).

On the other hand, this equation of motion indicates at once the conservation of (generalized) momentum for the force-free motion of a body in a homogeneous space. Indeed, there is a very tight interconnection of symmetries and conserved quantities in general, as stated in Noether's (1882–1935) theorem, the mechanical and field-theoretical applications of which being usually expressed by means of the Lagrange formalism. The principle of least action containing the Lagrange function is often even placed at the pinnacle of mechanics.

This development has strengthened the focus of physicists on the equations of motion and weakened their attention on the laws of state conservation, despite the extraordinary rôle of energy in quantum mechanics and Bohr's (1885–1962) emphasis on the fundamental rôle of the principles of state conservation and of state change [2]. Indeed, there are derivations of Newton's equation of motion from the energy law, e.g., in [3, 4, 5]; a deduction of Hamilton's (1805–1865) equation of motion from Euler's principles of classical mechanics can be found in [6, 7].

Thus, there are two traditional lines of thought,

- the "physics of conserved quantities": Parmenides (ca. 515 BC — ca. 445 BC) — Descartes — Leibniz (1646–1716), and

- the "physics of laws of change": Heraclites (ca. 388 BC — ca. 315 BC) — Galileo (1564–1642) — Newton.

In the end, both lines are equivalent, leading eventually to the same results, as first shown by Daniel Bernoulli (1700–1782) [8].

2.2 Motion vs stationary states

In classical mechanics, if an external force ceases to act upon a body or conservative system, the latter remains in that stationary state it has assumed at that moment. Non-

stationary motion is a continuous sequence of stationary states. Consequently, the set of stationary states of a system determines both its stationary and its non-stationary motions and, in particular, its set of possible configurations. For instance, the turning points of a pendulum are determined by its energy.

In quantum mechanics, the situation is somewhat more complicated. The set of stationary states is (quasi-)discontinuous. The external influence vanishes most likely at an instant, when the wave function of the system is *not* equal to one of the stationary states. However, it can be constructed from the stationary wave functions. According to Schrödinger (1887–1961) [9], the transition between two states is characterized by contributions to the wave function from both states. It's like climbing a staircase without jumping, i.e., the one foot leaves the lower step only after the other foot has reached the higher step. In this sense, the fashionable term "quantum leap" is a fiction. Therefore, the quantum motion, too, is largely determined by the stationary states.

2.3 State variables vs quantum numbers

A freely moving body exhibits 3 Newtonian state variables (e.g., the 3 components of its momentum vector; c.f. Laws 1 and 2), but 6 Laplacian state variables (e.g., the 6 components of its velocity and position vectors; c.f. Laplace's demon [10]). A freely moving spinless quantum particle exhibits 3 quantum numbers (e.g., the 3 components of its momentum vector).

The planets revolving around the sun à la Kepler (1571–1630) exhibit 3 Newtonian state variables (e.g., the total energy and 2 components of the angular momentum), but 6 Laplacian state variables (e.g., those of free bodies, given above). Neglecting spin, the one-electron states of atoms are labeled by 3 quantum numbers (1 for the energy plus 2 for the angular momentum). The same applies to the three-dimensional classical and quantum oscillators, respectively.

The example of these three basic systems of mechanics, both classical and quantum, clearly demonstrates that the Newtonian notion of state — corresponding largely to the modern notion of stationary states — is much more appropriate for comparing classical and quantum systems than the Laplacian notion of state. It should be enlightening to draw these parallels for field theory.

3 (In)Distinguishability

3.1 Permutation symmetry of Newtonian state functions

Two classical bodies are equal if they possess the same mass, size, charge, etc. [11]. A simple example is given by the red balls of snooker (a kind of billiards; I abstract, of course, from deviations caused by the production process). Due to the unique locus of a body, they can be distinguished by

their locations and, thus, are not identical. For the outcome of a snooker game, however, this does not play any rôle. Similarly, for recognizing a player of the own team, only the color of the tricot is important, not its size. In other words, it is not the totality of properties that matters, but just that subset which is important for the current situation.

The Hamilton function of a system of equal bodies is invariant under the interchange of two bodies (permutation of the space and momentum variables). More generally, given only the Newtonian state variables of a system, the classical (!) bodies in it are indistinguishable. This allows for discussing the issue of (in)distinguishability within classical dynamics. Equal quantum particles are also not identical, if they can be distinguished through their localization.

3.2 Distribution functions vs energy spectrum

In his 1907 paper "Planck's theory of radiation and the theory of specific heat of solids" [12], Einstein (1879–1955) not only founded the quantum theory of solids, but demonstrated also, that the differences between the classical and quantum occupation of states result from the different character of the energy spectra of classical and quantum systems, respectively; and he defined quantization as a selection problem [6, 7].

Wien's (1864–1928) classical distribution law he obtained by using the continuous energy spectrum of a classical oscillator, while Planck's (1858–1947) non-classical distribution law emerges from the discrete energy spectrum of a quantum oscillator.

In a perfect crystal, the atoms oscillate around localized lattice positions and, therefore, are distinguishable. Their interaction, however, leads to collective oscillations called normal modes. In these common states, the individual lattice atoms become indistinguishable. It is these normal modes that were actually used by Einstein. However, due to the use of Newton's notion of state Einstein was able to derive Planck's distribution law by means of "classical" arguments.

3.3 Gibbs' paradox

Consider a box filled uniformly with a gas in thermal equilibrium. When putting a slide sufficiently slowly into it, dividing the box into two parts, no macroscopic quantity of the box as a whole should change. However, within conventional classical statistical mechanics, the entropy changes drastically, because the interchange of two molecules from now different parts of the box is regarded as being significant. This is called Gibbs' (1839–1903) paradox [13]. In conventional representations, it is argued that, actually, the molecules are quantum particles and, thus, indistinguishable; the double counting is corrected ad hoc.

Now, as outlined above, if Newton's rather than Laplace's notion of state is used, an interchange of any two molecules of the same part or of different parts of the box, does not affect the state. Therefore, the artifact of Gibbs' paradox

can be avoided from the very beginning when working with Newton's notion of state, as can be seen from Einstein's 1907 paper discussed above.

4　Summary and discussion

Contrary to Einstein's results, Ehrenfest (1880–1933) [14] and Natanson (1864–1937) [15] explained the difference between the classical and quantum radiation laws by means of different counting rules for distinguishable and indistinguishable particles ([16], §1.4; [17], vol. 1, pt. 2, sect. V.3). Apparently supported by the uncertainty relation, in particular, after its "iconization" as the "uncertainty principle", this view prevailed for most of the 20th century. Only at its end was it realized more and more that it is not the (in)distinguishability of particles that matters, but that of the states (e.g. [18], sects. 1 and 2.1; [19], sect. 4.1). Using Newton's rather than Laplace's notion of state, the statistical reasoning in [18, 19] can be physically-dynamically substantiated.

It needs, perhaps, a congenial mixing of physics and philosophy, like that of von Weizsäcker, to recognize and stress the importance of notions within physics. As the notions are the tools of our thinking, the latter cannot be more accurate than the former.

Both Newton's and Laplace's notions of state exhibit advantages [20]. The proper use of them makes classical statistical mechanics self-consistent.

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Carl Friedrich von Weizsäcker, 1983.

Biography*

Carl Friedrich Freiherr (Baron) von Weizsäcker (June 28, 1912, Kiel – April 28, 2007, Säcking near Starnberg) was a German physicist and philosopher. He was the longest-living member of the research team which tried, and failed, to develop a nuclear weapon in Germany during the Second World War.

Weizsäcker was born in Kiel, Germany, the son of the German diplomat Ernst von Weizsäcker. He was the elder brother of the former German President Richard von Weizsäcker, father of the physicist and environmental researcher Ernst Ulrich von Weizsäcker and father-in-law of the former General Secretary of the World Council of Churches Konrad Raiser.

From 1929 to 1933, Weizsäcker studied physics, mathematics and astronomy in Berlin, Göttingen and Leipzig supervised by and in cooperation, e.g., with Werner Heisenberg and Niels Bohr. The supervisor of his doctoral thesis was Friedrich Hund.

His special interest as a young researcher was the binding energy of atomic nuclei, and the nuclear processes in stars. Together with Hans Bethe he found a formula for the nuclear processing in stars, called the Bethe-Weizsäcker formula and the cyclic process of fusion in stars (Bethe-Weizsäcker process, published in 1937).

Note regarding personal names: *Freiherr* is a title, translated as *Baron*, not a first or middle name. (The female forms are *Freifrau* and *Freiin*.)

During the Second World War, he joined the German nuclear energy project, participating in efforts to construct an atomic bomb. As a protegee of Heisenberg, he was present at a crucial meeting at the Army Ordinance headquarters in Berlin on 17 September 1939, at which the German atomic weapons program was launched. In July 1940 he was co-author of a report to the Army on the possibility of "energy production" from refined uranium, and which also predicted the possibility of using plutonium for the same purpose. He was later based at Strasbourg, and it was the American capture of his laboratory and papers there in December 1944 that revealed to the Western Allies that the Germans had not come close to developing a nuclear weapon.

Historians have been divided as to whether Heisenberg and his team were sincerely trying to construct a nuclear weapon, or whether their failure reflected a desire not to succeed because they did not want the Nazi regime to have such a weapon. This latter view, largely based on postwar interviews with Heisenberg and Weizsäcker, was put forward by Robert Jungk in his 1957 book *Brighter Than a Thousand Suns*. Weizsäcker states himself that Heisenberg, Wirtz and he had a private agreement to study nuclear fission to the fullest possible in order to "decide" themselves how to proceed with its technical application. "There was no conspiracy, not even in our small

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three-men-circle, with certainty not to make the bomb. Just as little, there was no passion to make the bomb . . . " (cited from: C. F. von Weizsäcker, *letter to Mark Walker*, August 5, 1990).

The truth about this question was not revealed until 1993, when transcripts of secretly recorded conversations among ten top German physicists, including Heisenberg and Weizsäcker, detained at Farm Hall, near Cambridge in late 1945, were published. The *Farm Hall Transcript* revealed that Weizsäcker had taken the lead in arguing for an agreement among the scientists that they would claim that they had never wanted to develop a German nuclear weapon. This story, which they knew was untrue, was called among themselves *die Lesart* (the Version). Although the memorandum which the scientists drew up was drafted by Heisenberg, one of those present, Max von Laue, later wrote: "The leader in all these discussions was Weizsäcker. I did not hear any mention of any ethical point of view" (cited from: John Cornwell, *Hitler's Scientists*, Viking, 2003, p. 398). It was this version of events which was given to Jungk as the basis of his book.

Weizsäcker was allowed to return to Germany in 1946 and became director of a department for theoretical physics in the Max Planck Institut for Physics in Göttingen (successor of Kaiser Wilhelm Institut). From 1957 to 1969, Weizsäcker was professor of philosophy at the University of Hamburg. In 1957 he won the Max Planck medal. In 1970 he formulated a *Weltinnenpoltik* (world internal policy). From 1970 to 1980, he was head of the Max Planck Institute for the Research of Living Conditions in the Modern World, in Starnberg. He researched and published on the danger of nuclear war, what he saw as the conflict between the first world and the third world, and the consequences of environmental destruction. In the 1970's he founded, together with the Indian philosopher Pandit Gopi Krishna, a research foundation "for western sciences and eastern wisdom". After his retirement in 1980 he became a Christian pacifist, and intensified his work on the conceptual definition of quantum physics, particularly on the Copenhagen Interpretation.

His experiences in the Nazi era, and with his own behavior in this time, gave Weizsäcker an interest in questions on ethics and responsibility. He was one of the Gättinger 18 — 18 prominent German physicists — who protested in 1957 against the idea that the Bundeswehr should be armed with tactical nuclear weapons. He further suggested that West Germany should declare its definitive abdication of all kinds of nuclear weapons. However he never accepted his share of responsibility for the German scientific community's efforts to build a nuclear weapon for Nazi Germany, and continued to repeat the version of these events agreed on at Farm Hill. Some others believe this version to be a deliberate falsehood.

In 1963 Weizsäcker was awarded the Friedenspreis des Deutschen Buchhandels (peace award of the German booksellers). In 1989, he won the Templeton Prize for Progress in Religion. He also received the Order Pour le Mérite. There is a Gymnasium named after him, in the town of Barmstedt, which lies northwest of Hamburg, in Schleswig-Holstein, the Carl Friedrich von Weizsäcker Gymnasium im Barmstedt.

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