Microscopic Foundations of Ohm and Joule's Laws – The Relevance of Thermodynamics

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We give a brief historical account on microscopic explanations of electrical conduction. One aim of this short review is to show that Thermodynamics is fundamental to the theoretical understanding of the phenomenon. We discuss how the 2nd law, implemented in the scope of Quantum Statistical Mechanics, can be naturally used to give mathematical sense to conductivity of very general quantum many—body models. This is reminiscent of original ideas of J.P. Joule. We start with Ohm and Joule's discoveries and proceed by describing the Drude model of conductivity. The impact of Quantum Mechanics and the Anderson model are also discussed. The exposition is closed with the presentation of our approach to electrical conductivity based on the 2nd law of thermodynamics as passivity of systems at thermal equilibrium. It led to new rigorous results on linear conductivity of interacting fermions. One example is the existence of so—called AC—conductivity measures for such a physical system. These measures are, moreover, Fourier transforms of time correlations of current fluctuations in the system. I.e., the conductivity satisfies, for a large class of quantum mechanical microscopic models, Green–Kubo relations.

Keywords: Ohm's law, Joule's law, conductivity measure, 2nd law, fermions.

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1. Electrical Conductivity and Classical Physics

1.1. The Genesis of Ohm and Joule's laws

G.S. Ohm was born in 1789 in Erlangen and came from a modest background (son of a master locksmith). Nevertheless, he succeeded in learning basic mathematics and sciences and became for about a decade teacher of mathematics and physics in Cologne. During this time, he had been able to elaborate his own experiments on electrical resistivity. He was originally inspired by J. Fourier's work, published in 1822, about heat theory. Indeed, G.S. Ohm drew a comparison of heat conduction with the electrical one in a metallic bar. Based on this intuition, he published a few papers on experimental outcomes about electrical resistivity in metals. He concluded his work on electrical conduction by his famous theory, which was a theoretical deduction of his law from "first principles". Indeed, he states that the current in the steady regime is proportional to the voltage applied to the conducting material. The

proportionality coefficient is the conductivity (or inverse resistivity) of the physical system. It is an empirical law which looks almost obvious nowadays.

At that time, however, his writings were almost unknown. His book¹ was at best completely ignored and at worst treated really negatively. Rather than scientific, some critics were more ethical as they were based on a priori conceptions on what science and nature are, probably on what L. Daston and P. Galison have called *truth-to-nature*.² Quoting [3, p. 243]:

...Ohm's theory, to quote one critic, was "a web of naked fancies", which could never find the semblance of support from even the most superficial observation of facts; "he who looks on the world", proceeds the writer, "with the eye of reverence must turn aside from this book as the result of an incurable delusion, whose sole effort is to detract from the dignity of nature". ... where he had looked for commendation he found at best complete indifference, and at worst open abuse and derision. ... The influence of this opposition (some school official) reached the Minister of Education himself, and he, speaking officially, definitely pronounced it as his opinion that "a physicist who professed such heresies was unworthy to teach science".

Retrospectively, such comments in "a country so well represented in the world of science by men of eminence and knowledge" are marks of revolutionary ideas, but it was a real bitter blow for G.S. Ohm: He gave up his teacher position at Cologne and started six years of hard times. His work was nevertheless occasionally cited and rumors about Ohm's theory started to appear in different places. This includes America where the famous physicist J. Henry asked in 1833 his colleagues: "Could you give me any information about the theory of Ohm? Where is it to be found?" J. Henry succeeded in having this information by going to England in 1837 at a time when Ohm's work had already become famous, particularly outside his own country.

Although at the origin of Ohm's intuition, the relation between heat and electrical conduction has not been established by himself, but J.P. Joule, who was born in 1818 in England. The pivotal ingredient was the wide concept of energy. Joule's intuition seems to have been that the different physical properties appearing in nature can be tracked by the concept of energy. He thus studied different forms of energy in order to relate them. The conversion of mechanical work into heat is a famous topic of such studies. His works, although also very controversial at the beginning, were seminal and yielded the 1st law of Thermodynamics, see, e.g., Ref. 4. Recall also that all mechanical work can be converted to heat but the converse is not true, in general. This observation refers to the 2nd law of Thermodynamics and the concept of entropy invented by R.J.E. Clausius in 1865.

Applied to electricity theory, Joule's intuition allowed to establish a relation between heat and electrical conduction. Indeed, more than one decade after Ohm's discovery¹ on linear electrical conduction, the physicist J. P. Joule observed⁵ in 1840 that the heat (per second) produced within an electrical circuit is proportional to

the electrical resistance and the square of the current:

...the calorific effects of equal quantities of transmitted electricity are proportional to the resistances opposed to its passage, whatever may be the length, thickness, shape, or kind of metal which closes the circuit: and also that, coeteris paribus, these effects are in the duplicate ratio of the quantities of transmitted electricity; and consequently also in the duplicate ratio of the velocity of transmission.

[Joule, 1840]

Nowadays, electrical conductivity usually refers to Ohm and Joule's laws. They are indeed among the most resilient laws of (classical) electricity theory. Materials are called ohmic or nonohmic, depending on whether they obey Ohm's law. Both assertions are empirical laws and, as usual, they generated at least as many theoretical problems as they solved. From a mathematically rigorous point of view, the microscopic origin of the phenomenological behavior of macroscopic conductors described by these laws is still not completely understood, specially in the DC regime. Moreover, as recent experiments show, Ohm's law is not only valid at macroscopic scales. Indeed, the validity of Ohm's law at the atomic scale for a purely quantum system has experimentally been verified⁶ in 2012. Such a behavior was unexpected:⁷

...In the 1920s and 1930s, it was expected that classical behavior would operate at macroscopic scales but would break down at the microscopic scale, where it would be replaced by the new quantum mechanics. The pointlike electron motion of the classical world would be replaced by the spread out quantum waves. These quantum waves would lead to very different behavior. ... Ohm's law remains valid, even at very low temperatures, a surprising result that reveals classical behavior in the quantum regime.

[D.K. Ferry, 2012]

1.2. Towards a microscopic theory of electrical conduction

In the end of the nineteenth century, the so–called classical physics reached a very high level of completeness with Classical Mechanics, Electrodynamics, and Thermodynamics. However, borderline problems became manifestly more and more important and eventually led to the scientific revolution of the beginning of the twentieth century. For instance, the study of the link between Classical Mechanics and Thermodynamics yielded the so–called Statistical Physics via Gibbs and Boltzmann's genius intuitions.

Classical Mechanics is indeed a causal theory based on elementary physical objects satisfying Newton's laws of motion. The exceptional success of this theory together with new technologies like photography had propagated a new view point on science during the last part of the nineteenth century with the so–called *mechanical objectivity*.² By contrast, Thermodynamics emphasizes the concepts of energy

and entropy of macroscopic systems. It speaks about reversible and irreversible processes, but it does not care about the concrete system under consideration. Classical Mechanics is in some sense a bottom—up or "local" approach, whereas Thermodynamics is a top—down or global one.

In order to bridge the gap between both theories, L. Boltzmann successfully tried to go from Classical Mechanics towards Thermodynamics via statistical or probabilist methods. His H-theorem (1872) was undoubtedly an important achievement as it has provided a mechanical explanation of the 2nd law of Thermodynamics from the dynamics of rarefied gases. Boltzmann's vision of "atoms" as the physical objects satisfying Newton's laws was however again very controversial for a long time: "have you seen any?" said the famous physicist and philosopher E. Mach as a reply to the issue of atoms. E. Mach had indeed a philosophical approach centered on the world of sensations in a similar spirit of mechanical objectivity, whereas L. Boltzmann also focussed on mathematical structures. See later the development of structural objectivity² (M. Planck (1906), B. Russell, H. Poincaré, C.S. Peirce, etc.). Similar ethical oppositions appeared in other sciences: S. Ramón y Cajal and C. Goldi were together Nobel laureates in 1906, but C. Goldi violently opposed S. Ramón y Cajal's theory of neurons (similar to Boltzmann's theory of atoms) to explain the global system which is the brain. The opposite conceptions of science were in this case truth-to-nature (Goldi) and mechanical objectivity (Ramón y Cajal) as well as continuous (Goldi) versus discontinuous (Ramón y Cajal) visions, see Ref. 2. For more details on Boltzmann's legacy, see also Ref. 8.

In the same spirit as Boltzmann, it was natural to rise the question of the microscopic origin of Ohm and Joule's laws. In 1846, W. Weber conjectured that currents were a flow of charged fluids and in 1881, H. von Helmholtz argued the existence of positive and negative charges as "atoms of electricity". The discovery of the electron took place in the last years of the nineteenth century by J.J. Thomson and others. It is the first discovered elementary particle. Based on the vision that current is a flow of electrons, the celebrated Drude model (P.L. Drude, 1863–1906) was next proposed in 1900 to give a mechanical explanation of the phenomenon of conductivity. This model or its extension, the Drude–Lorentz model (1905), are still used as microscopic explanations of conductivity in textbooks. Indeed, although the motion of electrons and ions is treated classically and the interaction between these two species is modeled by perfectly elastic random collisions, this quite elementary model provides a qualitatively good description of DC– and AC–conductivities in metals.

2. Electrical Conductivity and Quantum Mechanics

2.1. Emergence of Quantum Mechanics

The main principles of physics were considered as well-founded by the end of the nineteenth century, even with, for instance, no satisfactory explanation of the phenomenon of thermal radiation, first discovered in 1860 by G. Kirchhoff. In contrast

to classical physics, which deals with continuous quantities, Planck's intuition was to introduce an intrinsic discontinuity of energy to explain thermal radiation. Assuming the existence of a quantum of action h, the celebrated Planck's constant, he derived the well–known Planck's law of thermal radiation. Inspired by Planck's ideas, Einstein presented his famous discrete (corpuscular) theory of light to explain the photoelectric effect.

Emission spectra of chemical elements had also been known since the nineteenth century and no theoretical explanation was available at that time. It became clear that electrons play a key role in this phenomenon. However, the classical solar system model of the atom failed to explain the emitted or absorbed radiation. Following again Planck's ideas, N. Bohr proposed in 1913 an atomic model based on discrete energies that characterize electron orbits. It became clear that the main principles of classical physics are unable to describe atomic physics.

Planck's quantum of action, Einstein's quanta of light (photons), and Bohr's atomic model could not be a simple extension of classical physics, which, in turn, could also not be questioned in its field of validity. N. Bohr tried during almost a decade to conciliate the paradoxical looking microscopic phenomena by defining a radically different kind of logic. Bohr's concept of complementarity gave in 1928 a conceptual solution to that problem and revolutionized the usual vision of nature. See, e.g., Ref. 9. Classical logic should be replaced by quantum logic as claimed by G. Birkhoff and J. von Neumann in 1936.

On the level of theoretical physics, until 1925, quantum corrections were systematically included, in a rather *ad hoc* manner, into classical theories to allow explicit discontinuous properties. Then, two apparently complementary directions were taken by W.K. Heisenberg and E. Shrödinger, respectively, to establish basic principles of the new quantum physics, in contrast with the "old quantum theory" starting in 1900. Indeed, even with the so–called correspondence principle of N. Bohr, "many problems, even quite central ones like the spectrum of helium atom, proved inaccessible to any solution, no matter how elaborate the conversion", see [10, p. 18].

2.2. Quantum Fermi liquids

Electric current is carried by electrons, purely quantum objects (W.E. Pauli, 1925; E. Fermi, 1925; P.A.M. Dirac, 1929), whereas the Drude model describes non-interacting classical particles interacting with impurities via perfectly elastic collisions. Quantum Mechanics, which governs the microscopic world, represents a radical transformation of usual principles of classical physics and it is therefore not at all satisfactory to see the Drude (or the Drude–Lorentz) model as a proper microscopic explanation of conductivity, even with good agreements with experimental data. As one can see from the existence of superconducting phases first discovered in 1911, electrons can show collective behaviors while satisfying the celebrated Pauli exclusion principle.

A. Sommerfeld and H. Bethe modified in 1933 the Drude model to take into account quantum effects. Essentially, they replaced the classical point–like particles of Drude, carriers of electrical current, with fermions. In particular, the carriers present quantum coherences and obey the Fermi–Dirac statistics. However, the Drude–Sommerfeld model describes a system of non–interacting fermions although electrons strongly interact with each other via the Coulomb repulsion. A formal explanation of the success of this model is given by L.D. Landau in the fifties. His theory is based on the concept of *Landau Fermi liquids* (or Fermi liquids).

Landau's idea is, in a caricatured view, that the low-energy exited states of a Fermi system with interparticle interactions can be mapped onto the states of an effective non-interacting (or ideal) Fermi system. The theoretical justification of such a behavior, i.e., the fact that the electron-electron scattering remains negligible to change the momentum distribution, results from the Pauli exclusion principle for energies near the Fermi level. More precisely, if the system is at initial time in a state closed to an ideal system (weakly excited), then its time-dependent state can be uniquely described by occupation numbers of quasiparticles (as approximated quantum numbers). Moreover, L.D. Landau postulates the existence of a function $f_{k,k'}$, the so-called Landau interaction function, which quantifies the energy change of a quasiparticle of quasimomentum k in the presence of a quasiparticle of quasimomentum k'. The effective mass, another parameter of Fermi liquids, determines the dispersion relation of quasiparticles, i.e., the energy of quasiparticles as a function of their quasimomenta. This effective (or phenomenological) theory has been very successful in explaining the physics of some electron systems, called Fermi liquids. Fermion systems are called non-Fermi liquids if their behavior does not correspond to Landau's predictions. Non-Fermi liquid behaviors usually appear in low dimensions. For instance, in one dimension, the celebrated Luttinger liquid replaces the (Landau) Fermi liquid. For more details, see Ref. 11.

2.3. From theoretical physics to mathematics: The Anderson model

Resistivity of metals is believed to be due to interparticle interactions but also to inhomogeneities of the conducting crystal. Disordered electron liquids are therefore an important issue in this context. The theory of Fermi liquids can be extended to disordered systems but major differences appear as compared to the (space) homogeneous systems. New properties like the so–called *Anderson localization* are consequence of strong space inhomogeneities, even in the absence of interparticle interactions.

Anderson localization corresponds to the absence of electron transport at strong disorder and has been predicted by the physicist P.W. Anderson in 1958. This allows to guess a metal—insulator transition in three dimensions. This theory has experimentally been investigated and P.W. Anderson, together with N.F. Mott and J.H. van Vleck, won the 1977 Nobel price in physics for "their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems".

The Anderson model corresponds to a single quantum particle within a random potential. It is one of the most important types of random Schrödinger operators, which constitute nowadays an advanced and relatively mature branch of mathematics. In fact, random Schrödinger operators start to be studied in the seventies. The Anderson localization for an one–dimensional model was first proved by I. Goldsheid, S. Molchanov and L. Pastur in 1977, while a similar result for the one–dimensional Anderson model was obtained in 1981 by H. Kunz and B. Souillard. It is known that, in general, the one–dimensional Anderson model only has purely point spectrum with a complete set of localized eigenstates (Anderson localization) and it is thus believed that no steady current can exist in this case. For more detailed introduction to the Anderson model and more general random Schrödinger operators, see for instance the lecture notes of Ref. 12.

Nevertheless, mathematical studies usually focus on the existence of (dynamical or spectral) Anderson localizations and, even in absence of interactions, there are only few mathematical results on transport properties of such random models that yield Ohm's law in some form.

In 2007, A. Klein, O. Lenoble and P. Müller introduced¹³ for the first time the concept of a "conductivity measure" for a system of non–interacting fermions subjected to a random potential. More precisely, the authors considered the Anderson tight–binding model in presence of a time–dependent spatially homogeneous electric field that is adiabatically switched on. The fermionic nature of charge carriers – electrons or holes in crystals – as well as thermodynamics of such systems were implemented by choosing the Fermi–Dirac distribution as the initial density matrix of particles. In Ref. 13 only systems at zero temperature with Fermi energy lying in the localization regime are considered, but it is shown in Ref. 14 that a conductivity measure can also be defined without the localization assumption and at any positive temperature. Their study can thus be seen as a mathematical derivation of Ohm's law for space–homogeneous electric fields having a specific time behavior.

Ref. 15 is another mathematical result on free fermions proving Ohm's law for graphene–like materials subjected to space–homogeneous and time–periodic electric fields. Joule's law and heat production are not considered, at least not explicitly, in these mathematical studies.

3. Electrical Conductivity and 2nd Law of Thermodynamics

Via Refs. 13,14 one sees that measures (instead of functions or other types of distributions) are the natural mathematical objects to be used to describe conductivity starting form microscopic quantum dynamics. We claim that this is so because of the 2nd law of Thermodynamics. Indeed, such a principle guarantees the positivity of certain quadratic forms on external electric fields, which naturally appears by considering linear response. By Bochner's theorem, in a convenient form, such quadratic forms define measures. In the case of current response to external electric fields, one gets AC–conductivity measures. This approach permits to tackle the

mathematical problem of a rigorous microscopic description of the phenomenon of linear conductivity starting from first principles. Moreover, it is general enough to be applied to interacting systems. We implement the 2nd law of Thermodynamics in the scope of algebraic Quantum Mechanics, by using the remarkable results¹⁶ of W. Pusz and S. L. Woronowicz: We consider the 2nd law as a first principle of Physics which supplements Quantum Mechanics in the sense that it singles out special states of the considered systems. Indeed, states of infinite systems that are compatible with the 2nd law exist for a huge class of dynamics.

In fact, the 2nd law is "one of the most perfect laws in physics" [17, Section 1] and it has never been faulted by reproducible experiments. Its history starts with works of S. Carnot in 1824. Different popular formulations of the same principle have been stated by R.J.E. Clausius, W. Thomson or Lord Kelvin (and M. Planck), and C. Carathéodory. Our study is based on Kelvin–Planck statement while avoiding the concept of "cooling" [17, p. 49]:

No process is possible, the sole result of which is a change in the energy of a simple system (without changing the work coordinates) and the raising of a weight.

Using this formulation of the 2nd law, we define the concept of thermal equilibrium states by using algebraic Quantum Mechanics as mathematical framework. It is a well–known approach – originally due to J. von Neumann (cf. von Neumann algebras, C^* –algebras) – that extends the Hilbert space formulation of Quantum Mechanics. One important result of the theory of C^* –algebras, obtained in the forties, is the celebrated GNS (Gel'fand–Naimark–Segal) representation of states, which permits a natural relation between the new algebraic formulation and the usual Hilbert space based formulation of Quantum Mechanics to be established. Indeed, I.E. Segal proposed to leave the Hilbert space approach to consider quantum observables as elements of certain involutive Banach algebras, now known as C^* –algebra. The GNS representation has also led to very important applications of the Tomita–Takesaki theory, developed in seventies, to Quantum Field Theory and Statistical Mechanics. These developments mark the beginning of the algebraic approach to Quantum Mechanics and Quantum Field Theory. For more details, see, e.g., Ref. 18.

The algebraic formulation turned out to be extremely important and fruitful for the mathematical foundations of Quantum Statistical Mechanics and have been an important branch of research during decades with lots of works on quantum spin and Fermi systems. See, e.g., Refs. 19,20 (spin) and Refs. 21–23 (Fermi). Basically, it uses some C^* -algebra \mathcal{X} , the self-adjoint elements of which are the so-called observables of the physical system. States on the C^* -algebra \mathcal{X} are, by definition, continuous linear functionals $\rho \in \mathcal{X}^*$ which are normalized and positive, i.e., $\rho(\mathbf{1}) = 1$ and $\rho(A^*A) \geq 0$ for all $A \in \mathcal{X}$. They represent the state of the physical system.

To define the notion of equilibrium state, Ref. 16 is pivotal because it defines the notion of equilibrium by using the Kelvin–Planck statement. It is directly related

to the notion of passive and completely passive states. In fact, completely passive states are defined to be thermal equilibrium states in our setting. [16, Theorem 1.4] shows that thermal equilibrium states defined in such a way are exactly the KMS^{19} (Kubo–Martin–Schwinger) states of the corresponding C^* -dynamical system.

The approach to linear response we propose has the following technical and conceptual advantages, even in the non–interacting case:

- The positivity required for the existence of the AC–conductivity measure is directly related to the passivity property of thermal equilibrium states on the CAR algebra.
 - In other words, the existence of AC-conductivity results from the 2nd law of Thermodynamics in connection with the full quantum microscopic dynamics of the considered system.
- The conductivity measure naturally appears as the Fourier transform of current–current time correlations, that is, four–point correlation functions, in this framework. This means that Green–Kubo relations are generally valid, from first principles.
- The algebraic formulation allows a clear link between macroscopic transport
 properties of fermion systems and the CCR algebra of current fluctuations
 associated to that systems. The latter is related to non-commutative central
 limit theorems.
- Moreover, this approach can be naturally used to define and analyze conductivity measures for *interacting* fermions as well.

In Refs. 24,25 we study free lattice fermions subjected to a static bounded potential and a time—and space—dependent electromagnetic field. Refs. 24,25 establish a form of Ohm and Joule's laws valid at microscopic scales, uniformly with respect to the size of the region on which the electric field is applied. It is in accordance with the validity of Ohm's law in the quantum world, i.e., at microscopic scales, see Ref. 6. Refs. 26,27 extend the results of Refs. 24,25 to macroscopic scales and are reminiscent of Refs. 13,14. For more details, see the discussions in Ref. 26. Part of the phenomenology of the Drude model can be derived from our more detailed study²⁷ of macroscopic conductivity measures of free—fermions in disordered media.

Therefore, Refs. 24–27 give a complete, mathematically rigorous, microscopic derivation of the phenomenon of linear conductivity from first principles of Thermodynamics and Quantum Mechanics, only. These studies are restricted to non–interacting fermion systems. However, it is believed in theoretical physics that electric resistance of conductors should also result from the interactions between charge carriers, and not only from the presence of inhomogeneities (impurities). In Refs. 28,29, we succeed to extend our previous results to fermion systems with interactions.

To conclude, we think that such an approach can be useful in other contexts since it gives appropriate tools to tackle mathematically what is known in Physics

as excitation spectrum. Indeed, the concept of excitation spectrum is usually associated with the spectrum of a self-adjoint operator describing the energy of the system. In condensed mater physics, this notion mainly comes from superfluid helium 4, a quantum boson liquid which can be described by the spectrum of collective excitations via the celebrated Bogoliubov theory.³⁰ However, there is a plethora^{31,32} of other types of elementary excitations not covered by the Bogoliubov theory. We show^{25,26,28} that the notion of conductivity measure we defined is nothing else than a spectral measure of the generator of dynamics in an appropriate representation.

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