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# A SEMICLASSICAL APPROACH TO OHM'S LAW

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**Abstract:** A voltage source is modeled by a semiclassical perturbation of the quantum momentum operator. Applying the quantum formalism we obtain a formula for the electric current in a 1-dimensional piece of metal. It turns out that for the model based dependence between voltage and current Ohm's law is valid for a realistic range of voltages.

**AMS Subject Classification:** 81V99, 81-04

**Key Words:** Hamiltonian, quantum Gibbs state, expectation of the velocity operator

## 1. Introduction

Recently (cf. [1],[2],[3]) quantum models based on a discrete position space have drawn some attention. These models entail that quantum observables that are modeled by self-adjoint operators, can be represented by Hermitian matrices. This approach turns out to be attractive from computational viewpoint and enables us to build bridges between mathematical models, statistical evaluations of computer experiments and outcomes of laboratory measurements.

In the present contribution we model a microscopic voltage source by a formula for the momentum of an electron which depends in particular on temperature (Section 2). In Section 3 we present a lattice which serves as a discrete position space and construct a semiclassical momentum operator perturbed by the action of the voltage source. We

introduce the corresponding quantum Gibbs state and show a possibility of computing the values of an electric current indicator depending linearly on the voltage of the source (Sections 4 and 5). A graphical comparison between the model predictions and empiric values of resistivity is presented in Section 6. We conclude with Section 7 where the model prediction of the dependence of electric resistance on temperature is presented and discussed.

## 2. A Characterization of a DC-Voltage Source by the Momentum of the Electrons

Let

$$e = 1.60219 \cdot 10^{-19} \text{ C}$$

denote the elementary electric charge. (The charge of an electron can be approximated by  $-e$ ).

For modeling a voltage source of spatial extent  $a > 0$  and at temperature  $T > 0$  we assume that a homogeneous electrostatic field of strength  $E$  is present in the source, which corresponds to the voltage

$$(2.1) \quad U = E \cdot a.$$

Let  $m = 9.109534 \cdot 10^{-31} \text{ kg}$  denote the electron mass and  $k_B = 1.3806488 \cdot 10^{-23} \text{ J/K}$  the Boltzmann constant.

In Section 3 quantity  $a$  will be interpreted as a distance between adjacent atom rumps in a lattice  $L_a$  which electrons are also confined within. Therefore we call quantity

$$(2.2) \quad \gamma := \frac{(m \cdot k_B \cdot T)^{1/2}}{a}$$

as coefficient of thermal impediment of electrons moving within lattice  $L_a$  where  $(m \cdot k_B \cdot T)^{1/2}$  is the Maxwell-Boltzmann dispersion of the thermal momentum of an electron.

Let  $v(t)$  denote the velocity of an electron as function of time. The differential equation representing the balance of forces acting on the electron ist given by

$$(2.3) \quad m \cdot \frac{d}{dt}v(t) + \gamma \cdot v(t) = -E \cdot e.$$

The term  $\gamma \cdot v(t)$  in (2.3) may be interpreted as the frictional force which ist opposed to the motion of the electron. The time asymptotic

velocity  $\bar{v}$  in (2.3) is given by

$$(2.4) \quad \bar{v} = \lim_{t \rightarrow \infty} v(t) = -\frac{E \cdot e}{\gamma}$$

which corresponds to the asymptotic momentum

$$(2.5) \quad \bar{p} = m \cdot \bar{v} = -\frac{E \cdot e \cdot m \cdot a}{(m \cdot k_B \cdot T)^{1/2}}$$

imposed on the electron (cf. (2.1) and (2.2)) by the voltage source.

### 3. Finite Lattice and the Momentum Operator

Let us consider a finite lattice

$$L_a := \{na | n = 1, \dots, N\}$$

of  $N$  points modeling a discrete position space; parameter  $a > 0$  is called lattice constant.  $L_a$  serves as a model of an 1-dimensional conductor. A quantum state of an electron confined within the conductor is described by a function  $\varphi : L_a \rightarrow \mathbb{C}$  satisfying the condition

$$\sum_{n=1}^N |\varphi(na)|^2 = 1.$$

In this context  $|\varphi(na)|^2$  is interpreted as the probability of spatial association of the electron with lattice point  $na \in L_a$ . By a standard identification, the set of all states of the electron can be viewed as the unit sphere in  $\mathbb{C}^N$ .

The unperturbed quantum momentum operator  $\hat{p}^{(0)} : \mathbb{C}^N \rightarrow \mathbb{C}^N$  is defined by

$$(3.1) \quad (\hat{p}^{(0)}\varphi)(na) = -i\hbar \cdot \frac{\varphi((n+1)a) - \varphi((n-1)a)}{2a} \quad (n = 1, \dots, N)$$

where  $\hbar$  denotes Planck's constant; in (3.1) the convention

$$\varphi(na) = 0 \quad \text{for } n < 1 \quad \text{and for } n > N$$

is applied and can be interpreted as Dirichlet boundary condition (cf. [2], p. 28ff).  $\hat{p}^{(0)}$  is self-adjoint and serves as a discrete central difference approximation of the 1-dimensional momentum operator

$$-i\hbar \cdot \frac{d}{dx}$$

for the position space modeled by the real line.

Let us assume that at the site  $na = Na/2$  a microscopic DC voltage source is active and perturbs the momentum operator  $\hat{p}^{(0)}$  by  $\hat{p}^{(1)}$  whose matrix representation is given by

$$(3.2) \quad \hat{p}_{jk}^{(1)} = \begin{cases} \bar{p} & \text{for } j = k = N/2 \\ 0 & \text{elsewhere} \end{cases}$$

where  $\bar{p}$  is the semiclassical momentum modeling the action of the voltage source, cf. (2.5). Accordingly, the perturbed momentum operator  $\hat{p}$  is given by

$$(3.3) \quad \hat{p} = \hat{p}^{(0)} + \hat{p}^{(1)}.$$

Let  $e^{(j)}$  denote the  $j^{\text{th}}$  canonical unit vector in  $\mathbb{C}^N$  for  $j = 1, \dots, N$ . To illustrate the perturbed momentum operator  $\hat{p}$  we point out that

$$\langle e^{(j)}, \hat{p}e^{(j)} \rangle = \delta_{jn} \cdot \bar{p}$$

holds where  $\delta_{jk}$  and  $\langle \cdot, \cdot \rangle$  denotes the Kronecker symbol and the scalar product of  $\mathbb{C}^N$ , respectively, and  $n = N/2$  indicates the location of the voltage source.

**Remark 3.1.**

The matrix representing operator  $\hat{p}$  is Hermitean.

#### 4. The Gibbs State of the Electron

Let us consider the Hamiltonian

$$H_{\bar{p}} = \frac{\hat{p}^2}{2m}.$$

Operator  $H_{\bar{p}}$  describes the energy of an electron confined within lattice  $L_a$ .

Let  $T > 0$  denote the temperature of the lattice. The operator  $G_{T, \bar{p}} : \mathbb{C}^N \rightarrow \mathbb{C}^N$  modeling the Gibbs state of the electron is given by

$$(4.1) \quad G_{T, \bar{p}} = \frac{1}{Z(T, \bar{p})} \cdot \exp \left( -\frac{1}{k_B \cdot T} \cdot H_{\bar{p}} \right)$$

where

$$(4.2) \quad Z(T, \bar{p}) := \text{trace} \left( \exp \left( -\frac{1}{k_B \cdot T} \cdot H_{\bar{p}} \right) \right)$$

denotes the partition function.  $G_{T, \bar{p}}$  is a positive operator whose trace is equal to 1. Operator  $G_{T, \bar{p}}$  is motivated by the entropy principle

(cf. [4], p. 384) and describes the thermal equilibrium state of the electron confined within lattice  $L_a$  with the interpretation of the diagonal entry  $G_{T,\bar{p}}(j, j)$  as the probability of spatial association of the electron with lattice point  $ja$ .

## 5. The Electric Current and its Dependence on $U$

The operator  $\hat{v} : \mathbb{C}^N \rightarrow \mathbb{C}^N$ ,

$$\hat{v} := \frac{\hat{p}}{m},$$

describes the velocity of the electron confined within lattice  $L_a$  where  $\hat{p}$  is the perturbed momentum operator introduced in Section 3.

The quantum expectation  $\mathbb{E}_q(\hat{v})$  of the velocity of the electron whose state is described by  $G_{T,\bar{p}}$ , is given by

$$(5.1) \quad \mathbb{E}_q(\hat{v}) = \text{trace}(G_{T,\bar{p}}\hat{v}).$$

Since the operators  $G_{T,\bar{p}}$  and  $\hat{v}$  are self-adjoint, the expectation in (5.1) is a real number.

The current indicator

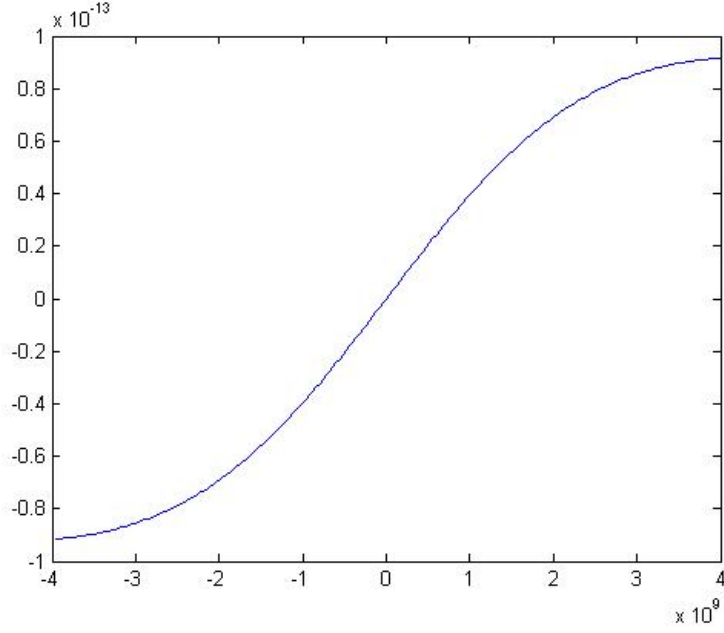
$$(5.2) \quad I = -\frac{\mathbb{E}_q(\hat{v}) \cdot Ne}{Na} = -\frac{\mathbb{E}_q(\hat{v}) \cdot e}{a}$$

is equal to the quantum expectation of the velocity multiplied by the density of the mobile electric charge present in the lattice.

Equations (2.1),(2.5),(5.1) and (5.2) enable us to relate the voltage  $U$  of the source with the corresponding current  $I$  in the lattice.

### Example 5.1.

*Put  $N = 300, a = 10^{-10}m, T = 300K$ . In a computer experiment we let the voltage  $U$  of the source vary and compute for each value of  $E$  the corresponding value  $I$  of the current indicator.*



**Fig. 1:**  $U - I$ -diagram

In Figure 1 the horizontal axis corresponds to strength  $E$  of the electric field (the physical unit is V/m) modeling the voltage source (cf. (2.1)) and the vertical axis to the quantum current  $I$  in A, cf. (5.2). The diagram shows that the current is a linear function of  $U$  for the values of the electric field  $E$  from the interval  $[-10^9 \text{ V/m}, 10^9 \text{ V/m}]$  which complies with Ohm's law. The departure from linearity in Fig. 1 occurs only for very strong electric fields which are difficult to explore empirically.

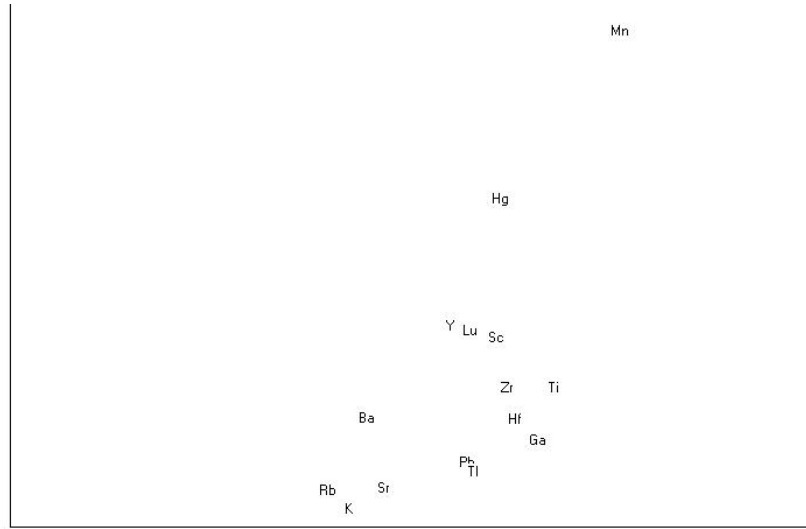
## 6. Model Based vs. Empiric Electric Resistivity

Since the linearity in Fig. 1 extends over the whole interval  $[-10^9 \text{ V/m}, 10^9 \text{ V/m}]$  we can select an arbitrary value  $E$  thereof, compute the corresponding current  $I$  and estimate the resistance  $R$  of the lattice according to

$$(6.1) \quad R = \frac{U}{I}.$$

The indicator  $s_m$  of the resistivity is then given by

$$(6.2) \quad s_m = \frac{R}{N \cdot a}.$$



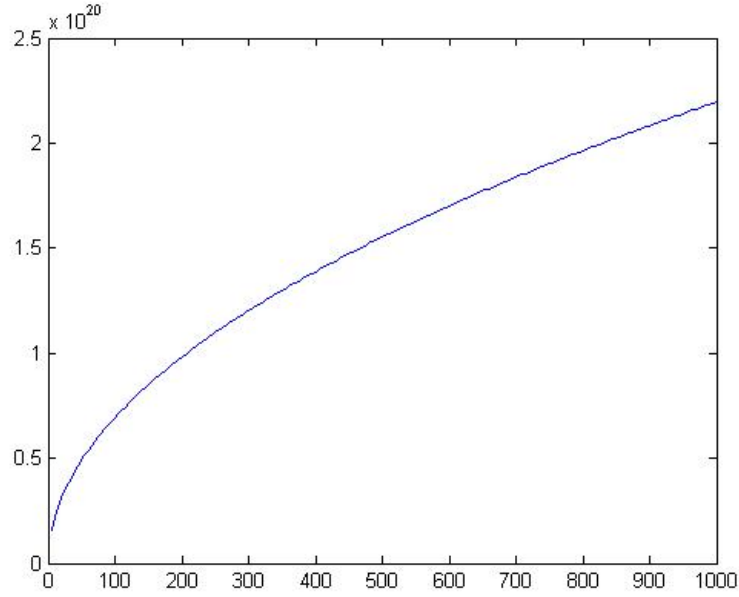
**Fig. 2:** Model Based vs. Empiric Resistivity

Fig. 2 shows a comparison between the model based and the empiric resistivity for a selection of metals yielding the correlation coefficient 0.66 between  $s_m$  and its empiric pedant. Although we cannot claim that our semiclassical model predicts the empiric resistivity for all metals, we emphasize the fact that lattice constant  $a$  is the only material specific quantity involved in the computation of the r. h. s. of (6.2).

## 7. Model Based Resistance vs. Temperature

In this Section we would like to show the dependence of electric resistance  $R$  (cf. (6.1)) of the lattice  $L_a$  on temperature. In Fig. 3 the horizontal axis corresponds to the temperature of the lattice in the range 0-1000 K and the vertical one to the electric resistance determined for our model. The diagram shows that the model resistance is reduced for low temperatures which is in a qualitative agreement with empiric observations.





**Fig. 3:** Model Based Resistance vs. Temperature

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### References

- [1] H.L. Cycon, R.G. Froese, W. Kirsch, B. Simon, *Schrödinger operators*. Springer, Berlin, Heidelberg, New York (2008).
- [2] M. Disertori, W. Kirsch, A. Klein, F. Klopp, V. Rivasseau, *Random Schrödinger Operators*. Panoramas et Synthèses, Societe Mathématique de France, Paris (2008).
- [3] E. Grycko, W. Kirsch, T. Mühlenbruch, Some quantum mechanical evidence for the amplification of thermal noise in an electrostatic field. *Int. J. Pure Appl. Math.* **69**, No. 4, (2011), 437-507.
- [4] W. Thirring, *Quantum Mathematical Physics*. Second edition, Springer, Berlin, Heidelberg, New York (2002).