Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 6-7

Artikel: Monte Carlo simulation in Fermi systems
Autor: Romanó, L. / Dallacasa, V.
DOI: https://doi.org/10.5169/seals-116154

MONTE CARLO SIMULATION IN FERMI SYSTEMS

L. Romanó,V. Dallacasa,Dipartimento di Fisica Viale delle scienze, Parma, Italy

Abstract We present an application of an ensemble Monte Carlo simulation for charge transport to a Fermi system to study the effects of the lattice interaction on the transport properties.

1. *Introduction*

In our MC simulations we use a semiclassical description in which the lattice effects are described by the first order perturbation theory neglecting the Pauli exclusion principle effects while an algorithm , first applied by Lugli and Ferry [1] for the description of degenerate semiconductor, takes into account of the Fermi statistic by means of the rejection technique. We present some results on the resistivity versus temperature which are in good agreement with the theory of metals at high and low temperatures indicating that it is possible to apply this technique to a normal state of the metal with reasonable computer time.

2. *The method and the results*

In our simulation we follow $N(\sim 10^5)$electrons with the initial energy distribution $g(\epsilon,0)$ for a given time interval t_m (corresponding to ~ 100 scattering events per electron), within a volume $V_c = \frac{N}{n} \simeq 10^{-17}cm^3$($n = 10^{22}cm^{-3}$)in a constant electrical field of the order of $1\frac{V}{cm}$, subjected to the lattice interaction.

To obtain the resistivity in the ohmic regime, we evaluate the transversal diffusion coefficients at very low fields and then obtain the mobility by means of the Einstein relation.

The collision frequencies for emission or absorption of a phonon by an electron of a metal as from [2]are:

$$\frac{1}{\tau} = \sum_{k'} S(\underline{k},\underline{k}') = A\sqrt{\epsilon \mp \hbar\omega}(n(\hbar\omega) + \frac{1}{2} \pm \frac{1}{2})$$

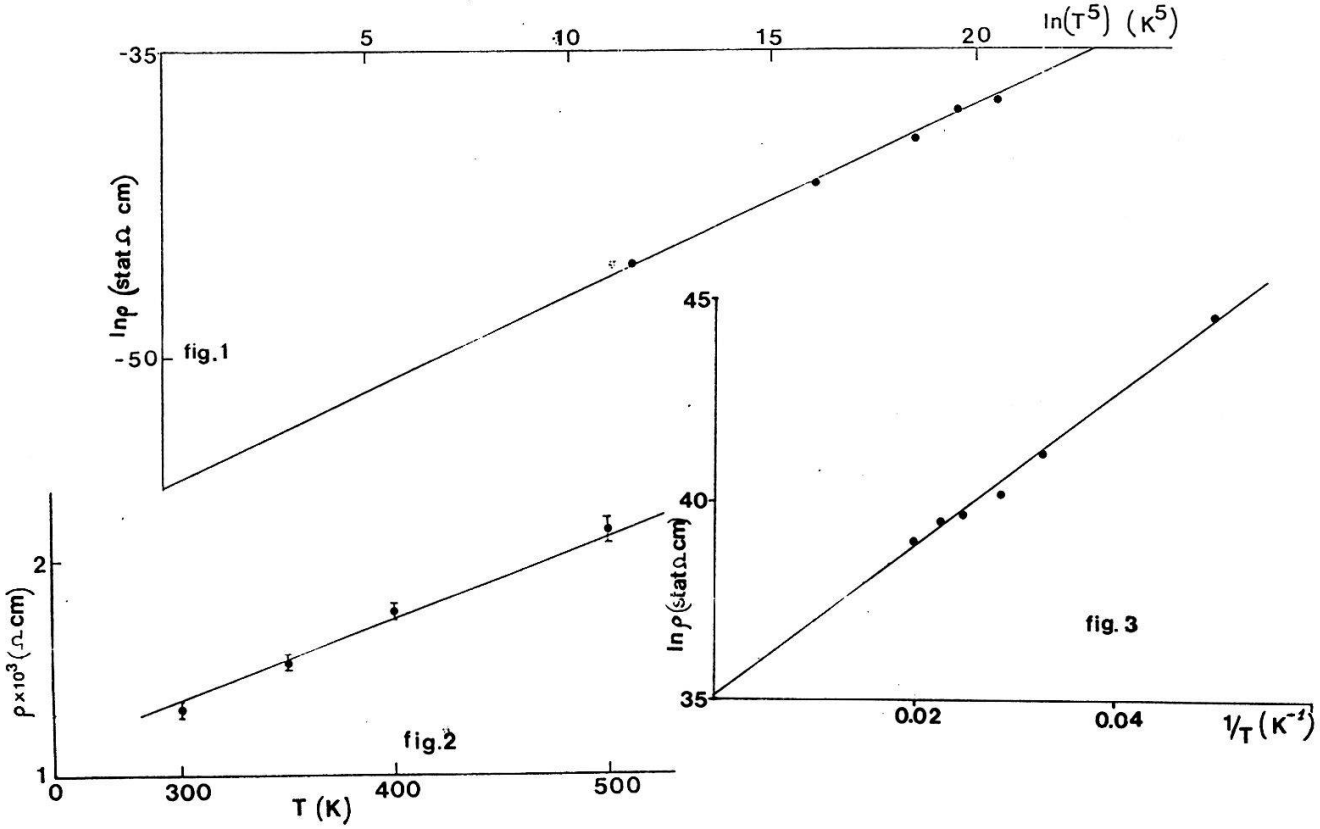
where $A = \frac{2.71*10^{13}V^2 m^{*3/2} q_D}{\rho v_s}$ (the density ρ of the crystal is in $\frac{gm}{cm^3}$, the sound velocity $v_s$is in $10^5\frac{cm}{sec}$, the Debye wave vector q_D in $10^8 cm^{-3}$ and the deformation potential V in eV). The coupling constant and the phonon frequency are assumed q-independent. In fig 1. we report the behaviour of the resistivity versus log T^5 at low temperature $T \ll \theta_D$ in a system in which $\epsilon_F = 0.1eV$ and $\theta_D = 116K$. The angular coefficient of

the straight line is $a = 3.2 * 10^{-25}$ in good agreement with the theory of the metals ($a_{th} = 2.97 * 10^{-25}$)[3]. In fig 2. we report the resistivity versus temperature for $T \gg \theta_D$ in the same system. The angular coefficient of the straight line is $b = 1.7 * 10^{-18}(b_{th} = 9.9 * 10^{-19}$[3])

In fig 3. we present the behaviour of the resistivity versus $\frac{1}{T}$ at low temperature obtained by our simulations with a renormalization of the electron self-energy which produces a shift of the energy ϵ of the electron:$\epsilon \rightarrow \epsilon + \Delta(\Delta = 7.7 * 10^{-3})$.

3.*Conclusions*

The MC technique appears a good method to study the transport properties of metals; and it seems to be suitable to investigate conditions of very low resistivity also in realistic situations like as the new superconducting materials.



References

[1] P.Lugli,K.Ferry,IEEE Trans.Electron.Devices,ED**32**,2431 (1985)

[2] B.K.Ridley, in *Quantum Processes in Semiconductors*, Clarendon Press, Oxford (1982)

[3] J.M.Ziman in *Principles of the Theory of Solids*, Cambridge University Press, Cambridge (1972)