Commun. math. Phys. 40, 197—213 (1975)

An Upper Bound on the Free Energy for Classical Systems with Coulomb Interactions in a Varying External Field

E. R. Smith and O. Penrose

Mathematics Department, University of Newcastle, New South Wales, Australia, and Mathematics Department, The Open University, Milton Keynes, England

Received July 4, 1974

Abstract. The thermodynamic limit is taken using a sequence of regions all the same shape as a given region ω of volume $|\omega|$, with a specified distribution of normal field component on $\partial\omega$. We show that with magnetostatic interactions the limiting free energy density is bounded above by

$$|\omega|^{-1} \inf_{\varrho(x)} \inf_{B(x)} \int_{\omega} \bar{f}(\varrho(x), B(x))\, d^3x$$

where $\bar{f}(\varrho, B)$ is the free energy density for a system of density ϱ in a uniform external field B and the "inf" is taken over all divergence-free fields B with given normal component on $\partial\omega$ and all densities $\varrho(x)$ compatible with particle number constraints of the form $\int_{\Gamma_i} \varrho(x)\, d^3x = |\Gamma_i| \varrho_i$ where Γ_i is a sub-region of ω. A physical argument suggests that this upper bound is the true thermodynamic limit, and that it takes account demagnetization effects. Electrostatic interactions can be treated similarly.

I. Introduction

In a previous paper [1] (hereafter referred to as $P-S$) we proved the existence of the thermodynamic limit of the free energy for a system of particles with Coulomb (electrostatic or magnetostatic) interactions in a uniform external field. The Coulomb contribution to the potential energy was calculated by considering a "microscopic" electric or magnetic field which was a superposition of the external field and the fields produced by the particles in the system. At the surface of the container which holds the particles, the normal component of the total field was set equal to the normal component of the uniform external field applied to the system. This boundary condition made it possible to prove the existence of the thermodynamic limit. The thermodynamic limit was found to be independent of the shape of the regions containing the particles.

In nature, systems with Coulomb interactions display shape-dependent effects in their free energy: the demagnetization or depolarization effects. These effects are due to non-uniformity of the total (macroscopic) magnetic field in the vicinity of the system, which can come about