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Asymptotic Free Energy of a System with Periodic Boundary Conditions

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Abstract. A ν-dimensional classical particle system in a torus, i.e., in a rectangular box with periodic boundary conditions, is considered in a canonical ensemble. Subject to mild restrictions over and above the usual stability and tempering conditions it is proved that the thermodynamic limit for the torus exists and is identical with that for systems contained in normal domains with boundaries or walls. If, in addition, the pair interaction potential $\varphi(r)$ decreases sufficiently rapidly (so that $r|\varphi(r)|$ is integrable at ∞), and satisfies some further regularity conditions, then the difference between the free energies of the torus and of the corresponding box is at most of the order of a surface term. Somewhat stronger results are indicated for the grand canonical pressure.

I. Introduction

The canonical free energy density of a system, namely

$$F(\Omega)/V(\Omega) = -\beta g(\beta, \varrho; \Omega), \tag{1.1}$$

is calculated in statistical mechanics from the partition function according to the relation

$$Z(\beta, N, \Omega) = e^{V(\Omega) g(\beta, \varrho; \Omega)}, \tag{1.2}$$

where $\beta = 1/k_B T$ measures the reciprocal temperature, and N is the number of particles contained in the ν-dimensional domain Ω, of (generalized) volume $V(\Omega)$, which represents a physical container with hard impenetrable walls. The density is defined for integral N by

$$\varrho = N/V(\Omega), \tag{1.3}$$

but the definition of $g(\beta, \varrho; \Omega)$ may readily be extended to general values of ϱ by linear interpolation (see Ref. [1]). We assume a particle Hamiltonian of the standard form

$$\mathscr{H}_N = \sum_{i=1}^{N} p_i^2/2m + U_N(\mathbf{r}_1, \ldots \mathbf{r}_n), \tag{1.4}$$