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The Inverse Problem in Classical Statistical Mechanics

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Abstract. We address the problem of whether there exists an external potential corresponding to a given equilibrium single particle density of a classical system. Results are established for both the canonical and grand canonical distributions. It is shown that for essentially all systems without hard core interactions, there is a unique external potential which produces any given density. The external potential is shown to be a continuous function of the density and, in certain cases, it is shown to be differentiable. As a consequence of the differentiability of the inverse map (which is established without reference to the hard core structure in the grand canonical ensemble), we prove the existence of the Ornstein-Zernike direct correlation function. A set of necessary, but not sufficient conditions for the solution of the inverse problem in systems with hard core interactions is derived.

1. Introduction

The inverse problem in classical statistical mechanics concerns the relationship between classical systems and their equilibrium single particle densities. Consider a finite temperature classical system of N particles characterized by an interaction $W(x_1, \ldots, x_N)$, where x_i denotes all the coordinates (e.g. space, spin, etc.) of the i^{th} particle. W is henceforth regarded as a fixed, given function. It need not be symmetric. If an external potential, $U(x)$, is applied to the system, the density of the i^{th} particle in the canonical distribution is

$$\varrho_i(U; x_i) = Z_U^{-1} \int \exp\left[-W(x_1, \ldots, x_N) - \sum_{j=1}^{N} U(x_j)\right] dx_1 \ldots \widehat{dx_i} \ldots dx_N, \qquad (1.1)$$

where $\widehat{dx_i}$ indicates that there is no integration over x_i, and

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