

First order perturbation calculation for the dynamical correlation function of a classical gas

Doctoral Thesis

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First Order Perturbation Calculation
for the Dynamical Correlation Function
of a Classical Gas

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First Order Perturbation Calculation for the Dynamical Correlation Function of a Classical Gas

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Abstract. For a classical gas with a finite twobody potential the dynamical correlation function has been evaluated to first order in the interaction. An extrapolation of this result is discussed for gases with more realistic interactions.

Zusammenfassung. Für ein klassisches Gas von identischen Teilchen, ohne innere Struktur, welche durch ein beschränktes Zweikörper-Potential wechselwirken, wird die dynamische Korrelationsfunktion in erster Ordnung der Kopplungskonstante berechnet. Das Resultat wird auf Gase mit einer realistischeren Wechselwirkung extrapoliert.

1. Introduction

In the theory of real gases and liquids various approximations and expansions for the static two-particle correlation [1, 2] have been given. Recently several approaches to a theory of the dynamical correlation have been discussed [1], [3-7]. The present paper proposes a perturbation expansion of the dynamical correlation function and evaluates the term linear in the interaction.

We consider a classical gas of identical particles without internal structure. We assume that the interaction between the particles is given by a finite two-body potential.

The dynamical correlation function for such a system is defined as:

$$\begin{aligned} G(\mathbf{r}, t) &= G_d(\mathbf{r}, t) + G_s(\mathbf{r}, t), \\ \rho G_d(\mathbf{r}, t) &= \frac{1}{N} \left\langle \sum_{i \neq j} \delta(\mathbf{r} + \mathbf{r}_i(0) - \mathbf{r}_j(t)) \right\rangle \\ \rho G_s(\mathbf{r}, t) &= \langle \delta(\mathbf{r} + \mathbf{r}_i(0) - \mathbf{r}_i(t)) \rangle. \end{aligned} \tag{1.1}$$

Here $\langle \dots \rangle$ is the canonical statistical average in the thermodynamic limit. N is the number of particles in the system, $\mathbf{r}_j(t)$ the position of the particle j at time t and ρ the particle density. The function $G_d(\mathbf{r}, t)$ is the distinct part and $G_s(\mathbf{r}, t)$ the self part of the dynamical correlation function.