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Further Properties of an Extremal Set of Uniqueness


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Mathematical analysis of the complete iterative inversion method. I. (English summary)

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In this paper, the authors give an interesting study of the famous complete iterative inversion method (CIIM) for solving the ill-posed inverse problem of recovering the pair potential from the second virial coefficient. More precisely, the potential energy $\varphi(r)$ between pairs of homogeneous gas molecules at distance r is related to the second virial coefficient $B(T)$ by the equation

$$(1) \quad B(T) = 2\pi N \int_0^{+\infty} \left(1 - \exp\left(-\frac{\varphi(r)}{kT}\right) \right) r^2 dr.$$

Here, T is the temperature of the gas, and k and N are the Boltzmann constant and the Avogadro number, respectively.

In this paper, the authors make two interesting contributions concerning the application and the validity of the CIIM for the reconstruction of the potential $\varphi(r)$, given by (1). The first contribution is given by Theorem 3.1 and provides a mathematical framework for examining the claims of the CIIM, by identifying a broad class of potentials for which the improper integrals in the CIIM converge, and the derivatives as well as the potential exist. The proof of this theorem is essentially based on the use of classical results from the theory of Lebesgue integration.

The second contribution, and perhaps the main result of this work, is the construction of a counter-example showing that the CIIM fails to reconstruct the pair potential in the attractive region, even when the second virial coefficient is known and φ_0, φ belong to \mathcal{C}^∞ . Here, φ_0 is the short range repulsive branch of the potential. The counter-example given is based on Theorem 4.1 and provides an alternate expression for the characteristic length of smooth admissible potentials with a short-range repulsive branch and a long-range attractive branch.

Reviewed by *Abderrazek Karoui*

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Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.