

DETERMINING PAIR INTERACTIONS FROM STRUCTURAL DATA: AN INVERSE PROBLEM IN STATISTICAL MECHANICS

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In a grand canonical ensemble of classical particles at equilibrium in continuous space we investigate the functional relationship between a given pair potential that determines the interaction of the particles and the molecular distribution functions. For certain admissible perturbations of the pair potential and sufficiently small activity we rigorously establish Frechet differentiability of this mapping in appropriate function spaces, and we provide explicit formulae for the derivative (integral) operator in the thermodynamical limit.

We utilize this information to study iterative methods for the reconstruction of the pair potential of a given system from measured data such as the equilibrium radial distribution function.