wave functions of all particles involved are mutually disturbed. Therefore, the interaction energy is not pair-additive. Accordingly, we attempted to evaluate the contribution of the non-additivity to the pair correlation function and thermodynamic functions of a fluid in the simplest case of triplet interactions.

The Hamiltonian is as follows:

$$H = \tfrac{1}{2} \sum_{i,j} \psi_{ij} + \frac{1}{3!} \sum_{i,j,k} \psi^{*}_{ijk}$$

where $\psi_{ij}$ is the pair (undisturbed by the presence of other particles) potential, $\psi^{*}_{ijk}$ is the non-additive part (perturbation) of the triple interaction potential. The solution of the problem was achieved in the framework of the BBGKY method and using the functional expansion of the Hamiltonian in non-additive three-particle potentials for diluted solutions both neutral and charged particles.

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## Theoretical Study on Solvation of a Neutral Molecule: $N_2$. Two Different Approaches

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A wide investigation has been performed in view of a theoretical study of the solvation of neutral molecules. $N_2$ as a test molecule and HF, $H_2O$, $NH_3$, $CH_4$ as solvents have been chosen.

In the former approach, the contour maps of interaction energy between $N_2$ and one solvent molecule have been evaluated, with fast semiempirical methods (Extended Hückel and CNDO), and compared with each other, in order to find a reliable but not too expansive calculation method. For $N_2$–$H_2O$ interactions, a map has been computed also *ab initio*. The maps are shown, and qualitative and quantitative differences are discussed.

The latter approach rests on building up clusters with one molecule of $N_2$ surrounded by a number (2 to 8) of solvent molecules and finding the structure of such clusters by energy minimization.

From the reported structures it results that they are determined mainly by steric factors, so that clusters optimized by means of different methods are quite similar.

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## Solvent Extrusion: A Pathway from Solvent Separated Ion Pairs to Tight Ion Pairs

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A simple model of two oppositely charged ions, embedded in a sea of hard sphere solvent dipoles (whose centers are fixed on a lattice) is implemented to study the recombination of ions in solution. The first step is the passage from 'solvent separated' ion pair to 'intimate' or 'tight' ion pair. A preliminary two dimensional calculation (restricted to purely electrostatic terms) of the potential energy surface for such a recombination reveals two minima, as required by the experimental observations of Winstein and others.

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## I.R. Experimental Studies of Dynamical Aspects of Water Structure: Effects of H–D Substitution and of Small Solutes

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Results on i.r. absorption spectra of $H_2O$, $D_2O$ and electrolytic solutions and their thermal modifications are presented. From the data, some parameters can be obtained which are suitable for a description of dynamical aspects of water structure. Solute induced changes of these parameters provide a quantitative, although phenomenologic description of the water–solute interaction.