Constructing high-dimensional neural network potentials (NNPs) to describe the solvation of protonated water clusters by superfluid helium

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Superfluid helium is a highly fascinating liquid where quantum effects are pervasive. It features many interesting properties such as zero viscosity, quantized vortex lines and vanishing friction that all can be explained by the Bose-Einstein-like condensation of the bosonic ^{4}He particles below the transition temperature of 2.17 K in the bulk phase. Helium also forms nanodroplets that feature superfluid behavior and can be used to solvate guest molecules. The gentle, ultracold environment easily picks up desired species and adjusts itself rapidly to the solute impurity. This allows one to examine the solute with e.g. infrared spectroscopy as performed in HENDI experiments [1]. However, at temperatures on the order of one Kelvin, nuclear quantum effects govern the properties and can not be neglected, if quantitative and even qualitative conclusions are of interest.

Here quantum simulation techniques employing path integrals can be used to treat the quantum nature of the nuclei exactly [2]. Only recently these techniques were extented to treat reactive solute species by coupling bosonic PIMC simulations of helium to *ab initio* PIMD simulations of the solute [3, 4]. This allows one for the first time, to study interesting systems such as microsolvated HCl/water clusters [4] or protonated water clusters including their full reactivity solvated by superfluid helium. These simulations, however, require very accurate interaction potentials to link the two regimes [5, 6].

Here we show how artificial neural networks [7, 8] can be applied to develop interaction potentials for the solvation of protonated water clusters by superfluid helium. The intrinsic nature of neural networks does not only allow to represent the reference coupled cluster energies with very high accuracy, but also provides the opportunity to easily identify missing points in configuration space and thus to keep the number of reference calculations to a minimum. This offers the opportunity for an unbiased and elegant access to solute-He interaction energies.

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