

Better Variational Density Matrices

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Restricted path integral Monte Carlo at an inverse temperature β needs a trial nodal surface for all inverse temperatures between 0 and $\beta/2$.

These nodal surfaces typically come from a series of trial thermal density matrices. While there has been decades of work writing down classes of variational wave-functions, there has been significantly less experience in generating variational density matrices.

In this talk, we demonstrate an approach for constructively generating the required matrix elements from a set of variational density matrices using only a class of variational wave-function as input. The resulting variational density matrices are not compactly representable.