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Solving Hydrogen Systems in a Gaussian-Sinc Mixed Basis[1] JONATHAN JERKE, C.J. TYMCZAK, YOUNG LEE, Texas Southern University — We introduce a Gaussian-Sinc electronic structure mixed basis calculation scheme. We solve the Schrödinger's wave equation with a uniform magnetic field for a single electron in Hydrogen Systems in three dimensions. The scheme is inherently unbiased since most of the field is digital under the Sinc basis and the Gaussian are only meant to capture the cusp of atomic states. The entire scheme is translational invariant and the potentials are calculated properly and are necessarily off diagonal. In the absence of magnetic fields the scheme is variational bound. We generally find under arbitrary configurations of protons that we can achieve four significant digits after the decimal.

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