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Exact quantum dynamics calculations using a symmetrized Gaussian basis THOMAS HALVERSON, BILL POIRIER, Texas Tech University — In a series of earlier articles, a new method was introduced for performing exact quantum dynamics calculations. The method uses a "weylet" basis set (orthogonalized Weyl-Heisenberg wavelets), combined with phase space truncation, to defeat the exponential scaling of CPU effort with system dimensionality that has long plagued such calculations. Here, we present results obtained using a basis of momentum-symmetrized Gaussians. Despite being non-orthogonal, symmetrized Gaussians do exhibit collectively locality, allowing for effective phase space truncation. Application to both isotropic uncoupled harmonic oscillators and coupled anharmonic oscillators are discussed. Results for uncoupled systems up to 15 dimensions are compared with previous weylet calculations and found to be essentially just as efficient. A "universal" code has been written, which is dimensionally independent, and which also exploits massively parallel algorithms. Using the new codes, calculations up to 27 dimensions have been achieved. Lastly, symmetrized Gaussian calculations for coupled anharmonic oscillators are analyzed, and compared to first order degenerate perturbation theory.

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