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Quantum Energy Level Calculations of Molecules Using Weyl-Heisenberg Wavelets and Classical Phase Space RICHARD LOMBARDINI, BILL POIRIER, Texas Tech University — New methods are examined regarding the quantum-mechanical calculations of the nuclear dynamics of polyatomic systems. The first of these, introduced earlier in a series of articles, involves compact orthogonal wavelets as the basis set which is subsequently truncated using the guidance of a classical phase space picture of the system. This poster presents the first application of this technique to real molecular systems, more specifically, the calculation of the rovibrational energy levels of the neon dimer. The second technique involves further optimizations of the latter method using phase space region operators which improve the efficiency K/N of the basis set where N represents the number of basis functions needed to calculate K eigenvalues at a desired accuracy. Finally, for systems that produce sparse Hamiltonian matrices in the wavelet basis, a new parallel algorithm for matrix diagonalization is introduced which uses the subspace iteration method.

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