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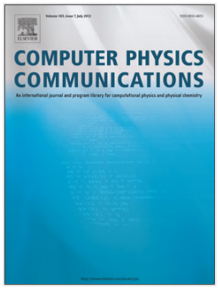

Optimized spatial matrix representations of quantum Hamiltonians

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Optimized spatial matrix representations of quantum Hamiltonians

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We examine the accuracy of several approaches to represent the quantum mechanical Schrödinger, Klein-Gordon and Dirac Hamilton operators by optimized spatial matrices. Two of the approaches are based on periodic and reflecting boundaries and have an error scaling with the number of spatial grid points that is significantly better than the ones based on the usual approaches where the momentum operator is approximated by finite-difference schemes. These N×N matrices are optimum in the sense that their eigenvalues and eigenvectors are exact representations on the spatial grid for the continous solutions of the corresponding force-free Hamiltonian. As an example, we apply these techniques to compute the vacuum's polarization charge density from the Dirac and Foldy-Wouthuysen theory.