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Using the Feynman-Kac Path Integral Method in Finding Excited States of Helium. NAIL G. FAZLEEY, JAMES M. REJCEK, JOHN L. FRY, Department of Physics, University of Texas, Arlington — Group theory considerations and properties of a continuous path are used to define a failure tree procedure for finding eigenvalues of the Schrodinger equation using stochastic methods. The procedure is used to calculate the lowest excited state eigenvalues of eigenfunctions possessing anti-symmetric nodal regions in configuration space using the Feynman-Kac path integral method. Within this method the solution of the imaginary time Schrodinger equation is approximated by random walk simulations on a discrete grid constrained only by symmetry considerations of the Hamiltonian. The required symmetry constraints on random walk simulations are associated with a given irreducible representation and are found by identifying the eigenvalues for the irreducible representation corresponding to symmetric or antisymmetric eigenfunctions for each group operator. The method provides exact eigenvalues of excited states in the limit of infinitesimal step size and infinite time. The numerical method is applied to compute the eigenvalues of the lowest excited states of the helium atom that transform according to specific irreducible representations associated with explicitly determined symmetry groups.

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