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Computational Approaches for Solving the Second Quantized Schroedinger Equation Using Non-Orthogonal Basis Sets<sup>1</sup> ANDREW GIUSTINI, BRIAN GRANGER, Santa Clara University — The second quantized approach to quantum mechanics provides an efficient method of incorporating the exchange symmetry of the many body wavefunction. The usual formulation, however, requires that field operators be expanded in an orthogonal basis. Using the theory developed by Artacho and del Bosch (PRA 43, 5770 (1991)) we have developed a numerical method for solving the second quantized Schroedinger equation using nonorthogonal basis sets, such as B-splines and finite elements. We present an implementation of this approach in the Python programming language and discuss preliminary results of the efficiency and performance of the method.

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