Energies of the Li Atom Using Undergraduate Quantum Mechanics*

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An article usually includes an abstract, a concise summary of the work covered at length in the main body of the article.

The Li atom, with 3 electrons, is the lightest and simplest atom whose energy levels are radically constrained by the Pauli Exclusion Principle. For the 2 electron He atom,... Thus the energy levels of 2-electron atoms can be calculated in a straightforward manner using a simple product basis [1].

In the following I will present a calculation of the low-lying energy levels of the Li atom using a variationally chosen basis of Slater determinants.

I. THE PAULI EXCLUSION PRINCIPLE

A naive version of the Pauli principle, namely that the three electrons must have unique quantum numbers, erroneously leads to the conclusion that the 6 permutations of the state $|1sd; 1su; 2su\rangle$ would be all be valid quantum states... The solution to the Li Hamiltonian in such a basis results in one solution that is completely symmetric upon exchange of any pair of electrons, one totally anti-symmetric solution, and four solutions of mixed exchange symmetry.

The full Pauli principle requires that only the totally anti-symmetric solution is valid. This solution is compactly represented by the Slater determinant

$$|||ad; bu; cd||\rangle = \frac{1}{\sqrt{6}}(1 + \mathcal{L} + \mathcal{R})(1 - P_{23})|n_1sd; n_2su; n_3su\rangle \tag{1}$$

Here P_{ij} is the exchange operator for electrons i and j, $\mathcal{L} = P_{12}P_{23}$ is a cyclic left-rotation of the spin orbitals, *i.e.* $\mathcal{L}|a; b; c\rangle = |b; c; a\rangle$, and $\mathcal{R} = \mathcal{L}^\dagger$ is a cyclic right-rotation.

II. MATRIX ELEMENTS OF SLATER DETERMINANTS

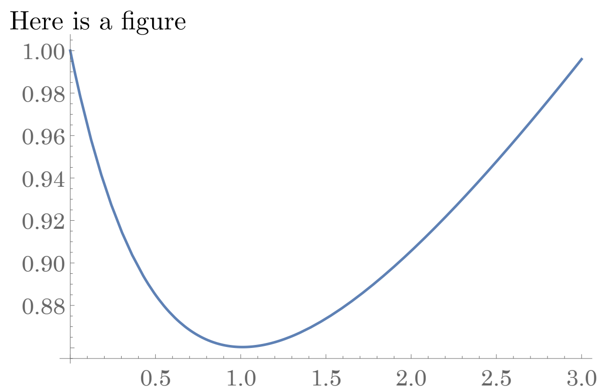

FIG. 1. Caption

III. VARIATIONAL ANALYSIS OF THE LI $1s^22s$ STATE.

IV. REPRESENTATION OF THE LI HAMILTONIAN IN A BASIS OF SLATER DETERMINANTS

V. QUANTUM DEFECT ANALYSIS OF LI

VI. CONCLUSIONS

[1] Robert Massé and Thad G. Walker, "Accurate energies of the He atom with undergraduate quantum mechanics", Am. J. Phys. 83, 730 (2015).

* A footnote to the article title