

Energies of the Li Atom Using Undergraduate Quantum Mechanics

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This paper demonstrates the calculation of the low-lying energies levels of the Li atom through the introductory quantum mechanics[1] and software such as MATHEMATICA[7]. Given that the Li atom has 3 electron, an appropriate wavefunction can be constructed based on the Pauli exclusion principle. The matrix elements of the Hamiltonian of the Li atom will be determined from the components of the Slater determinant. Besides, the variational analysis of the Li $1s^2 2s$ states helps restrict the limit of the ground state energy. The Hamiltonian of the Li atom can then be represented through the low-lying energy states. The result of the ground state energy can be improved to 0.7599% error by comparing with the experimental results in the Energy Level Database of the National Standards of Science and Technology (NIST).[2] Finally, a quantum defect analysis helps study on the excited states energy.

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, the matrix diagonalization can be used to evaluate the energies of $1s2s$ singlet and triplet states. Thus the energy levels of 2-electron atoms can be calculated in a straightforward manner using a simple product basis [5].

The Hamiltonian of the Li atom [1] can be written as

$$\hat{H} = \hat{H}^{++}(1) + \hat{H}^{++}(2) + \hat{H}^{++}(3) + \frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \quad (1)$$

To begin, we can obtain an approximate form of the wavefunction for the Li atom by considering the Hamiltonian of the Li ions. We can begin with a wavefunction in the form of

$$P_{n,l}(r) = \sqrt{zz} P_{n,l}(zz \ r) \quad (2)$$

Here $P_{n,l}(r)$ is the radial wavefunction for the Li atom and zz is a variational parameter that can be alternated when the particular energy states are calculated.

It needs to be noted that in this paper all energy terms are written in the atomic units. Specifically, 1 Hartrees equal to 2 Rydbergs and also equal to 27.2114 eV.[3]

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; however, not all of the permutations are allowed. 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, which is A very common method to ensure that multi-electron wavefunctions are antisymmetric on exchange is to expand the wavefunctions in a series of Slater determinants, each of which is constructed to be anti-symmetric and such an expansion guarantee that our wavefunctions obey the Pauli exclusion principle. The Slater determinant $||ad; bu; cd||$, [4] in general, can be calculated by

$$\det \begin{vmatrix} \phi[a]d(1) & \phi[b]u(1) & \phi[c]u(1) \\ \phi[a]d(2) & \phi[b]u(2) & \phi[c]u(2) \\ \phi[a]d(3) & \phi[b]u(3) & \phi[c]u(3) \end{vmatrix}$$

Here ϕ denotes different orbital functions. Since the spin parts are different in the first 2 columns, $\phi[a]$ and $\phi[b]$ (or $\phi[a]$ and $\phi[c]$) can be the same orbital function.

It can also be written as

$$||ad; bu; cd|| = \frac{1}{\sqrt{6}}(1 + \mathcal{L} + \mathcal{R})(1 - \hat{P}_{23})|n_1sd; n_2su; n_3su\rangle \quad (3)$$

Here \hat{P}_{ij} is the exchange operator for electrons i and j , $\mathcal{L} = \hat{P}_{12}\hat{P}_{23}$ 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. With the notations defined, we are able to prove that if $|\psi\rangle$ is an eigenvector of \hat{P}_{12} and \hat{P}_{23} with eigenvalue -1, it is also an eigenvector of \hat{P}_{13} with eigenvalue -1. Let $\hat{Q} = \hat{P}_{23}\hat{P}_{12}$. With $\hat{P}_{12} = -|\psi\rangle$ and $\hat{P}_{23} = -|\psi\rangle$, it follows that

$$\begin{aligned} \hat{Q}|\psi\rangle &= \\ \hat{P}_{23}\hat{P}_{12}|\psi\rangle &= \hat{P}_{23}(\hat{P}_{12}|\psi\rangle) = \\ \hat{P}_{23}(-|\psi\rangle) &= -(\hat{P}_{23}|\psi\rangle) = -(-|\psi\rangle) = |\psi\rangle \end{aligned} \quad (4)$$

The above proof shows that given the exchange operators \hat{P}_{12} , \hat{P}_{13} and \hat{P}_{23} which commute with the Hamiltonian, all of their eigenvectors are also valid to be the

eigenvectors of the Hamiltonian without violating the Pauli exclusion principle, with eigenvalues -1 for each. And with such a verification, the method to calculate the matrix elements for the Slater determinant for the Li Hamiltonian can be constructed.

II. MATRIX ELEMENTS OF SLATER DETERMINANTS

From the Eq. (3), we are able to derive a general method to calculate the matrix elements for Slater determinant in general. Recall that $\mathcal{L} = \hat{P}_{12}\hat{P}_{23}$ is a cyclic left-rotation of the spin orbitals and $\mathcal{R} = \mathcal{L}^\dagger$ is a cyclic right-rotation; we can define $||ad; bu; cd|| = \frac{1}{\sqrt{6}}(1 + \mathcal{L} + \mathcal{R})(1 - \hat{P}_{23})|n_1sd; n_2su; n_3su\rangle = \frac{1}{\sqrt{2}}\mathcal{A}|ad, bu, cd\rangle$, where the operator \mathcal{A} is considered as an "antisymmetrizer" as it converts a product state into a Slater determinant. We can further show that

$$\begin{aligned} & \frac{1}{6}\langle ad, bu, cd | \mathcal{A}^\dagger \hat{H} \mathcal{A} | ad, bu, cd \rangle = \\ & \frac{1}{2}\langle ad, bu, cd | (1 - P_{23})^2 \hat{H} | ad, bu, cu \rangle = \\ & \langle a, b, c | \hat{H} | A, B, C \rangle - \langle a, b, c | \hat{H} | A, C, B \rangle \end{aligned} \quad (5)$$

Here both $|a, b, c\rangle$ and $|A, B, C\rangle$ are the spin-orbitals of Li Hamiltonian. Therefore, the matrix elements of the Slater determinant for the 3-spin system can be constructed from the spatial orbitals. And the following integrals are obeyed $\langle n_1n_2n_3 | \hat{H} | n_4n_5n_6 \rangle = \int d^3r_1 d^3r_2 d^3r_3 P_{n_1l_1}(r_1) P_{n_2l_2}(r_2) P_{n_3l_3}(r_3) \frac{1}{r_{>}} P_{n_4l_4}(r_4) P_{n_5l_5}(r_5) P_{n_6l_6}(r_6)$.

In particular, if we take the Li atom as an example, the calculation of the matrix elements of its Slater determinant can be realized by MATHEMATICA codes (Ref. 7) shown in Fig. 1. The first line gives the radial eigenfunction which is also used by the Li ions, where zz represents a variational parameter which can be determined by variational analysis for the Li atom; the variational analysis of the Li $1s^22s$ is shown later in the part III. The lines in the second box indicates the unperturbed Hamiltonian and the potential energy terms for the 3-spin system from the spatial orbits. The line in the third box gives a total Hamiltonian. By applying this Hamiltonian to $1s^22s$ and $1s^23s$ states, we obtain the first 2×2 matrix elements for the Slater determinant

$$\begin{pmatrix} -7.05658 & -0.26949 \\ -0.26949 & -7.05438 \end{pmatrix}$$

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

A variational calculation of the ground state energy of Li can be realized through the MATHEMATICA codes

$P_{n_{i-1}, z, z_{zz}}[r_{-}] := \sqrt{zz} P_{n_i}[zz r]$
$H11a[\{n1_, n2_, n3_, \{n4_, n5_, n6_, zz_, Z_] :=$ $\delta_{n3, n6} \delta_{n2, n5} \text{NIntegrate}[P_{n1, 0, zz}[r] \left(\frac{-1}{2} \partial_{r, r} P_{n4, 0, zz}[r] - \frac{Z}{r} P_{n4, 0, zz}[r] \right), \{r, 0, \infty\}];$ $H11b[\{n1_, n2_, n3_, \{n4_, n5_, n6_, zz_, Z_] :=$ $\delta_{n3, n6} \delta_{n1, n4} \text{NIntegrate}[P_{n2, 0, zz}[r] \left(\frac{-1}{2} \partial_{r, r} P_{n5, 0, zz}[r] - \frac{Z}{r} P_{n5, 0, zz}[r] \right), \{r, 0, \infty\}];$ $H11c[\{n1_, n2_, n3_, \{n4_, n5_, n6_, zz_, Z_] :=$ $\delta_{n1, n4} \delta_{n2, n5} \text{NIntegrate}[P_{n3, 0, zz}[r] \left(\frac{-1}{2} \partial_{r, r} P_{n6, 0, zz}[r] - \frac{Z}{r} P_{n6, 0, zz}[r] \right), \{r, 0, \infty\}];$ $V12[\{n1_, n2_, n3_, \{n4_, n5_, n6_, zz_, Z_] := \delta_{n3, n6} \text{NIntegrate}[$ $P_{n1, 0, zz}[r1] P_{n2, 0, zz}[r2] \text{Min}[\frac{1}{r2}, \frac{1}{r1}] P_{n4, 0, zz}[r1] P_{n5, 0, zz}[r2], \{r2, 0, \infty\}, \{r1, 0, \infty\}];$ $V13[\{n1_, n2_, n3_, \{n4_, n5_, n6_, zz_, Z_] := \delta_{n2, n5} \text{NIntegrate}[$ $P_{n1, 0, zz}[r1] P_{n3, 0, zz}[r3] \text{Min}[\frac{1}{r3}, \frac{1}{r1}] P_{n4, 0, zz}[r1] P_{n6, 0, zz}[r3], \{r3, 0, \infty\}, \{r1, 0, \infty\}];$ $V23[\{n1_, n2_, n3_, \{n4_, n5_, n6_, zz_, Z_] := \delta_{n1, n4} \text{NIntegrate}[$ $P_{n2, 0, zz}[r2] P_{n3, 0, zz}[r3] \text{Min}[\frac{1}{r2}, \frac{1}{r3}] P_{n5, 0, zz}[r2] P_{n6, 0, zz}[r3], \{r2, 0, \infty\}, \{r3, 0, \infty\}];$
$H11d[\{n1_, n2_, n3_, \{n4_, n5_, n6_, zz_, Z_] :=$ $H11d[\{n1, n2, n3_, \{n4, n5, n6_, zz, Z\}] =$ $(H11a[\{n1, n2, n3_, \{n4, n5, n6_, zz, Z\}] + H11b[\{n1, n2, n3_, \{n4, n5, n6_, zz, Z\}] +$ $H11c[\{n1, n2, n3_, \{n4, n5, n6_, zz, Z\}] + V12[\{n1, n2, n3_, \{n4, n5, n6_, zz_, Z\}] +$ $V13[\{n1, n2, n3_, \{n4, n5, n6_, zz_, Z\}] + V23[\{n1, n2, n3_, \{n4, n5, n6_, zz_, Z\}]) -$ $(H11a[\{n1, n2, n3_, \{n4, n6, n5_, zz, Z\}] + H11b[\{n1, n2, n3_, \{n4, n6, n5_, zz, Z\}] +$ $H11c[\{n1, n2, n3_, \{n4, n6, n5_, zz, Z\}] + V12[\{n1, n2, n3_, \{n4, n6, n5_, zz_, Z\}] +$ $V13[\{n1, n2, n3_, \{n4, n6, n5_, zz_, Z\}] + V23[\{n1, n2, n3_, \{n4, n6, n5_, zz_, Z\}]);$
$st11b = \text{Table}[\{1, 1, i\}, \{i, 2, 3\}]$ $\{\{1, 1, 2\}, \{1, 1, 3\}\}$
$\text{SlaterDet} =$ $\text{Quiet}[\text{Table}[\text{H11d}[\text{st11b}[\text{i}], \text{st11b}[\text{j}], 3, 3], \{i, \text{Length}[\text{st11b}]\}, \{j, \text{Length}[\text{st11b}]\}];$ $\text{SlaterDet} // \text{MatrixForm}$ $\begin{pmatrix} -7.05658 & -0.26949 \\ -0.26949 & -7.05438 \end{pmatrix}$

FIG. 1. The calculation in MATHEMATICA to obtain the Slater determinant matrix elements for the Li Hamiltonian. An executable and annotated version is available electronically (Ref. 5)

shown in the previous section. According to the Pauli exclusion principle, it is the most possible to write the lowest energy wavefunction as $\langle r_1, r_2, r_3 | 1s; 1s; 2s \rangle = P_1^z(r_1) P_2^z(r_2) P_3^z(r_3)$, where z is an adjustable parameter.

In practice, detailed calculations of the energy levels of multi-electron systems can be carried out by using the variational method. Townsend gives the process by taking the He atom as an example.[1] The same approach can be applied to the Li atom, and a part of the calculations can also be done by MATHEMATICA codes.

The steps of the calculation follow the convention of the variational method.[1] First, an expression for the Li $1s^22s$ state with respect to the variational parameter zz can be found by applying the method to calculation the matrix elements to the Li $1s^22s$ state. By starting from the assumption that $E_n \leq E_0$, with E_0 the exact ground-state energy. Thus for any state $|\psi\rangle$,

$$E_0 \leq \langle \psi | \hat{H} | \psi \rangle = \langle E \rangle \quad (6)$$

With choosing a trial state with the variational parameters, $P_{n,l}(r) = \sqrt{zz} P_{n,l}(zz)$, $\langle \psi | \hat{H} | \psi \rangle$ can be then calculated through the integral $\int d^3r P_{n,l}(r) \hat{H} P_{n,l}(r)$.

Second, the value of zz that minimizes the energy can

be calculated by letting the first derivative of the expression equal to 0, i.e. $\frac{\partial \langle E_{1s,1s,2s} \rangle}{\partial zz} = 0$, regarding to the energy states we are interested in. Fig.2 shows a MATHEMATICA calculation based on the coding we obtained in Fig.1; $zz = 2.54542$ is then obtained.

```
e0Li = H12d[{1, 1, 2}, {1, 1, 2}, zz, 3]
e0Li // N

5965 zz +  $\frac{9}{5832} (-6 + zz) zz$ 

1.02281 zz + 1.125 (-6. + zz) zz

Solve[ $\frac{\partial}{\partial zz} \left( \frac{5965 zz}{5832} + \frac{9}{8} (-6 + zz) zz \right) = 0, zz] // N$ 
{{zz -> 2.54542}}

Eval12 =  $\frac{5965 \times 2.54541990550221}{5832} + \frac{9}{8} (-6 + 2.54541990550221) 2.54541990550221$ 
-7.28906
```

FIG. 2. The calculation based on the variational principle, where the variable H12d is just the H11d given in Fig. 1. (Ref. 5)

Third, after plugging in the experimental values for Li atom and writing result in the atomic units, it turns out that the upper limit on the ground state energy of the Li atom approximately equals to -7.28906 Hartrees. The last line of Fig.2 shows the step to get this value. It has a 2.52637% error comparing to the NIST value.[2] The precision can be enhanced by adding more orbitals to the energy calculation, which is then shown in the following section about the representation of the Li Hamiltonian in a basis of Slater determinants.

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

Since we find the upper limit of the lowest energy for Li atom through the variational analysis which means we have a particular value for the variational parameter $zz = 2.54542$, we are able to construct the representation of the Li Hamiltonian in a basis of Slater determinants now. As shown in the section II, the matrix elements of Slater determinant for the Li atom can be calculated through MATHEMATICA codes. By calculating the matrix element in $1s^2 2s$ only, we obtained the ground state energy which equals to -7.2896 Hartrees and has an error around 2.52637%.

By adding a few more $1s2sns$ and even $2s1sns$ orbitals, we can numerically calculate the integrals more precisely, as shown in Fig. 3. It follows that the matrix elements of the Li Hamiltonian with respect to these states can be obtained, as the coding shown in Fig. 4. The results of the first few entries are

$$\begin{pmatrix} -7.26594 & -0.181188 & 0.0995244 & -0.0664833 & 0.0488127 \\ -0.181188 & -7.19778 & -0.114781 & 0.0690339 & -0.0485813 \\ 0.0995244 & -0.114781 & -7.19724 & -0.0762411 & 0.0484261 \\ -0.0664833 & 0.0690339 & -0.0762411 & -7.20213 & -0.053833 \\ 0.0488127 & -0.0485813 & 0.0484261 & -0.0538337 & -7.20646 \end{pmatrix}$$

```
st14 = {{1, 1, 2}, {1, 1, 3}, {1, 1, 4}, {1, 1, 5}, {1, 1, 6}, {1, 1, 7}, {1, 1, 8},
{1, 1, 9}, {1, 1, 10}, {1, 1, 11}, {1, 1, 12}, {1, 1, 13}, {1, 1, 14}, {1, 1, 15},
{1, 1, 16}, {2, 1, 2}, {2, 1, 3}, {3, 1, 2}, {1, 2, 3}, {2, 1, 4}, {4, 1, 2},
{1, 2, 4}, {2, 1, 5}, {5, 1, 2}, {1, 2, 5}, {2, 1, 6}, {6, 1, 2}, {1, 2, 6},
{2, 1, 7}, {7, 1, 2}, {1, 2, 7}, {3, 1, 4}, {4, 1, 3}, {1, 3, 4}}

(* If it is taking too long to run use this basis instead:
st14 = {{1, 1, 2}, {1, 1, 3}, {1, 1, 4}, {1, 1, 5}, {1, 1, 6}, {1, 1, 7}, {1, 1, 8}, {1, 1, 9},
{1, 1, 10}, {1, 1, 11}, {1, 1, 12}, {1, 1, 13}, {1, 1, 14}, {1, 1, 15}, {1, 1, 16},
{2, 1, 2}, {2, 1, 3}, {3, 1, 2}, {1, 2, 3}, {2, 1, 4}, {4, 1, 2}, {1, 2, 4}}
*)

(* Need pairs of combinations like in the He Perturbation Theory notebook...
st14 = {{1, 1, 2}, {1, 1, 3}, {1, 1, 4}, {1, 1, 5}, {1, 1, 6},
{1, 1, 7}, {1, 1, 8}, {1, 1, 9}, {1, 1, 10}, {1, 1, 11}, {1, 1, 12}, {1, 1, 13},
{1, 1, 14}, {1, 1, 15}, {1, 1, 16}, {2, 1, 2}, {2, 1, 3}, {2, 1, 4}, {2, 1, 5},
{2, 1, 6}, {2, 1, 7}, {2, 1, 8}, {3, 1, 4}, {3, 1, 5}, {4, 1, 5}, {5, 1, 6}}*)

{{1, 1, 2}, {1, 1, 3}, {1, 1, 4}, {1, 1, 5}, {1, 1, 6}, {1, 1, 7}, {1, 1, 8},
{1, 1, 9}, {1, 1, 10}, {1, 1, 11}, {1, 1, 12}, {1, 1, 13}, {1, 1, 14},
{1, 1, 15}, {1, 1, 16}, {2, 1, 2}, {2, 1, 3}, {3, 1, 2}, {1, 2, 3}, {2, 1, 4},
{4, 1, 2}, {1, 2, 4}, {2, 1, 5}, {5, 1, 2}, {1, 2, 5}, {2, 1, 6}, {6, 1, 2},
{1, 2, 6}, {2, 1, 7}, {7, 1, 2}, {1, 2, 7}, {3, 1, 4}, {4, 1, 3}, {1, 3, 4}}
```

FIG. 3. The $1s2sns$ and $2s1sns$ orbitals we choose to add to get more precise matrix elements of the Li atom. (Ref. 5)

```
H14 = Quiet[Table[H11d[st14[[i]], st14[[j]], 2.688776938, 3],
{1, Length[st14]}, {j, Length[st14]}]];

H14 // MatrixForm
```

FIG. 4. The MATHEMATICA codes to calculate the matrix elements of the Li Hamiltonian, where H14 is just the H11d in Fig.1. (Ref. 5)

The ground state energy is then calculated and it equals to -7.42115 Hartrees, with an improved 0.759904% error comparing the experimental results from the NIST data.[2]

V. QUANTUM DEFECT ANALYSIS OF LI

After verifying the precision of the energies of the $1s^2 2s$ state, we try to explore a qualitative behavior of the energies in the various excited states. We can begin with the semi-empirical formula of the energy levels for most atoms, and particularly for the alkali-metal atoms

$$E_n = E_\infty - \frac{1}{2(n-\delta)^2} \quad (9)$$

Here δ is called the "quantum defect" and E_∞ is the total energy of the atom when the most weakly bound electron is removed. For Li, E_∞ would be the ground-state energy of Li^+ and $n = 2, 3, 4, \dots$ is the principle

number of the outer electron. Subtracting the Li ground state energy E_2 from both sides of the equation gives

$$E_n - E_2 = IP - \frac{1}{2(n-\delta)^2} \quad (8)$$

Here $IP = E_\infty - E_2$, which is the ionization potential, and also the difference between the ground state energies of Li^+ and Li , and is therefore the amount of energy required to remove one electron from the Li atom.

First we compare the $1s^2 3s - 1s^2 2s$ energy difference with experiment. By using the Li Hamiltonian matrix provided in the previous section, we are able to obtain the eigenvalues, which are also the energy values for the $1s^2 3s$ and $1s^2 2s$ states. The energy difference based on the calculation is 0.121161 Hartrees, and the error is around 2.25787% after we compared with the data in NIST.[2]

After examining the NIST tables,[2] we plot the Li energies versus n which is shown by Fig. 5 and deduce the value of the quantum defect δ , which equals to 0.401185 Hartrees. The ionization potential is found to be 0.196953 Hartrees. We also find and plot the fitting function $n^* = \frac{1}{[2(E_\infty - E_n)]^2}$ in MATHEMATICA, which is in Fig. 6.

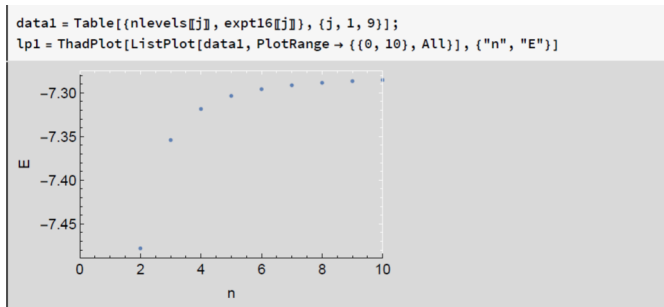
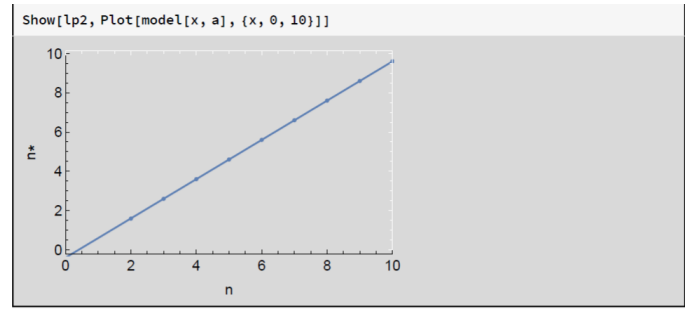


FIG. 5. The Li energies versus the principal quantum number n based on the NIST data (Ref. 5).



Furthermore, we plot the energies of Li atom based on our calculations and construct curve which fits the data. Then we compare our computed results with the experimental results from the NIST. The calculated quantum defect number δ equals to 0.408504, which has 1.82409% error comparing with the NIST data. The calculated ionization potential is 0.196953%, which is 0.599975% different from the experimental results.[2]

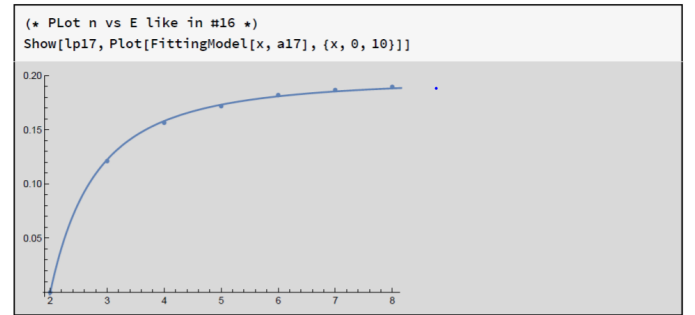


FIG. 7. A plot of the fit function of the calculated energies of Li atom(Ref. 5).

VI. CONCLUSIONS

The Li atom is an example of a realistic system that can be quantitatively understood using the methods learned in an introductory quantum mechanics course. By calculating the matrix elements based on Slater determinant, we are able to obtain the eigenvalues for the matrix, which represent for the low-lying energies. Moreover, the quantum defect analysis helps us study the excited states. With the MATHEMATICA codes, we improve the results of the ground state energies to 0.7599% error and to 1.8241% for the quantum defect number.

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