First Principle 2017-Fall Homework 3 Solution

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1. The following shows the result of Al and Na:

- Al

(1) a_0 using volume optimization:

$$a_0 = 4.05000$$

(2) Variation with different a_0:

a_0	E
3.90	-14.541085
3.95	-14.665726
4.00	-14.735369
4.05	-14.757538
4.10	-14.738699
4.15	-14.684395
4.20	-14.599834

(3) the following figure shows the energy (E) v.s. V :

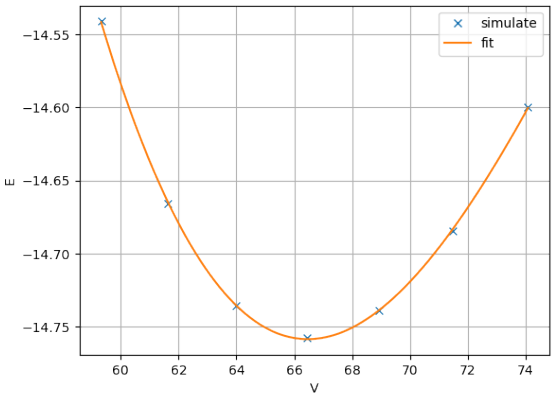

FIG. 1. Al-fcc E-V

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By using third order polyfit, and with the following formula, we can get the bulk-modulus B and the minimum a_0:

$$B = V\frac{\partial^2}{\partial V^2}E$$
$$V = a_0^3$$

$$a_0 = 4.050723 \ \ \mathring{A}$$
$$B = 74.608739 \ \ GPar$$

(4)

- Si