# Helium Binding Energy in Helium-Vacancy Clusters

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# Formation Energy Data

Formation energy files only for $V = 1, 2, 6, 14, 18, 19, 27, 32, 44$.

Example:

```
#V #He Ef
1  0   3.82644
1  1   5.14166
1  2   8.20919
1  3   11.5304
```

Binding energy formula:

$$E_b(He_X, V_Y) = E_f(He_{X-1}, V_Y) + E_f(He_1, 0) - E_f(He_X, V_Y)$$

# Binding Energy Data

Binding energy file for V up to 50.

Example:

| #He | #V | #I | E_He | E_V | E_I | E_t | E_mig | D_0 |
|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | Infinity | Infinity | Infinity | 8.270E+0 | 1.300E-1 | 2.950E+10 |
| 2 | 0 | 0 | 8.640E-1 | Infinity | Infinity | 6.120E+0 | 2.000E-1 | 3.240E+10 |
| 3 | 0 | 0 | 1.210E+0 | Infinity | Infinity | 4.440E+0 | 2.500E-1 | 2.260E+10 |
| 4 | 0 | 0 | 1.560E+0 | Infinity | Infinity | 3.180E+0 | 2.000E-1 | 1.680E+10 |

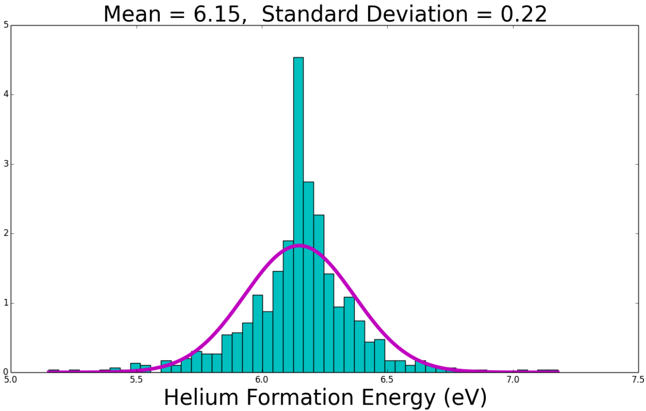
Here we are only interested in the helium binding energy.

# Helium Formation Energy

$E_f(He_1, 0)$ is missing from our data:

- can be computed with the formula and the data we have.

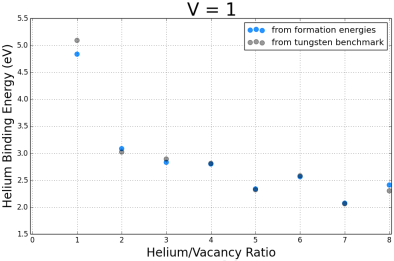
$$E_b(He_X, V_Y) = E_f(He_{X-1}, V_Y) + E_f(He_1, 0) - E_f(He_X, V_Y)$$

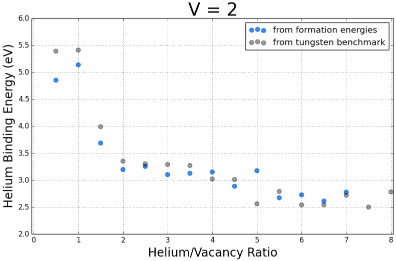


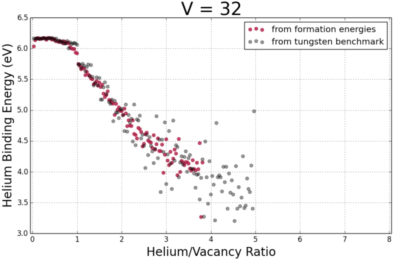

$E_f(He_1, 0) = 6.15$ eV will be used now.

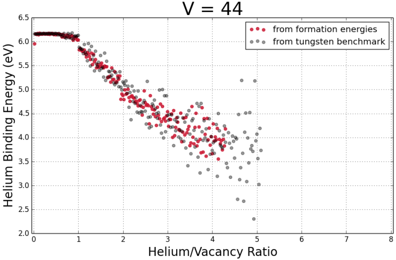
# Rebuilding Binding Energies

Using only the given formation energies, one can now compute new binding energies:

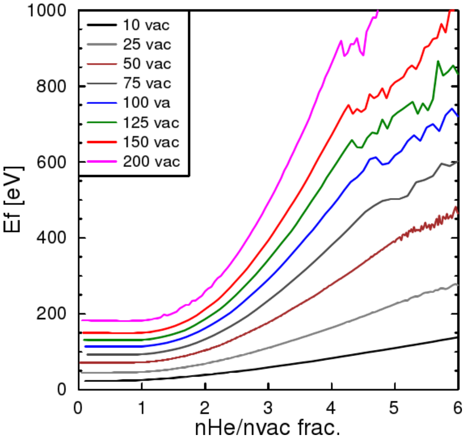


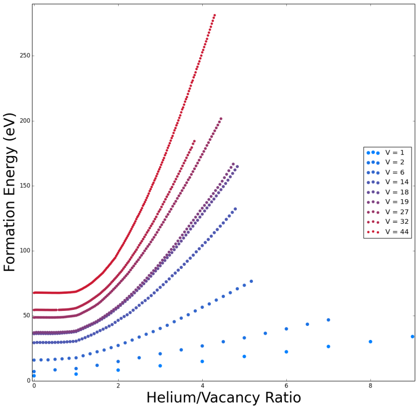



# Formation Energy Data

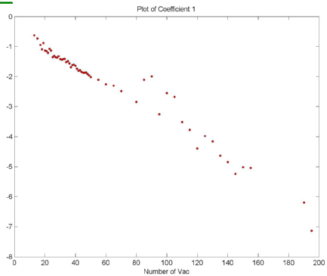


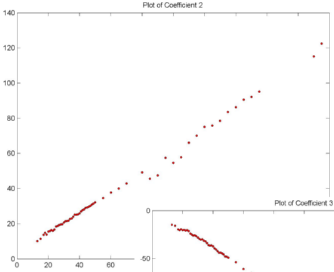



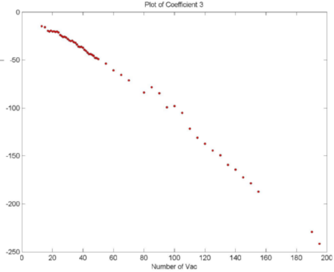
# From Juslin's Presentation

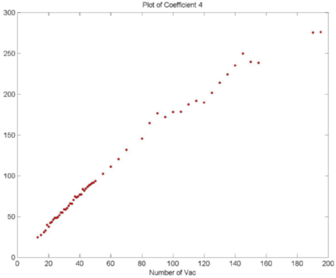
## *Polynomial fits*

- Formation energies:
  - $E^f = c_1 + c_2 x + c_3 x^2 + c_4 x^3$; $x = n_{He}/n_{vac}$



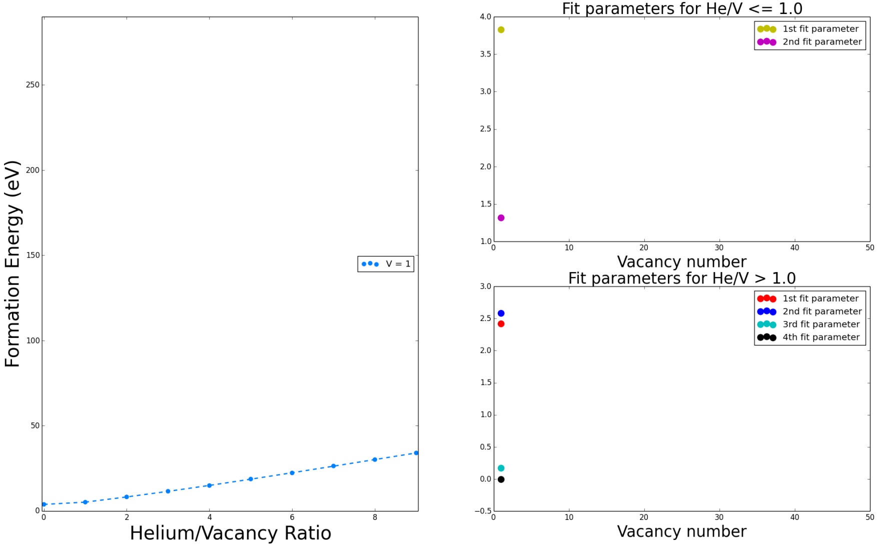
# Fitting Methods

- Piecewise 2D polynomials fit with a separation arround $He/V = 1$ where the order of the lower and higher parts can be chosen independently

- Two-step 1D polynomials fits:
  - Use only polynomials
  - Piecewise fit first on the formation energies as a function of $He/V$ with a separation arround $He/V = 1$
  - Fit then the parameters of those fits as a function of V
  - Each fit orders (4 in total) and the separation can be changed

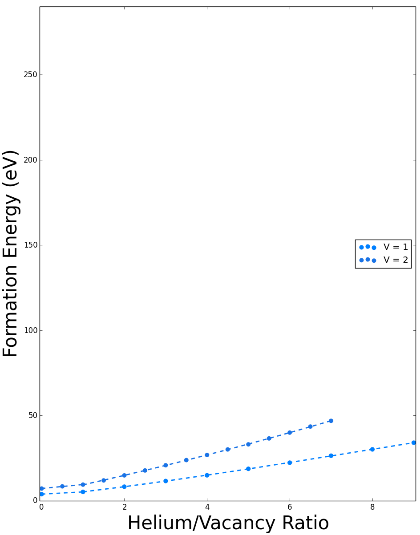
# Example of Two-Step fit:

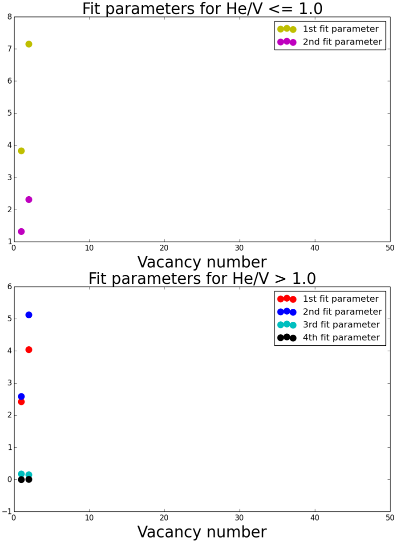
Order 1 and order 3 polynomials for V = 1



# Example of Two-Step fit:

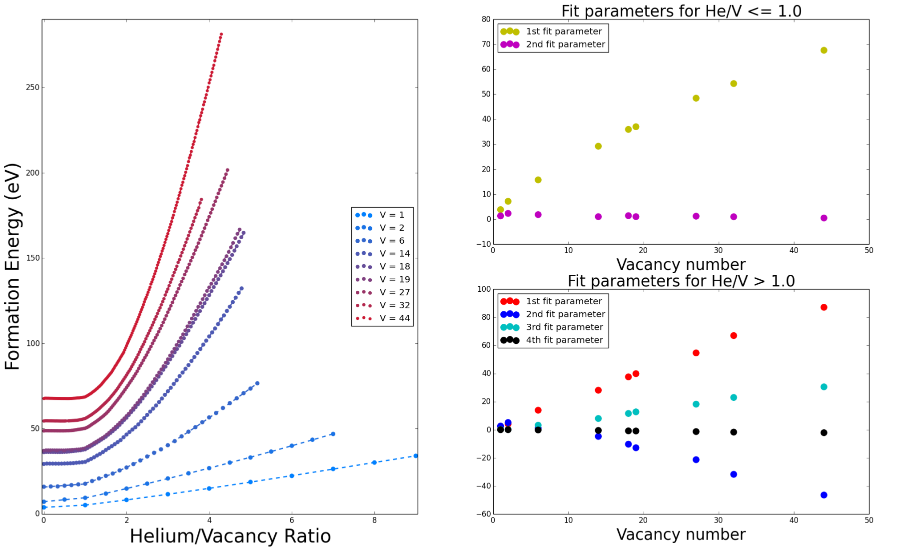
Order 1 and order 3 polynomials for V = 2



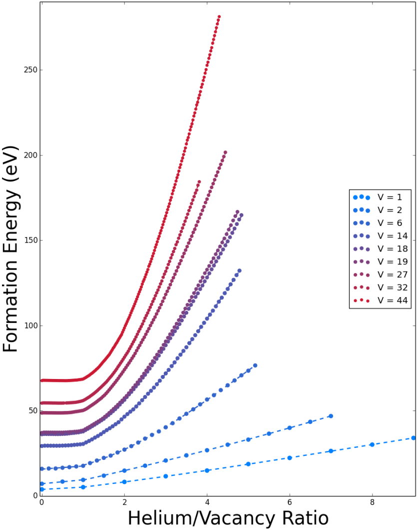
# Example of Two-Step fit:

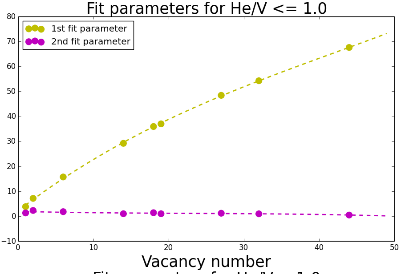
Order 1 and order 3 polynomials for all V

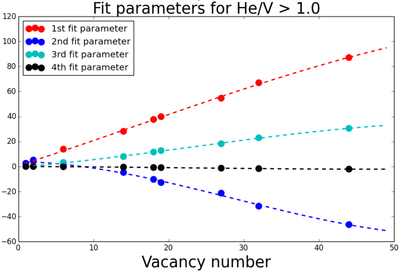


# Example of Two-Step fit:

Fit the parameters with order 3 polynomials

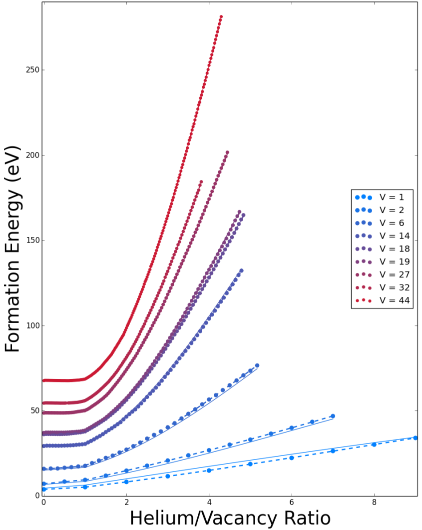


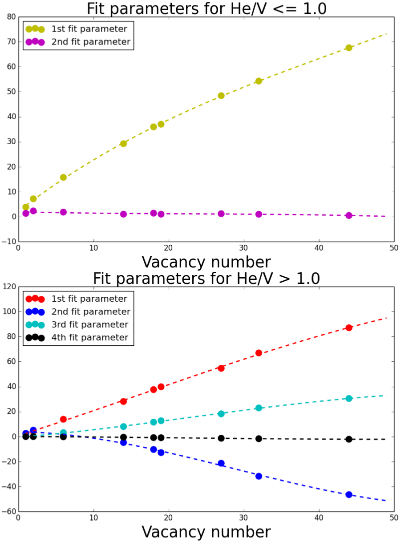



# Example of Two-Step fit:

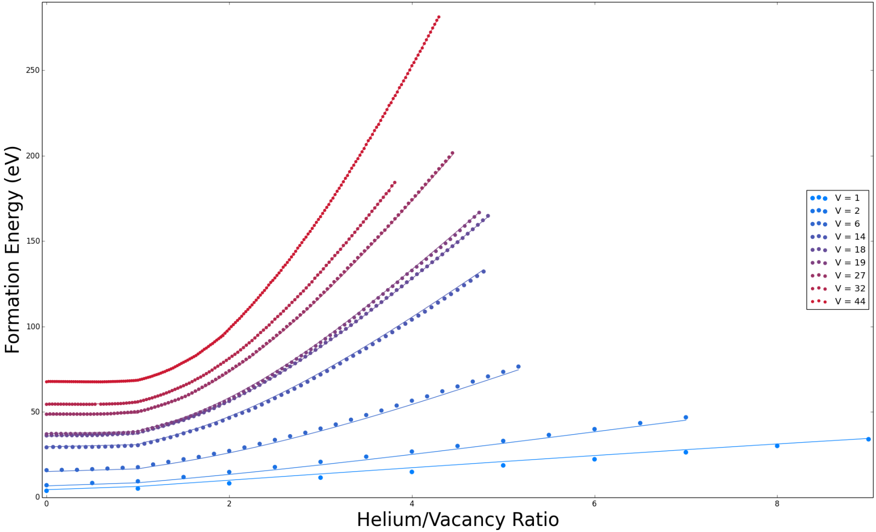
Use the obtained parameters to define a 2D function



# Example of Two-Step fit $(1., 1, 3, 3, 3)$

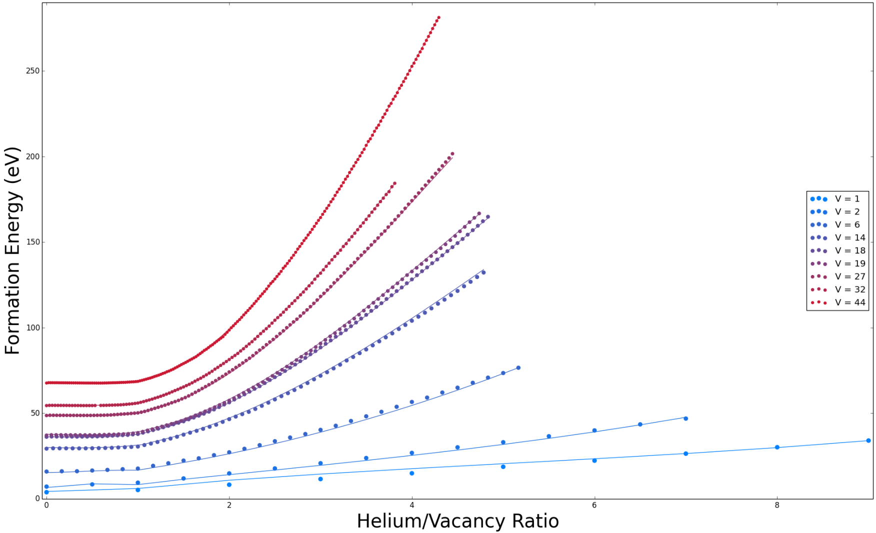
Result:



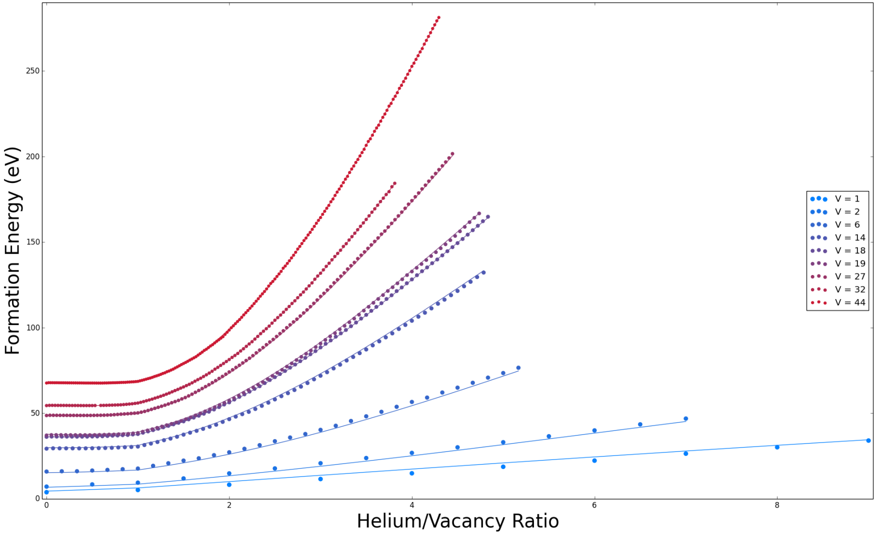
# Selection Criteria

- The closest to the formation energies.
- Polynomial orders lower or equal to 3.

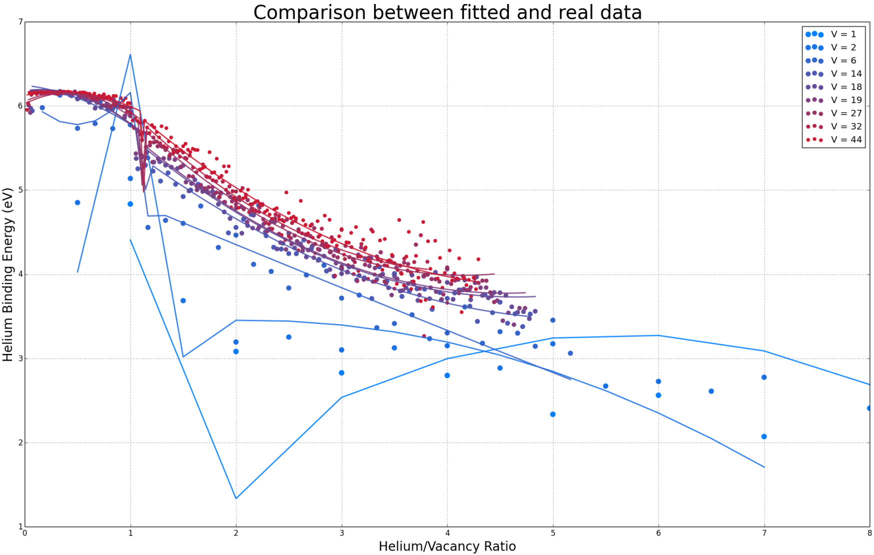
# Best 2D fit $(1.1, 3, 3)$



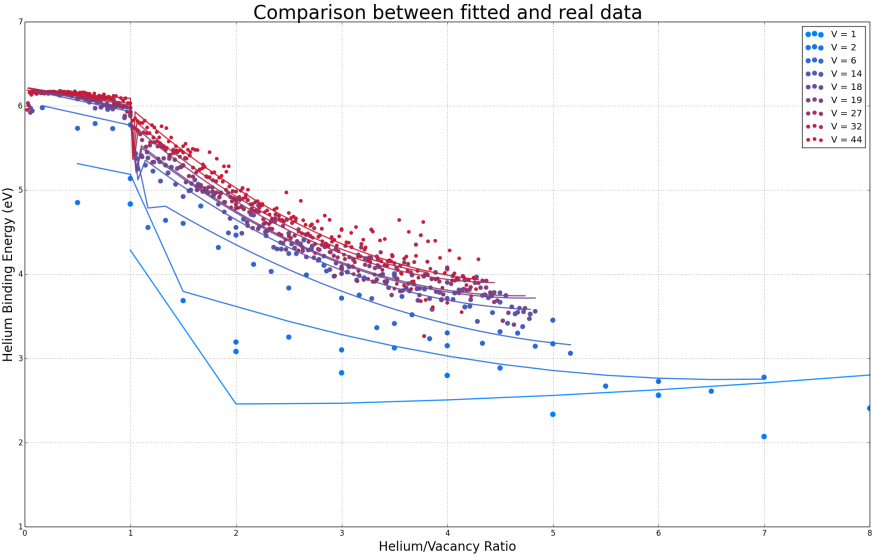
# Best Two-Step fit $(1., 2, 3, 3, 3)$



# Binding Energies, 2D fit $(1.1, 3, 3)$



# Binding Energies, Two-Step fit $(1., 2, 3, 3, 3)$

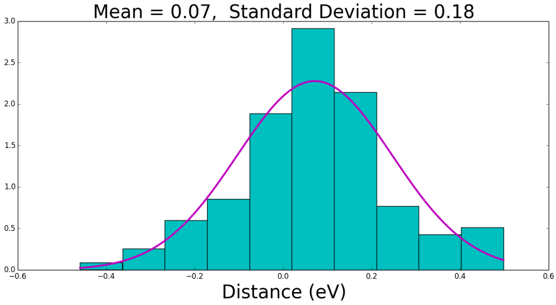


# Confidence Interval of the Fit

Compare the given formation energies to the fitted ones:

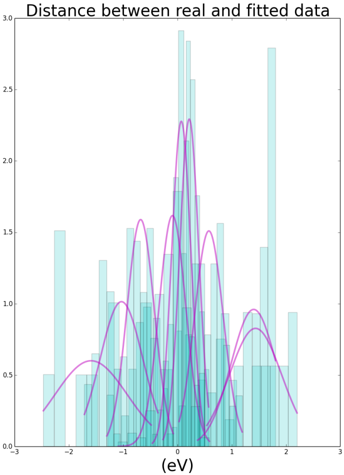
- compute the distance between them for each vacancy number
- plot it in a histogram and fit it with a normal distribution

Example for $V = 32$:

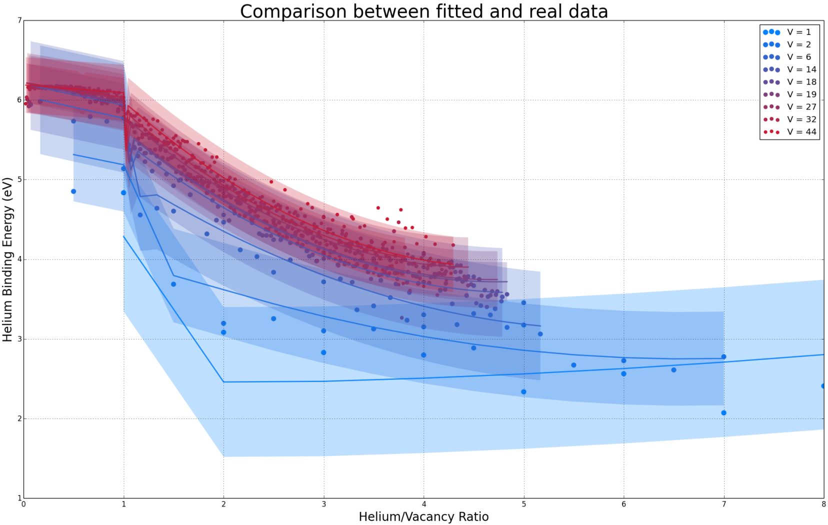


# Confidence Interval of the Fit

Summary for all vacancy numbers:




# Confidence Interval of the Fit



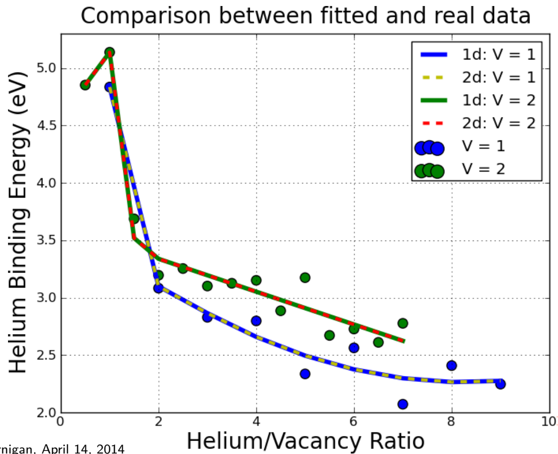
# Problem

Most of the fit tried to give a non-decreasing function of He for $V = 1$.

# Fitting binding energies for $V = 1, 2$

Two options...

- Due to the lack of data, use fit described in previous slides.
- Acquire a good fit for $V = 1, 2$ ONLY and use previously described fit for all $V > 2$



# Bayesian Inference Principle

$$P(H|E) \propto P(E|H) \cdot P(H)$$

- the **posterior** $P(H|E)$ (probability of the hypothesis $H$ given the evidence $E$) that is infered
- the **likelihood** $P(E|H)$ (probability of the evidence $E$ given the hypothesis $H$)
- and the **prior** $P(H)$ that gathers all the information one had before the evidence $E$ was observed

# Bayesian Inference in UQTk

Markov Chain Monte Carlo (MCMC) Method: Metropolis-Hastings algorithm with adaptive proposal distribution.

- Metropolis-Hastings: the step $Y$ at $t$ is kept with a probability $\alpha$

$$\alpha = \min(1, \frac{\pi(Y)}{\pi(X_{t-1})})$$

  with $\pi$ the target distribution.

- Adaptive part: the proposal distribution (to go from a step to the next one) is a function of all the previous step.

# Bayesian Inference in UQTk: Example

- Generate points from $-20$ to 20 following

$$f(x) = -1 + 0.4x - 0.12x^2 + 0.032x^3$$

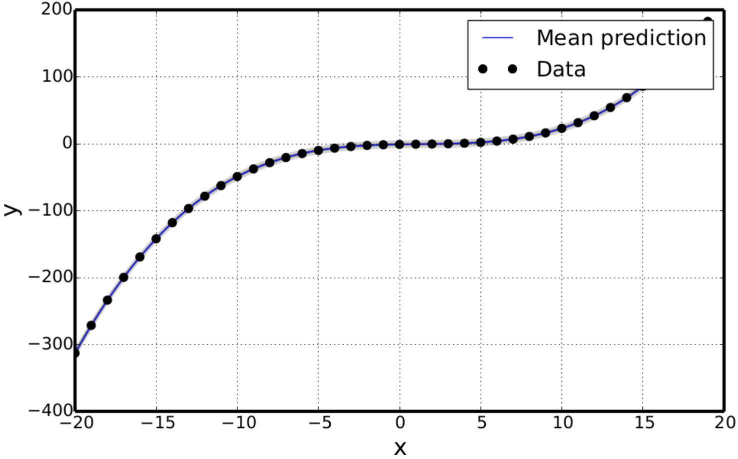
with a gaussian noise of amplitude 5.

- Model them with

$$M(x) = \texttt{param\_a} + \texttt{param\_b} \cdot x - \texttt{param\_c} \cdot x^2 + \texttt{param\_d} \cdot x^3$$

and the same gaussian noise.

# Bayesian Inference in UQTk: Example



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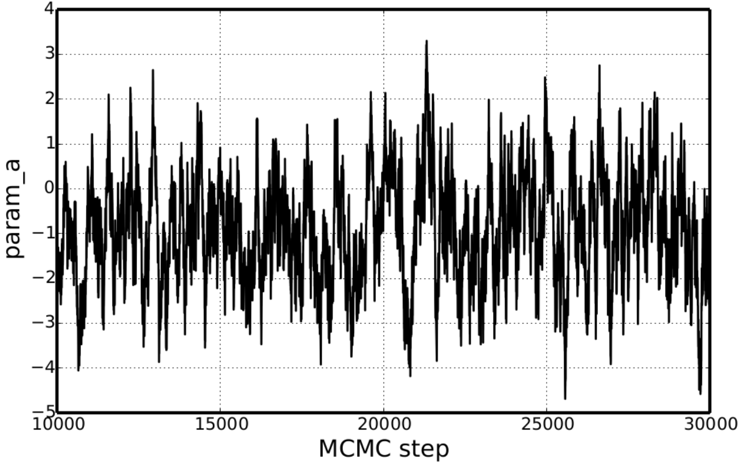

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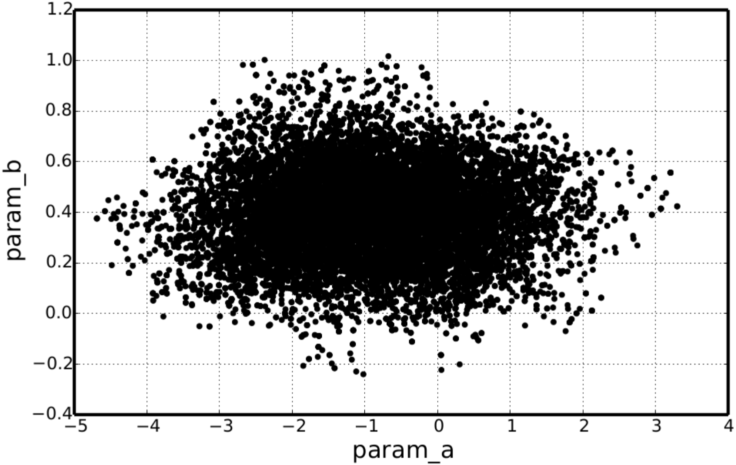
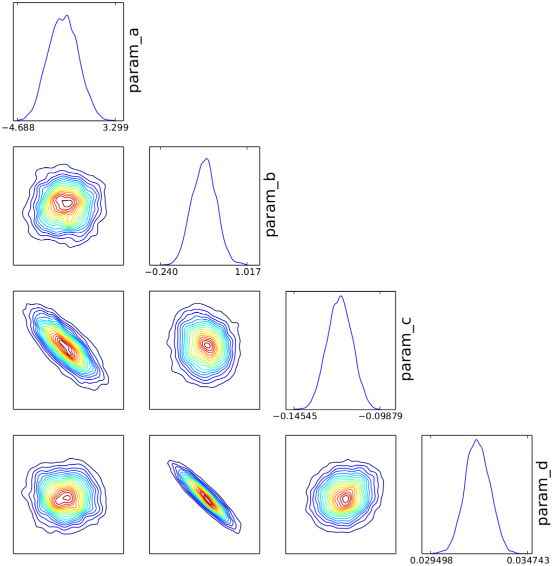
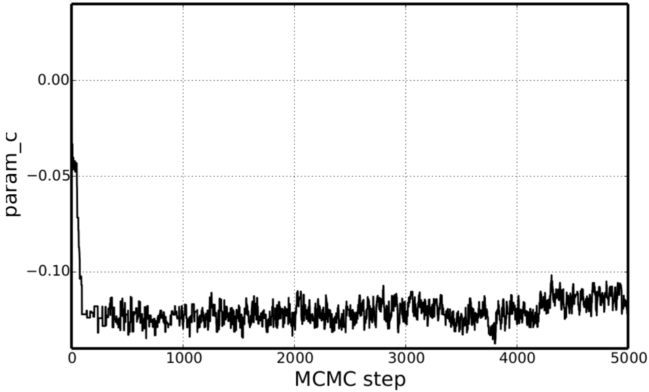


# Bayesian Inference in UQTk: Example



# Bayesian Inference in UQTk: Burn-in

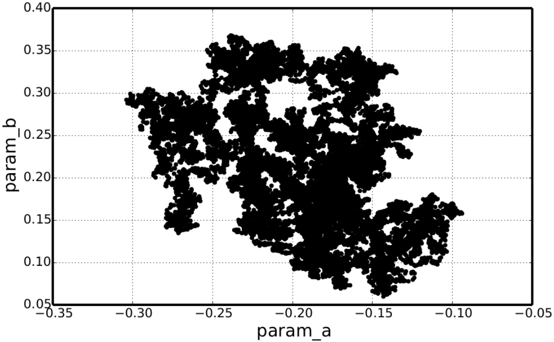
Steps needed for the chain to converge, must not be used to obtain the target distribution.



# Bayesian Inference in UQTk: $\gamma$ parameter

“Size of the step", needs to be fine tuned:

- if too small (high acceptance rate)




- if too big: low acceptance rate.

# Bayesian Inference in UQTk: $V = 27$ Formation Energies

- Suppose the following function is used to fit the data

$$f(x) = a + bx + cx^2 + dx^3 + gx^4 + hx^5$$

- Fitting the data using GNUplot gives

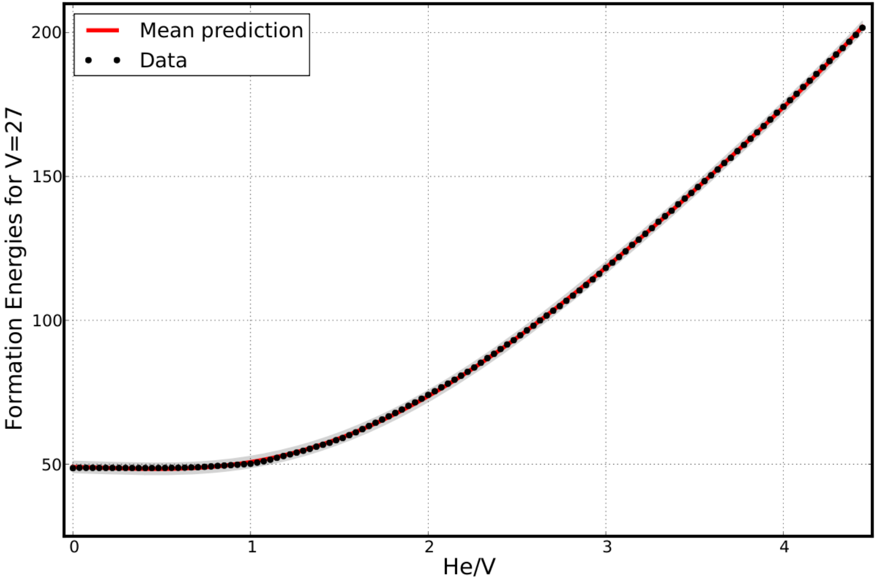
$$a = 49.0722, b = -1.0619, c = -4.87474, d = 9.92562,$$
$$g = -2.47767, h = 0.200702$$

- Model the data with

$$M(x) = \texttt{param\_a} + \texttt{param\_b} \cdot x - \texttt{param\_c} \cdot x^2 + 9.92562 \cdot x^3 - 2.47467 \cdot x^4 + 0.200702 \cdot x^5$$

to infer 3 parameters.

# Bayesian Inference in UQTk: V = 27



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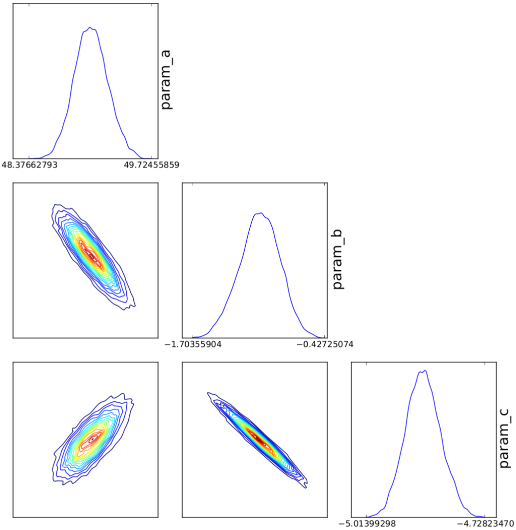
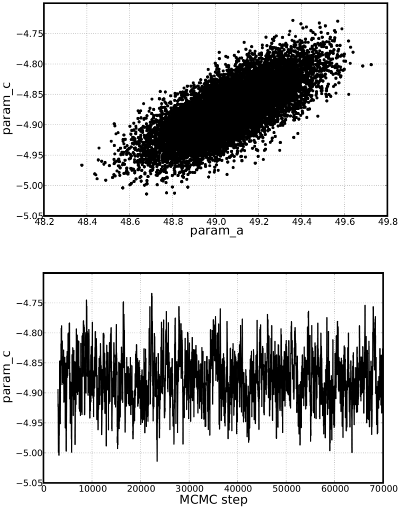



$\gamma = 0.1$



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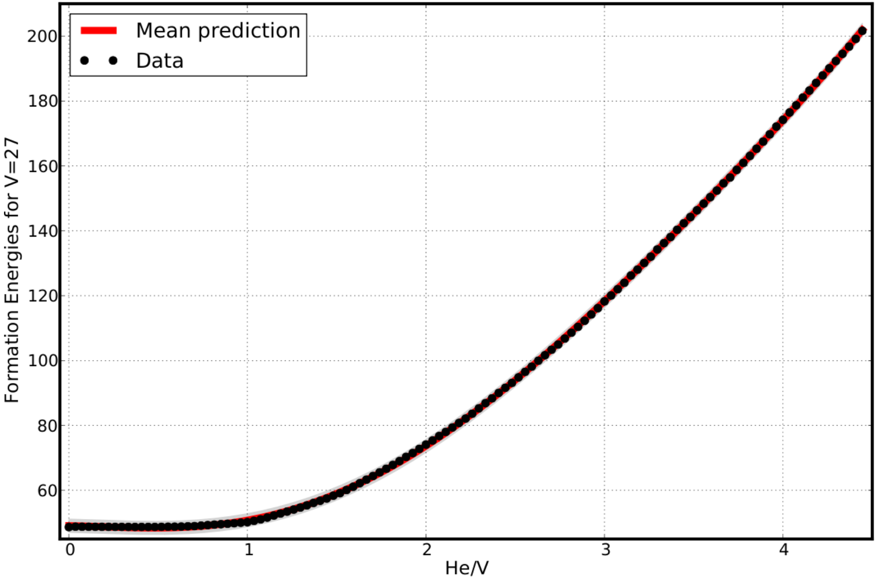
to infer 4 parameters.

# Bayesian Inference in UQTk: V = 27



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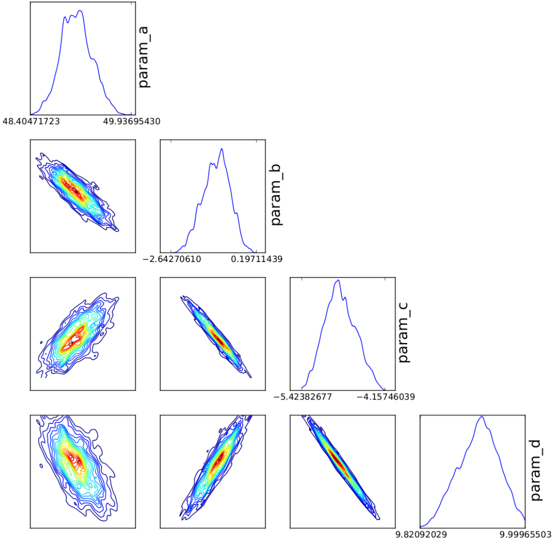
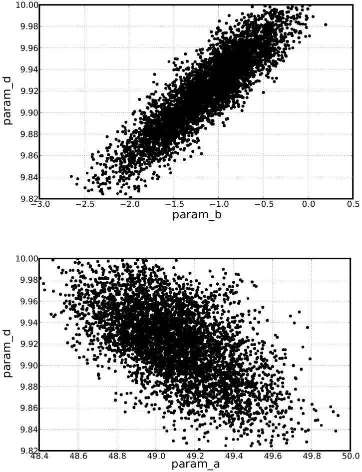



$\gamma = 0.1$



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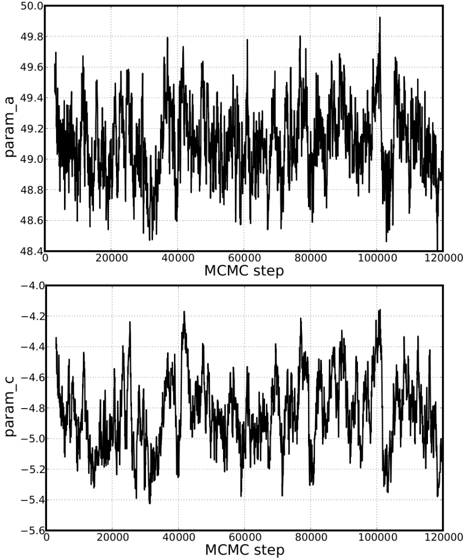
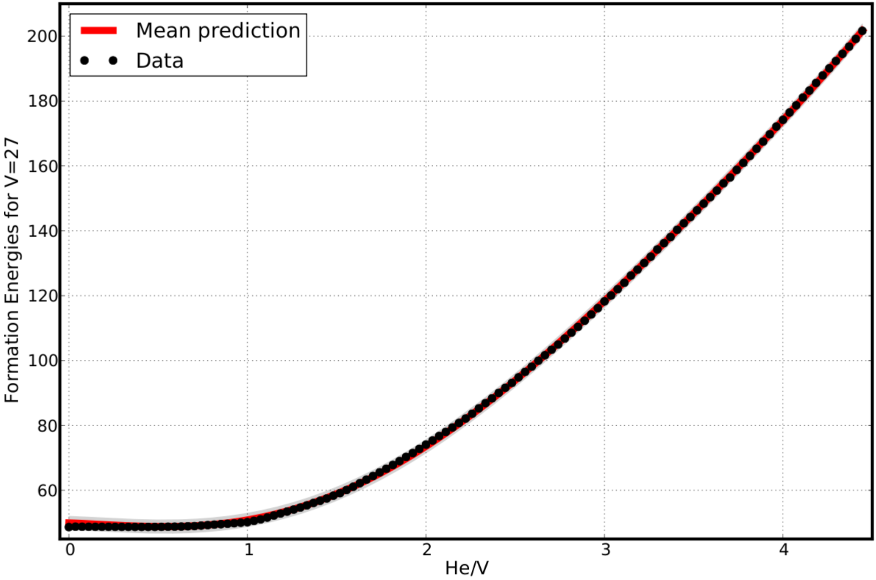


# Bayesian Inference in UQTk: V = 27, Infer 5 params



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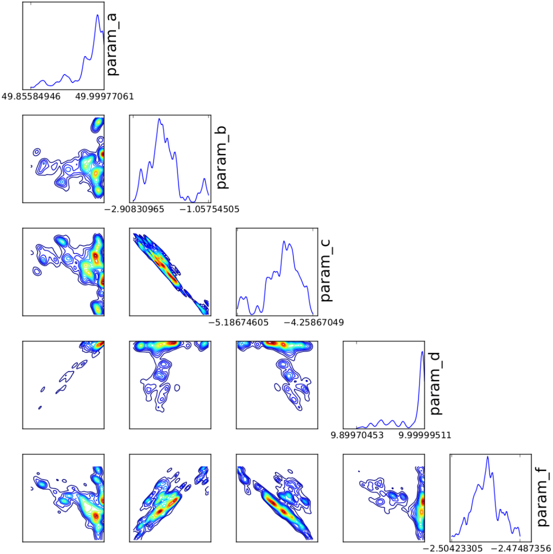
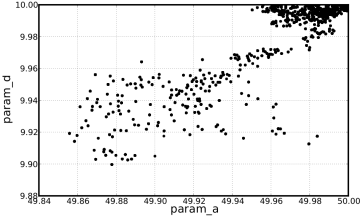
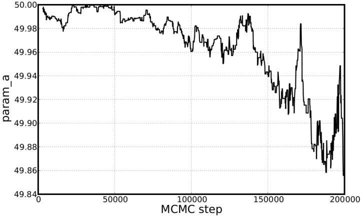



$\gamma = 0.1$

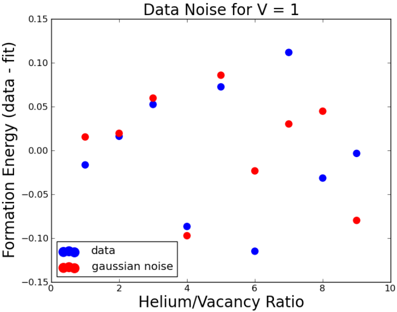


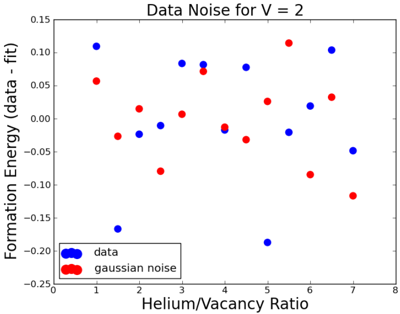



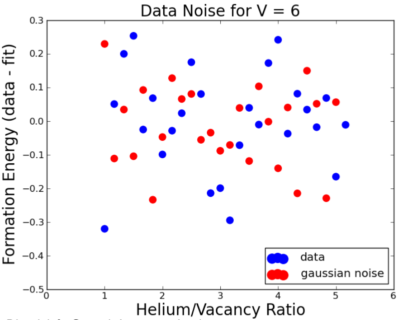
# Bayesian Inference on Formation Energies

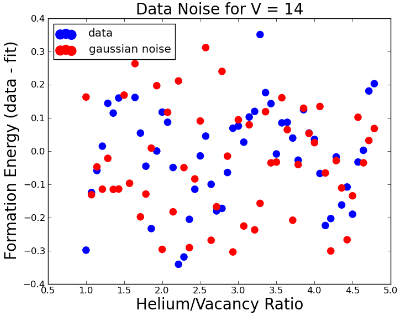
- Using Bayesian inference to infer the parameters of the formation energy fit has proven to be a nontrivial task
- After many unsuccessful attempts to infer the fit parameters for just one vacancy number further investigation into the formation energy noise was performed

# Formation Energy Noise for V = 1, 2, 6, 14



# Formation Energy Noise for V = 18, 19, 27, 32, 44