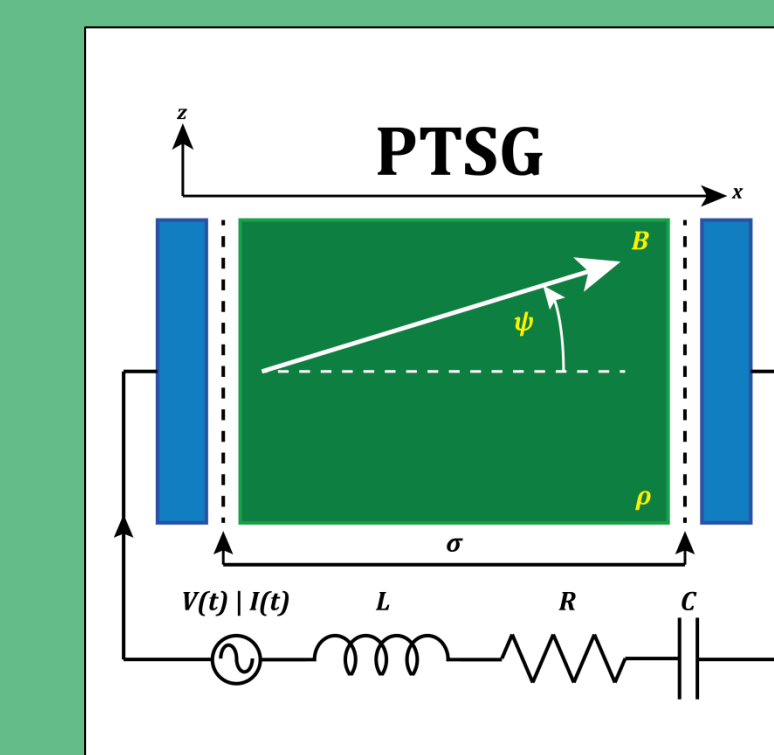# Effective Quantum Potentials for Atomic, Molecular and Scattering Processes in Dense Plasmas*

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Abstract

Atomic and molecular data calculations can be computationally very demanding as the complexity of the atom or molecule increases. In a strongly coupled plasma environment the interactions are of many-particle nature and cannot be approximated as simpler binary events [1]. A full quantum mechanical calculation would be prohibitive due to the vast number of particles involved. An alternative is to treat the quantum mechanical interactions in a classical framework using effective potentials as in the Fermion Molecular Dynamics method which incorporates the Heisenberg and Pauli principles through corresponding momentum dependent potentials [2]. This method has found success in atomic and molecular physics applications [3]. The limitation has been capturing the correct empirical quantities in the potentials which decide the extent of exclusion in phase space and are crucial for obtaining reasonable results. We present our approach of training these phase space parameters and calculation of ground state energies of some atoms. The computed energies match very well with Hartree-Fock (HF) calculations. The model has been extended to study excited states of Hydrogen atom.

Formulation

Quasi-classical Hamiltonian of an N electron atom [2]:

$$H_{QC} = H_0 + V_H + V_P$$

Classical Hamiltonian $\rightarrow$
$$H_0 = \sum_{i=1}^{N} \frac{p_i^2}{2} - \frac{Z}{r_i} + \frac{1}{2}\sum_{i,j\ i\neq j} \frac{1}{r_{ij}}$$

Heisenberg pseudo-potential $\rightarrow$
$$V_H = \sum_{i=1}^{N} \frac{\varepsilon_H^2}{4\alpha_H r_i^2} exp\left[\alpha_H\left(1 - \left(\frac{r_i p_i}{\varepsilon_H}\right)^4\right)\right]$$

Pauli pseudo-potential $\rightarrow$
$$V_P = \frac{1}{2}\sum_{i,j\ i\neq j} \delta_{s_i,s_j} \frac{\varepsilon_p^2}{4\alpha_P r_{ij}^2} exp\left[\alpha_P\left(1 - \left(\frac{r_{ij} p_{ij}}{\varepsilon_p}\right)^4\right)\right]$$

α_H, $\alpha_P \rightarrow$ Hardness parameters

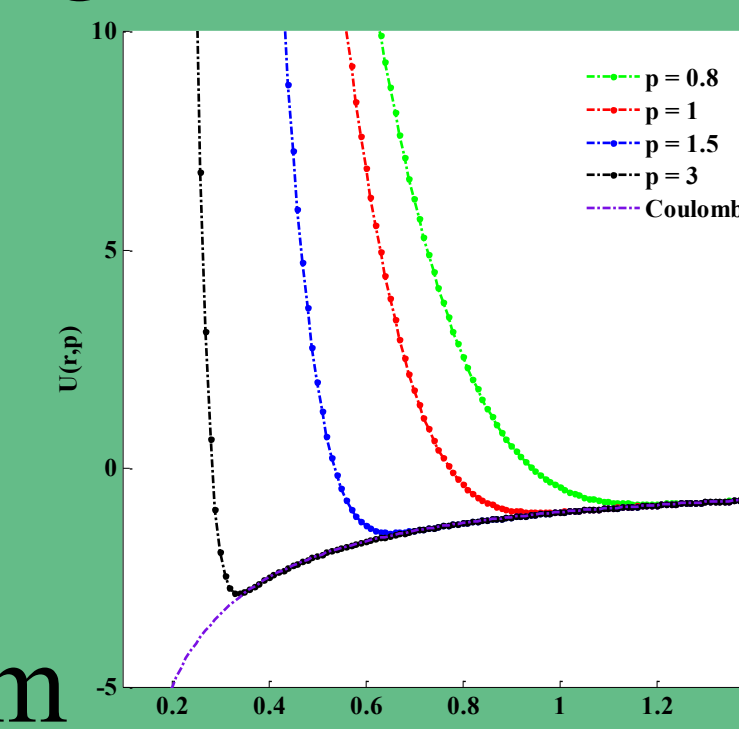ε_H, $\varepsilon_P \rightarrow$ Phase-space parameters

$\delta_{s_i,s_j} = $ 1, $s_i = s_j$

0, $s_i \neq s_j$

s_i, $s_j \rightarrow$ spin numbers

Results

I. Ground State Energy

- Effect of momentum dependent potential on the potential energy landscape is illustrated with Hydrogen atom
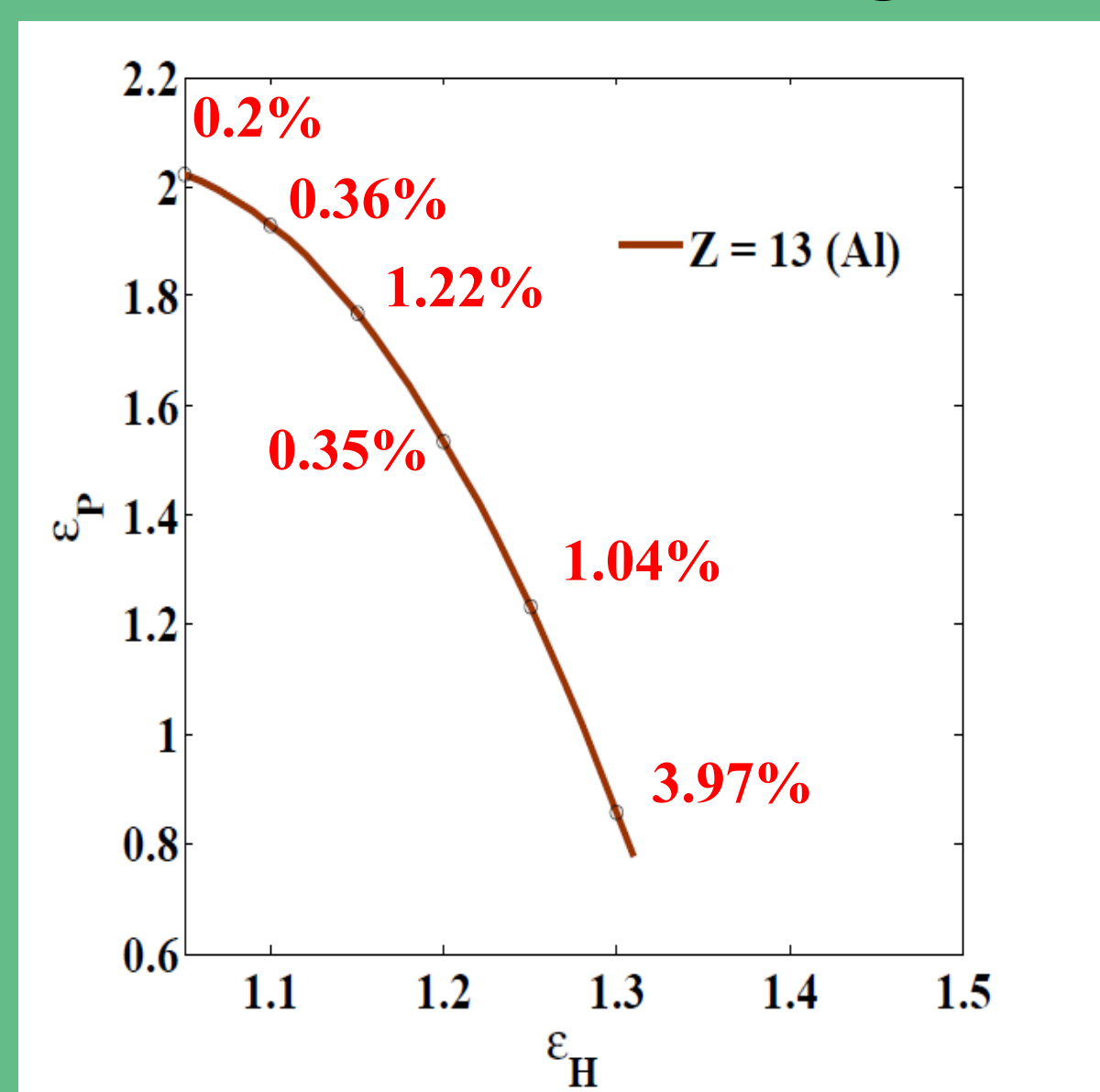
$$U(r, p) = -\frac{1}{r} + V_H(r,p)$$

- Net potential acquires the form of an asymmetric well with depth and position of the minimum altered by the momentum

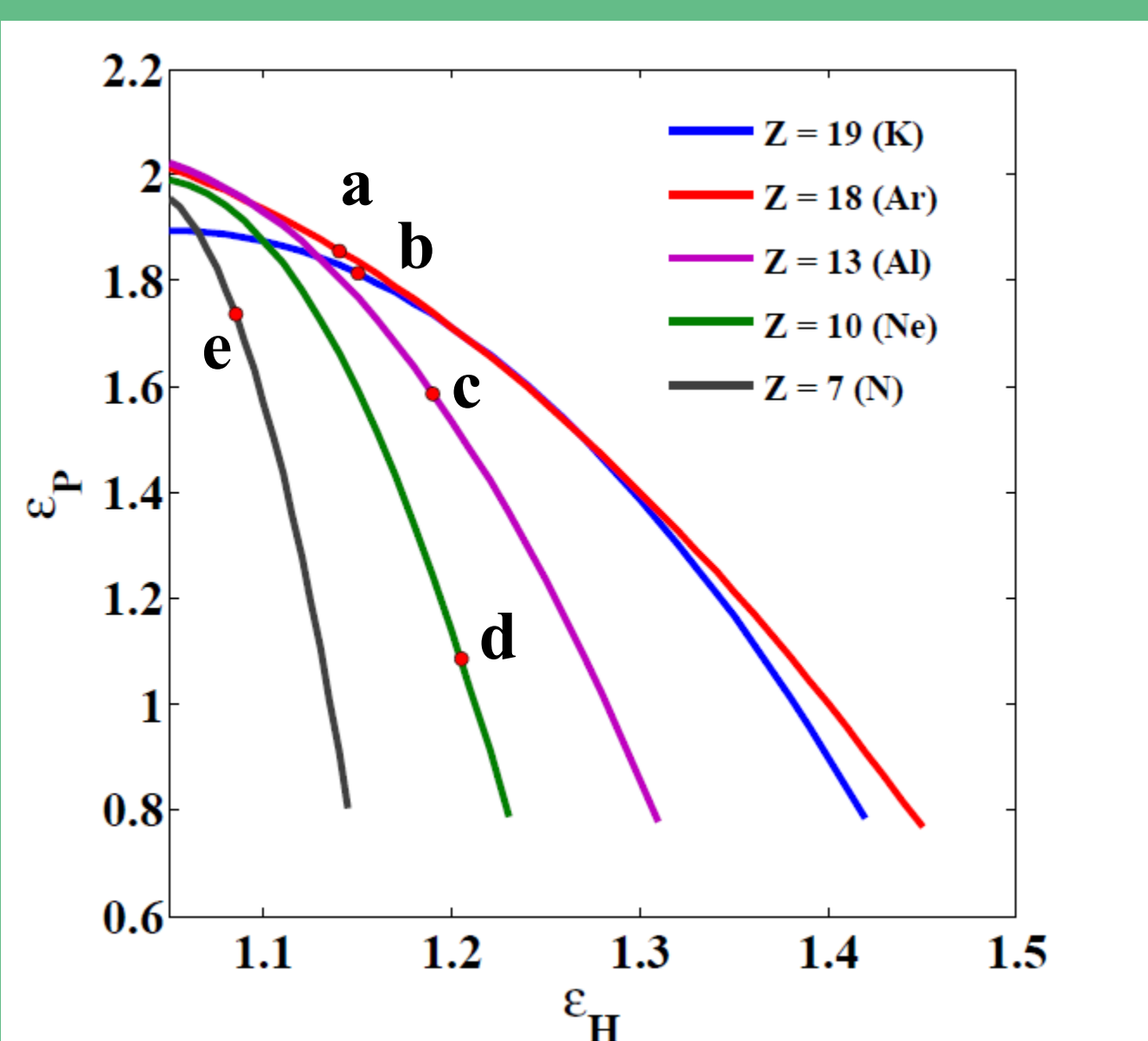### Correlated Phase Space parameters

- Correlation between the parameters that resulted in ground state atomic energies with < 10% deviation from HF

$$\Delta_{HF}(\%) = \left|\frac{E - E_{HF}}{E_{HF}}\right|$$

- Search in parameter space $\rightarrow$ search along curve: **EFFICIENT**
- Correlated values – motivation for physical reason

- Similar correlation for some other ground state atoms

Δ_{HF}(%)
a : 0.045%
b : 0.04%
c : 0.039%
d : 0.036%
e : 0.064%

- Min. deviation from HF value
- Accurate than those reported
- Much reduced computational cost
- Formulation simpler than HF

- Pattern in correlation with respect to Atomic number: Parabolic form $\varepsilon_P = A\ \varepsilon_H^2 + B\ \varepsilon_H + C$

- Coefficients extracted for intermediate Z

$A(Z)$

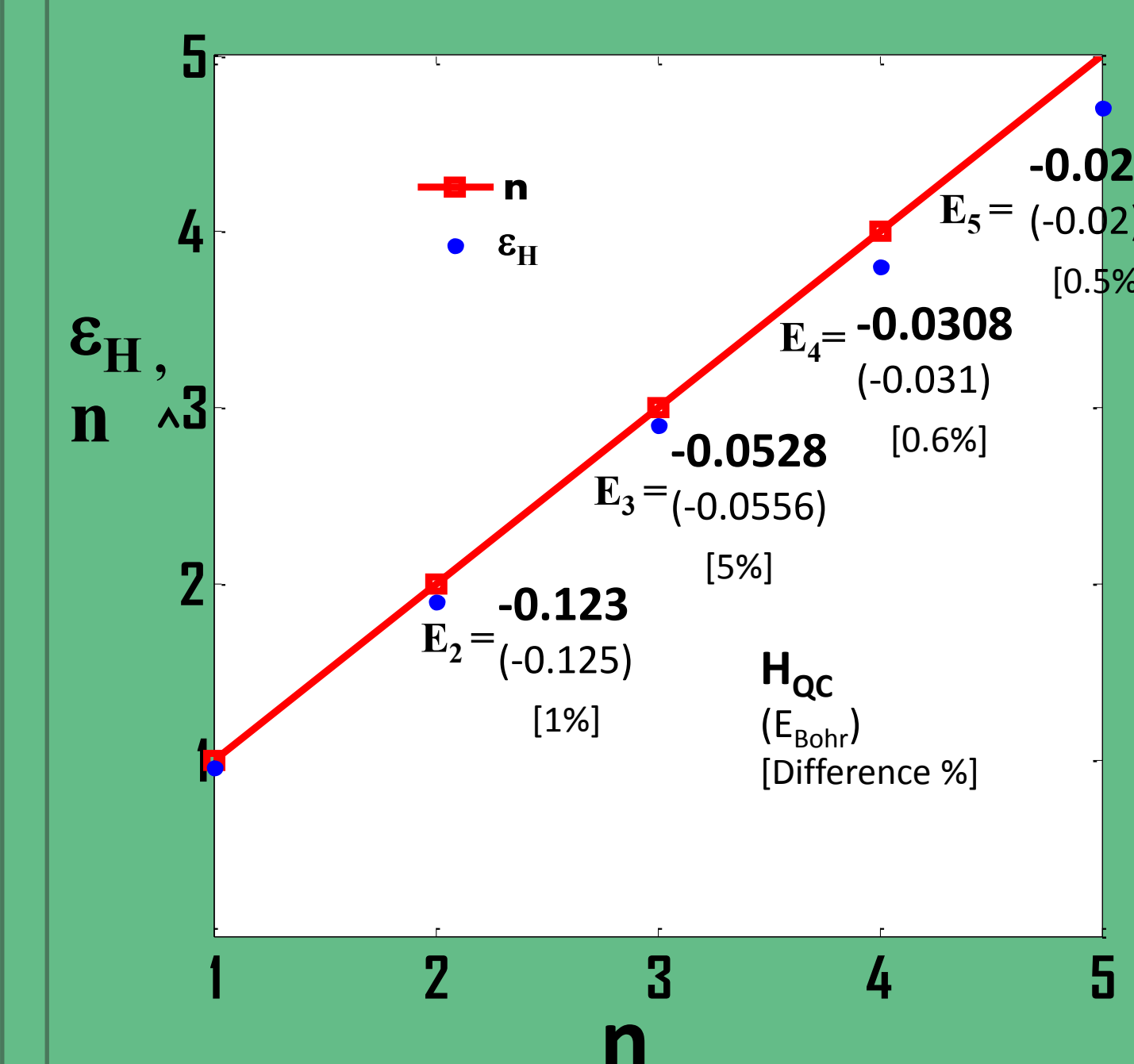$B(Z)$ — Data, 4th degree polynomial fit

$C(Z)$
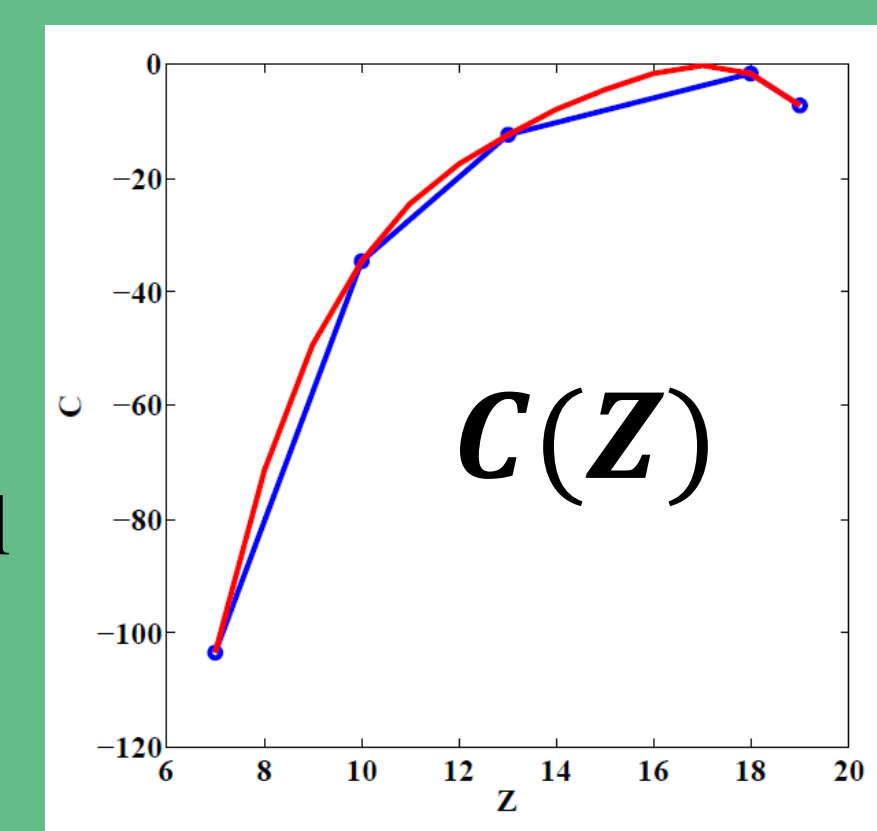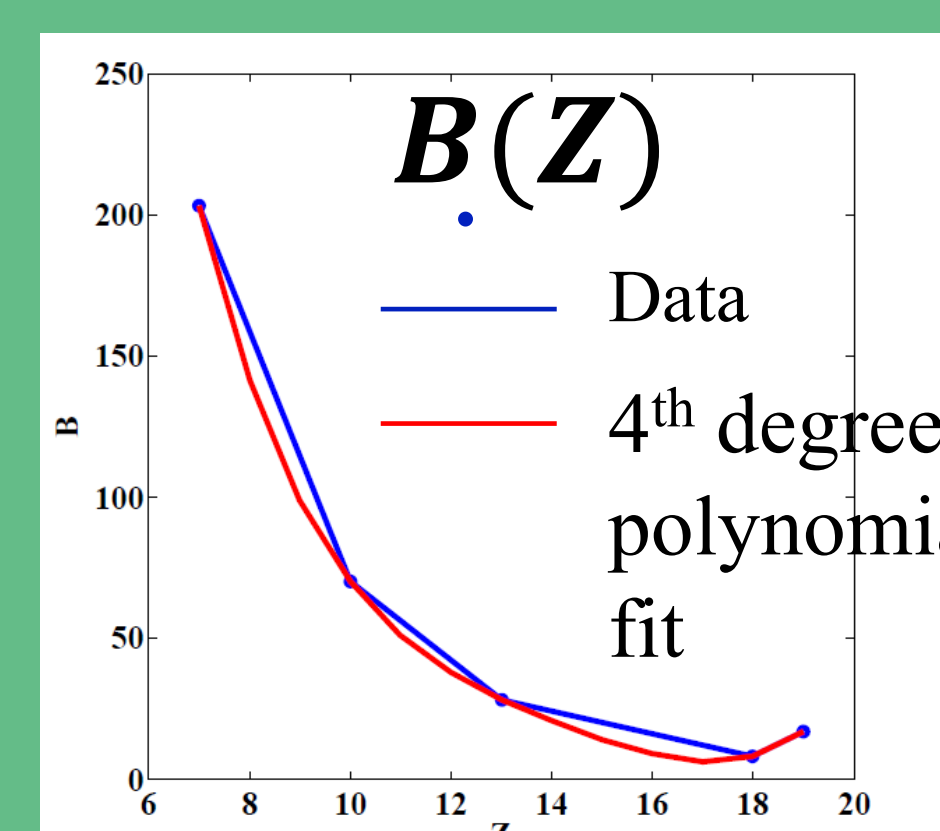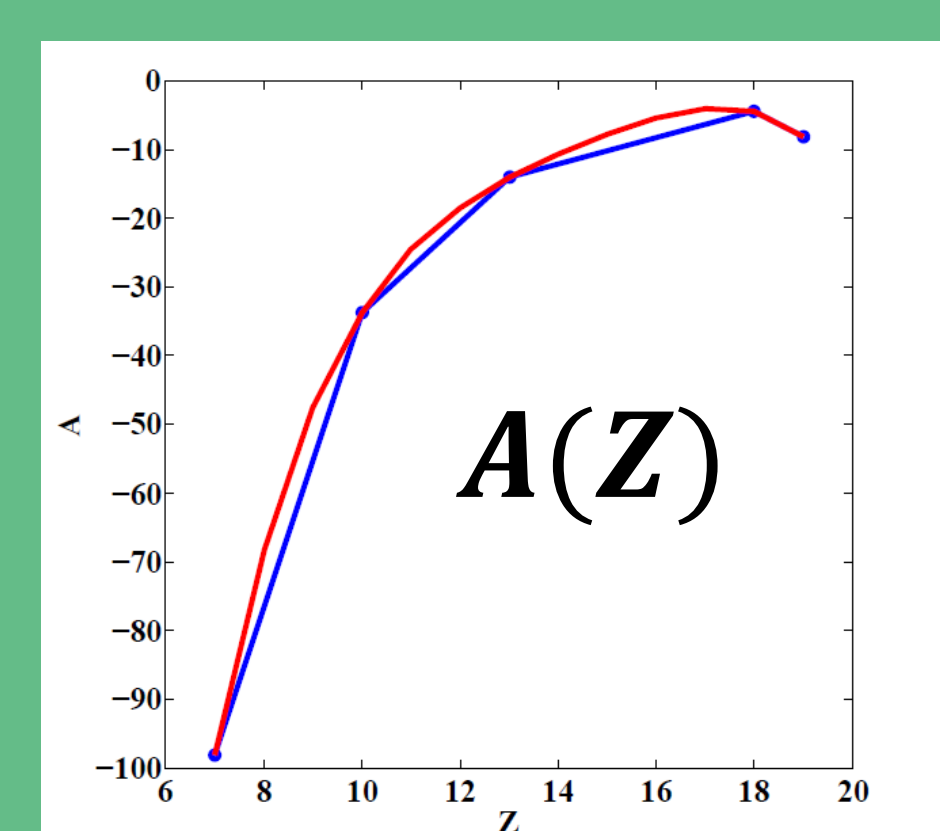
Predictability
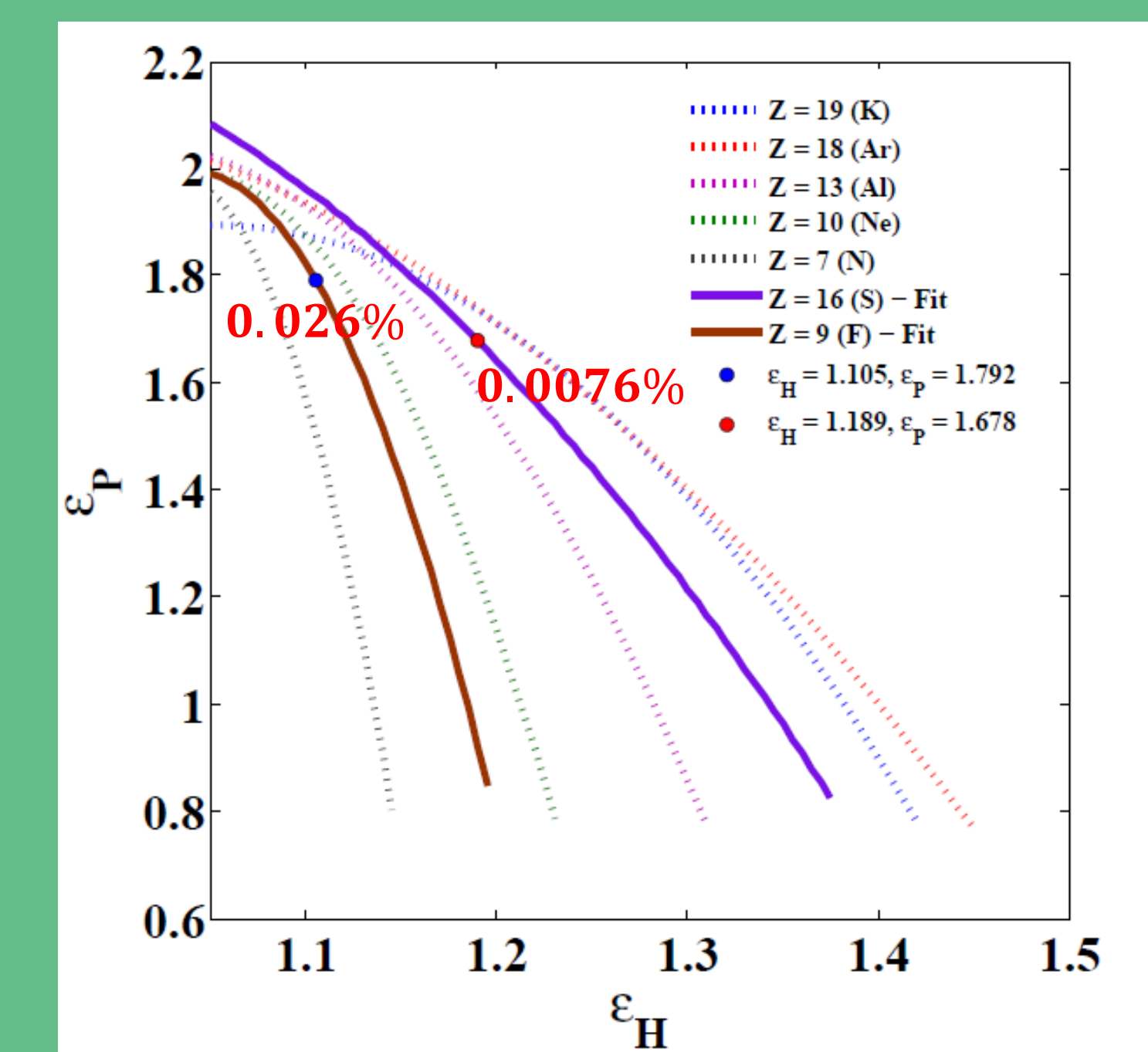
- Curves computed for F and S using the extracted coefficients
- Search along the curves $\rightarrow$ parameters that resulted in ground state energy with <0.03% deviation from HF

S: $\varepsilon_P = -5.29\varepsilon_H^2 + 8.97\varepsilon_H - 1.5$ F: $\varepsilon_P = -47.51\varepsilon_H^2 + 98.79\varepsilon_H - 49.4$

II. Excited State Energy

- Model extended to excited sates of Hydrogen – energy values in reasonable agreement with Bohr model
- Relationship between Heisenberg parameter and principal quantum number found to be almost linear

Conclusions & Future Work

- Correlation between phase-space parameters identified
- Studying the correlation resulted in identifying a pattern w.r.t. atomic number
- By extracting the pattern information, ground state energy of Sulphur and Fluorine were predicted within 0.03% of corresponding HF value
- Much reduced cost compared to Hartree-Fock method
- To understand the physical reason for correlation and to identify accurate functional form
- To understand the physical reason for the pattern in correlation w.r.t. atomic number

References

[1] M. S. Murillo and J. C. Weisheit, *Phys. Reports* **302**, 1 (1998).

[2] J. S. Cohen and L. Wilets, *Contemp. Phys.* **39**, 163 (1998).

[3] Y. Zhou et. al, *Phys. Rev. Lett.* **109**, 053004 (2012).