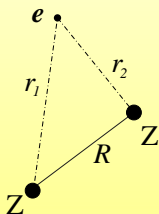


Critical Points Of Coulomb Systems

Héctor Medel

jointly with A. Turbiner

System: Z_2^+ Ion



Hamiltonian:

$$\mathcal{H}(Z) = -\frac{1}{2}\Delta_1 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{Z^2}{R}$$

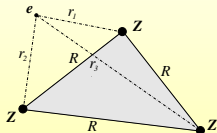
For $Z \in (0, Z_{cr})$ system is bound, $Z = 1 \rightarrow H_2^+$

Critical point: $Z_{cr} \approx 1.437$, Critical $R_{eq} \approx 2.89$ a.u.

Behavior (found by fit):

$$E_{total} = -1.8036 + 1.4082 (Z_{cr} - Z) + 0.0305 (Z_{cr} - Z)^{3/2} - 0.4265 (Z_{cr} - Z)^2 + \dots$$

System: Z_3^{++} Ion



Equilateral triangular configuration

$$\mathcal{H}(Z) = -\frac{1}{2}\Delta_1 - \frac{Z}{r_1} - \frac{Z}{r_2} - \frac{Z}{r_3} + Z^2\frac{3}{R}$$

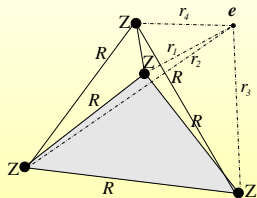
For $Z \in (0, Z_{cr})$ system is bound

Critical point: $Z_{cr} \approx 0.9539$, Critical $R_{eq} \approx 4.75$ a.u.

Behavior (found by fit):

$$E_{total} = -0.6960 + 0.3875(Z_{cr} - Z) - 2.1163(Z_{cr} - Z)^{3/2} \\ + 5.2306(Z_{cr} - Z)^2 - 5.7183(Z_{cr} - Z)^{5/2} + \dots$$

System: Z_4^{3+}



Tetrahedron configuration

$$\mathcal{H}(Z) = -\frac{1}{2}\Delta - \sum_{i=1}^4 \frac{Z}{r_i} + 6\frac{Z^2}{R}$$

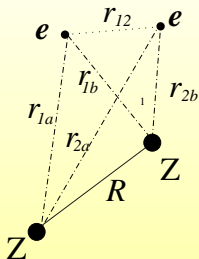
For $Z \in (0, Z_{cr})$ system is bound

Critical point: $Z_{cr} \approx 0.730$, Critical $R_{eq} \approx 6.31$ a.u.

Behavior (found by fit):

$$\begin{aligned} E_{total} &= -0.3388 - 0.5424(Z_{cr} - Z) + 0.0350(Z_{cr} - Z)^{3/2} \\ &\quad - 0.5423(Z_{cr} - Z)^2 - 0.7951(Z_{cr} - Z)^{5/2} + \dots \end{aligned}$$

System: Z_2 Molecule



$$\mathcal{H}(Z) = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \sum_{i=1}^2 \sum_{k=a}^b \frac{Z}{r_{ik}} + \frac{Z^2}{R}$$

For $Z \in (0, Z_{cr})$ system is bound,
 $Z = 1 \rightarrow H_2$

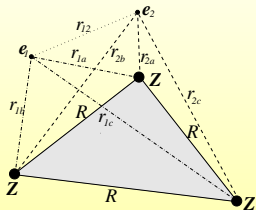
Critical point: $Z_{cr} \approx 2.2442$, Critical $R_{eq} \approx 1.51$ a.u.

Behavior (found by fit):

$$E_{total} = -8.6519 + 5.3812(Z_{cr} - Z) + 0.0855(Z_{cr} - Z)^{3/2} \\ - 0.3169(Z_{cr} - Z)^2 - 0.3659(Z_{cr} - Z)^{5/2} + \dots$$

System: Z_3^+ Ion

Equilateral triangular configuration



$$\mathcal{H}(Z) = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 - \sum_{i=1}^2 \sum_{k=a}^c \frac{Z}{r_{ik}} + 3\frac{Z^2}{R}$$

For $Z \in (0, Z_{cr})$ system is bound,
 $Z = 1 \rightarrow H_3^+$

Critical point: $Z_{cr} \approx 1.433$, Critical $R_{eq} \approx 1.96$ a.u.

Behavior (found by fit):

$$E_{total} = -3.6768 + 2.9047(Z_{cr} - Z) - 7.8009(Z_{cr} - Z)^{3/2} + 18.3164(Z_{cr} - Z)^2 - 12.5502(Z_{cr} - Z)^{5/2}$$