

The linear stability of the relative equilibria in the Coulomb $(n + 1)$ body problem

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The Kepler $(n + 1)$ -body problem

The $(n + 1)$ -body problem was introduced by J. Clerk Maxwell in his study of the rings of Saturn in 1858. The system consists of n bodies of mass 1 and one body have mass M interacting via gravity where $M \gg 1$.

Meyer's summary

The study of relative equilibria (r.e.) of the N -body problem has had a long history starting with the famous collinear configuration of the 3-body problem found by Euler (1767). Over the intervening years many different technologies have been applied to the study of r.e. In the older papers of Euler (1767), Lagrange (1772), Hoppe (1879), Lehmann-Filhes (1891), and Moulton (1910), special coordinates, symmetries, and analytic techniques were used. In their investigations, Dziobek (1900) used the theory of determinants; Smale (1970) used Morse theory; Palmore (1975) used homology theory; Simo (1977) used a computer; and Moeckel (1985) used real algebraic geometry. Thus, the study of r.e. has been a testing ground for many different methodologies of mathematics.

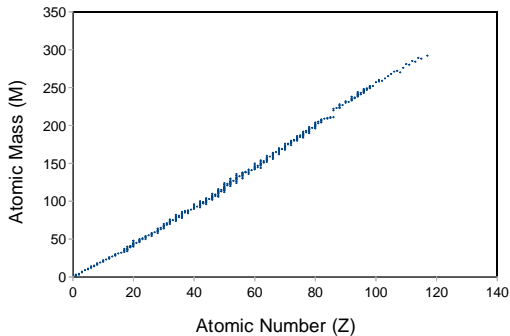
The Coulomb $(n + 1)$ -body problem

The Coulomb $(n + 1)$ -body problem was introduced by H. Nagaoka in his study of atomic structure in 1904. The system consists of n electrons of mass 1 and charge -1 and the nucleus having mass M with charge Z interacting via the electrostatic forces. (The gravitational forces are sufficiently weak that they can be neglected.)

$$1.8 \times 10^3 \leq M \leq 5.4 \times 10^5$$
$$1 \leq Z \leq 118$$

Atomic Mass vs Atomic Number

Atomic Number vs. Atomic Mass



The Hamiltonians

$$H = \frac{1}{2} \sum_{i=1}^n \left(p_{\rho_i}^2 + \frac{p_{\theta_i}^2}{\rho_i^2} + p_{z_i}^2 \right) - \sum_{i=1}^n \frac{\lambda}{\sqrt{\rho_i^2 + z_i^2}} \pm \sum_{i=1}^{n-1} \sum_{j=i}^n \frac{1}{\sqrt{(\rho_i^2 + \rho_j^2 - 2\rho_i\rho_j \cos(\theta_j - \theta_i)) + (z_j - z_i)^2}}$$

where for the Kepler problem $\lambda = M$ and the sign is taken to be negative. For the Coulomb problem $\lambda = Z$ and the sign is taken to be positive.

Linus Pauling: General Chemistry

“One of the most valuable parts of chemical theory is the **periodic law**. In its modern form this law states simply that **the properties of the chemical elements are not arbitrary, but depend upon the electronic structure of the atom and vary with the atomic number in a systematic way**. The important point is that this dependence involves a crude periodicity that show itself in the periodic recurrence of characteristic properties.”

Periodic Table

Periodic Table of the Elements

1 IA 1A																	18 VIIIA 8A	
1 H Hydrogen 1.008																	2 He Helium 4.002	
3 IIA 2A	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180	
11 Na Sodium 22.990	12 Mg Magnesium 24.305	3 III 3B	4 IV 4B	5 V 5B	6 VI 6B	7 VII 7B	8 VIII 8		9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.723	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 84.80	
37 Rb Rubidium 84.464	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29	
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71 Lanthanide Series		72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.084	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [209]	85 At Astatine [209]	86 Rn Radon [222]
87 Fr Francium 223.027	88 Ra Radium 226.025	89-103 Actinide Series		104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [263]	107 Bh Bohrium [264]	108 Hs Hassium [265]	109 Mt Meitnerium [266]	110 Ds Darmstadtium [265]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Nh Nihonium [278]	114 Fl Flerovium [277]	115 Uup Ununpentium [278]	116 Lv Livermorium [276]	117 Uus Ununseptium [278]	118 Uuo Ununoctium [276]
		57 La Lanthanum 138.905	58 Ce Cerium 140.115	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.966	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967		
		89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.083	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]		
		Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide							

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 www.ptable.com

I recommend the following web resource to my students:

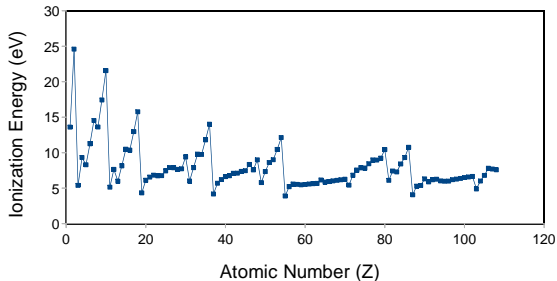
<http://www.ptable.com/>



Ionization Energy vs Atomic Number

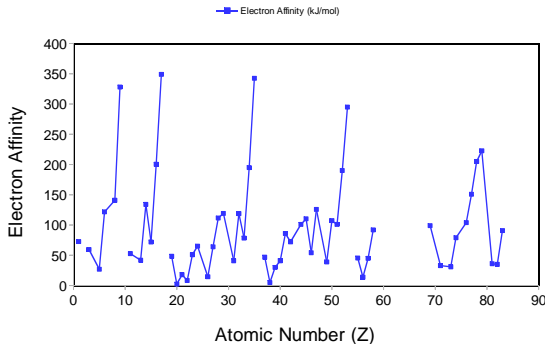
Ionization Energy vs Atomic Number

Data from Clementi et al (1967)

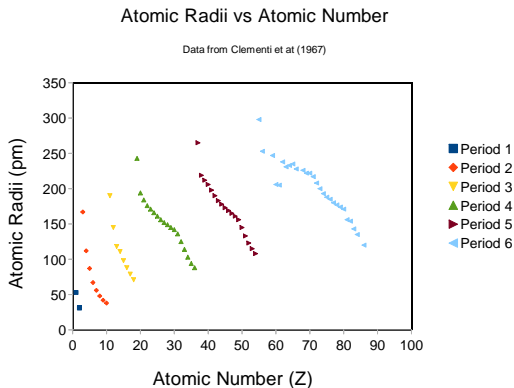


Electron Affinity vs Atomic Number

Electron Affinity vs Atomic Number



Atomic Radii vs Atomic Number



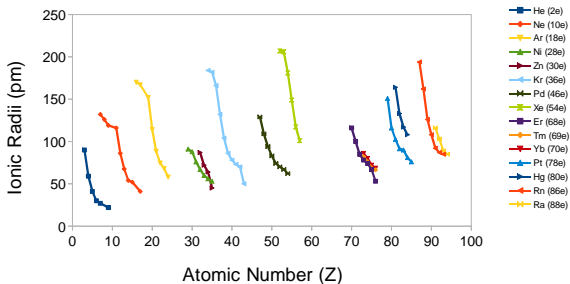
Isoelectronic Series

Keep the number of electrons n fixed while varying the nuclear charge Z .

Example for $n = 2$: H^{-1} , He , Li^{+1} , Be^{+2} , B^{+3} , C^{+4} , N^{+5} , O^{+6} ,
 F^{+7}

Ionic Radii for Isoelectronic Series

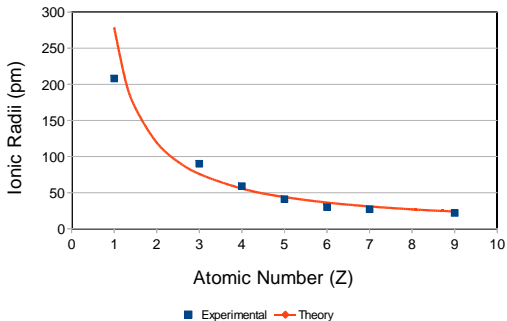
Ionic Radii for Isoelectronic Series



Ionic Radii for the He Isoelectronic Series

Ionic Radii

The He (2e) Isoelectronic Series



Linearized Equations of Motion

The stability of the relative equilibria is studied by first linearizing the equations of motion

$$\dot{z} = J\nabla Hz$$

where ∇H is the Hessian of the Hamiltonian, J is

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

and I is the $n \times n$ unit matrix. The stability is then determined by examining the eigenvalues of the Jacobian $J\nabla H$.

Diagonalization

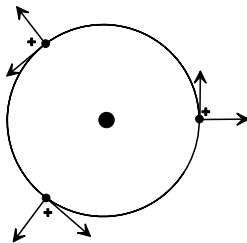
- 1 Transform to rotating frame.
- 2 Transform to symmetry variables.
- 3 Decouple the coordinates from the momenta.
- 4 Diagonalize and balance the Hessian via a sequence of rotations and scalings.
- 5 Transform to complex coordinates.
- 6 Multiply by J .

Criteria: The relative equilibrium is said to be linearly stable if none of the eigenvalues have positive real part.

Point Groups

The equilibrium configuration in the rotating frame has belongs to the C_{nh} point group. As an example consider $n = 3$ or C_{3h} .

C_{3h}	E	$2C_3$	σ_h	$2S_3$
A'	1	1	1	1
A''	1	1	-1	-1
E'	2	-1	2	-1
E''	2	-1	-2	1



$$\Gamma_{Li} = 2A' + A'' + 2E' + E''$$

Point Groups

For even n consider $n = 6$ or C_{6h} . As the in-plane and out-of-plane motion decouples, one can work in C_6 .

C_{6h}	E	$2C_6$	$2C_3$	C_2	σ_h	$2S_6$	$2S_3$	i	
A_g	1	1	1	1	1	1	1	1	A'
B_u	1	-1	1	-1	1	-1	1	-1	B'
E_{1u}	2	1	-1	-2	2	1	-1	-2	E'_1
E_{2g}	2	-1	-1	2	2	-1	-1	2	E'_2
A_u	1	1	1	1	-1	-1	-1	-1	A''
B_g	1	-1	1	-1	-1	1	-1	1	B''
E_{1g}	2	1	-1	-2	-2	-1	1	2	E''_1
E_{2u}	2	-1	-1	2	-2	1	1	-2	E''_2

Irreducible Representations

The irreducible representations for odd n :

$$\Gamma_H = 2A' + A''$$

$$\Gamma_{Li} = 2A' + A'' + 2E' + E''$$

$$\Gamma_B = 2A' + A'' + 2E'_1 + E''_1 + 2E'_2 + E''_2$$

$$\Gamma_N = 2A' + A'' + 2E'_1 + E''_1 + 2E'_2 + E''_2 + 2E'_3 + E''_3$$

Irreducible Representations

The irreducible representations for even n :

$$\Gamma_{He} = 2A' + A'' + 2B' + B''$$

$$\Gamma_{Be} = 2A' + A'' + 2B' + B'' + 2E' + E''$$

$$\Gamma_C = 2A' + A'' + 2B' + B'' + 2E'_1 + E''_1 + 2E'_2 + E''_2$$

$$\Gamma_O = 2A' + A'' + 2B' + B'' + 2E'_1 + E''_1 + 2E'_2 + E''_2 + 2E'_3 + E''_3$$

Block Diagonalization

- The introduction of symmetry variables block diagonalizes the Hessian matrix. Each block corresponding to one of the irreducible representations.

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- Irreducible representations with a single prime corresponds to in-plane motion. Those with double prime correspond to out-of-plane motion.

Block Diagonalization

- The introduction of symmetry variables block diagonalizes the Hessian matrix. Each block corresponding to one of the irreducible representations.
- Irreducible representations with a single prime corresponds to in-plane motion. Those with double prime correspond to out-of-plane motion.
- The $2A'$ modes leave the relative configuration of the system unchanged; one is the rotation about the z -axis and the other is the symmetric breathing mode.

The totally symmetric representation

- The A' irreducible representation is totally symmetric.
- Its block is a 4×4 with determinant is equal to zero.
- The eigenvalues are $(0, 0, \pm i\omega_0)$
- The two zeros are associated with the rotation. The complex pair is associated with the symmetric breathing mode.

The A'' representation

- The A'' representation corresponds to out-of-plane motion.
- The A'' representation corresponds to a 2×2 block with determinant not equal to zero.
- The eigenvalues are $(\pm i\omega_0)$ for $n = 1$ and $(\pm i\omega_1 = \pm ia/Z)$ for $n > 1$ where $a^3 = r_0$.

The B' representation

- The B' representation corresponds to in-plane motion.
- The B' representation corresponds to a 4×4 block with determinant not equal to zero.
- The eigenvalues are $(\pm\lambda, \pm i\omega_2)$.

The B'' representation

- The B'' representation corresponds to out-of-plane motion.
- The B'' representation corresponds to a 2×2 block with determinant not equal to zero.
- The eigenvalues are $(\pm i\omega_0)$ if $n = 2$ and $(\pm i\omega_3)$ for $n > 2$.

The E'_1 representation

- The E'_1 representation corresponds to in-plane motion.
- The E'_1 representation corresponds to an 8×8 block with determinant not equal to zero.
- It can be further reduced to two 4×4 blocks. The blocks being complex conjugates of each other.
- The eigenvalues are $(\pm i\omega_4, \pm i\omega_4, a \pm ib, -a \pm ib)$

The E_1'' representation

- The E_1'' representation corresponds to out-of-plane motion.
- The E_1'' representation corresponds to a 4×4 block with determinant not equal to zero.
- It can be further reduced to two 2×2 blocks. The blocks being complex conjugates of each other.
- The eigenvalues are $(\pm i\omega_0, \pm i\omega_0)$ if $n = 3$ and $(\pm i\omega_5, \pm i\omega_5)$ for $n > 3$

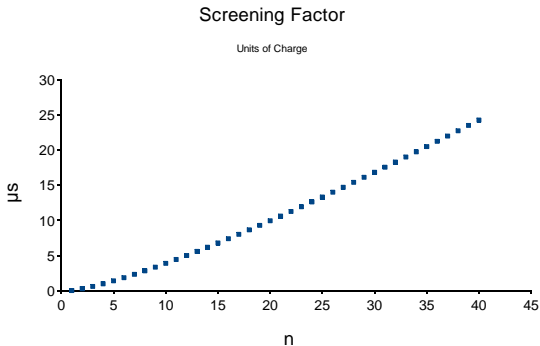
Summary

The principle relative equilibria for the Coulomb $(n + 1)$ -body problem is not linearly stable. In fact, it is a highly degenerate $(n - 1)$ -rank saddle.

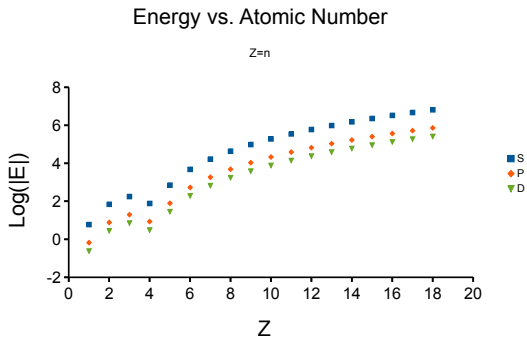
Degeneracies

n	Element	ω_0	Saddle	Single	Double	modes
1	H	2+1	0	0	0	3
2	He	2+1	1	2	0	6
3	Li	3+1	2	1	2	9
4	Be	3+1	3	3	2	12
5	B	3+1	4	1	6	15
6	C	3+1	5	3	6	18
7	N	3+1	6	1	10	21
8	O	3+1	7	3	10	24
9	F	3+1	8	1	14	27
10	Ne	3+1	9	3	14	30

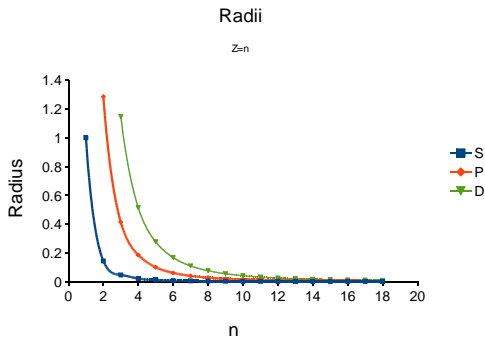
The Screening Factors



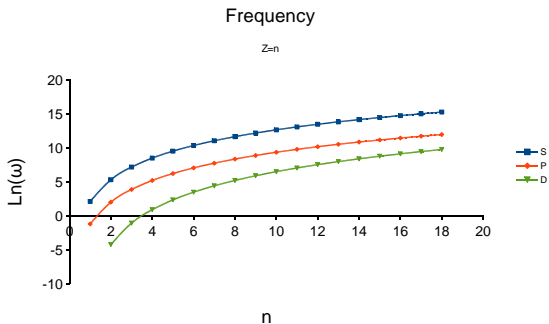
The Energies



The Radii



The Frequencies



The Future

- Other Relative Equilibria?
- Choreographies?
- Use correct symmetry to include quantum effects (permutation-inversion group).
- Unravel the dynamics of the complex quartic (a rotating saddle)!
- Semiclassical Quantization (already done for $n = 1$, submitted to Accounts of Theoretical Chemistry)!

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