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 $M >> 1$.

Meyer's summary

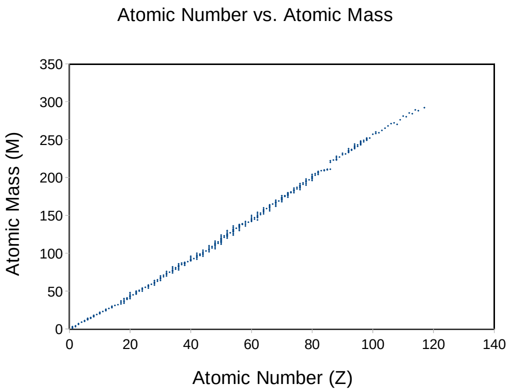
The study of relative equilibria (r.e.) of the N-body problem has had a long history starting with the famous collinear configuration of the 3-body problem found by Euler (1767). Over the intervening years many different technologies have been applied to the study of r.e. In the older papers of Euler (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.)

$$
\begin{aligned}
1.8 \times 10^3 &\leq M \leq 5.4 \times 10^5 \\
1 &\leq Z \leq 118
\end{aligned}
$$

Atomic Mass vs Atomic Number



The Hamiltonians

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

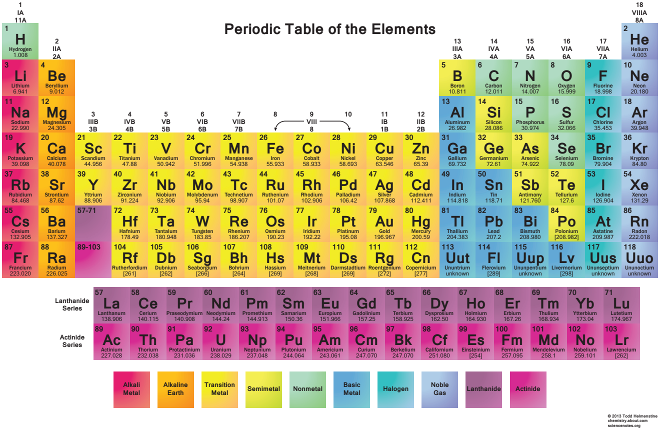
$$\pm \sum_{i=1}^{n-1}\sum_{j=i}^{n}\frac{1}{\sqrt{(\rho_i^2 + \rho_j^2 - 2\rho_i\rho_j\cos(\theta_j - \theta_i)) + (z_j - z_i)^2}}$$

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."

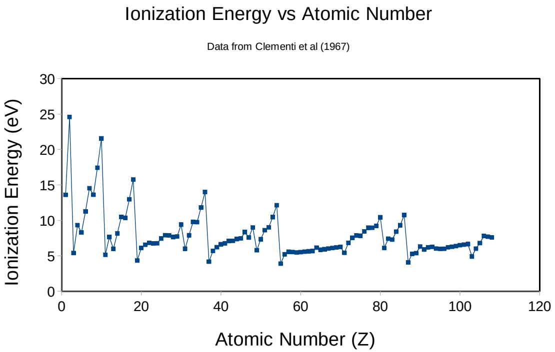
Periodic Table



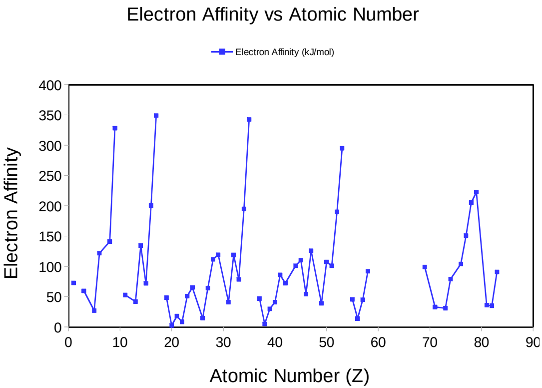
I recommend the following web resource to my students:

http://www.ptable.com/

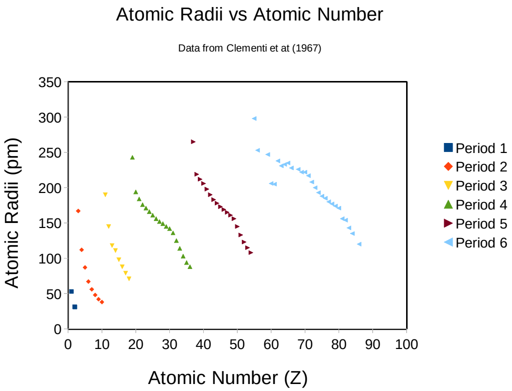
Ionization Energy vs Atomic Number



Electron Affinity vs Atomic Number



Atomic Radii vs Atomic Number

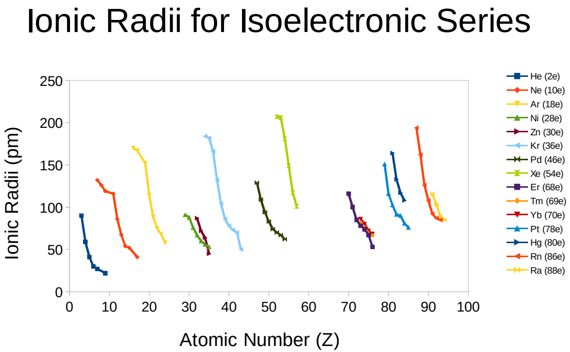


Isoelectronic Series

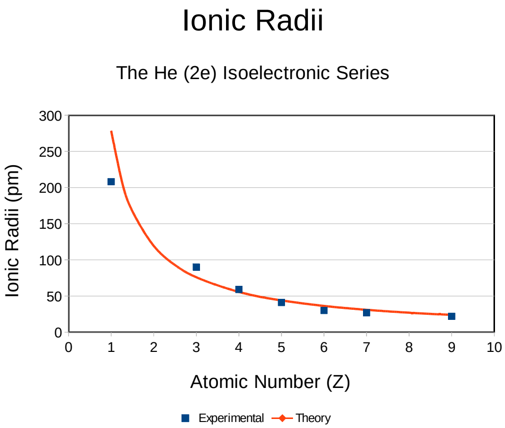
Keep the number of electrons n fixed while varying the nuclear charge Z.

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 the He Isoelectronic Series



Linearized Equations of Motion

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

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

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

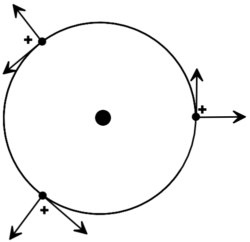
1. Transform to rotating frame.
2. Transform to symmetry variables.
3. Decouple the coordinates from the momenta.
4. Diagonalize and balance the Hessian via a sequence of rotations and scalings.
5. Transform to complex coordinates.
6. Multiply by J.

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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- 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 $n > 3$

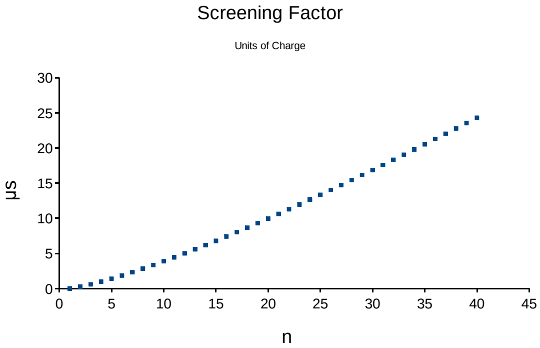
Summary

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.

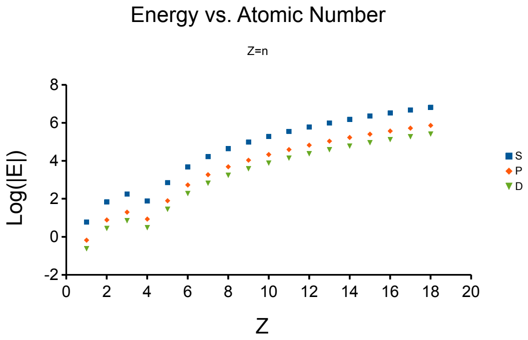
Degeneracies

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

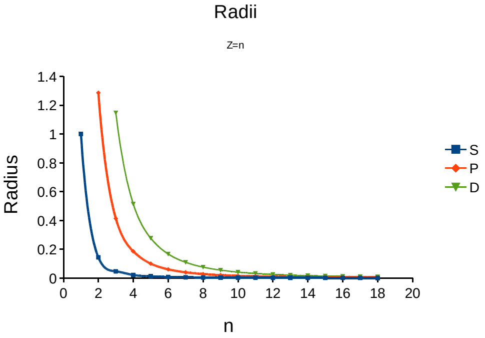
The Screening Factors



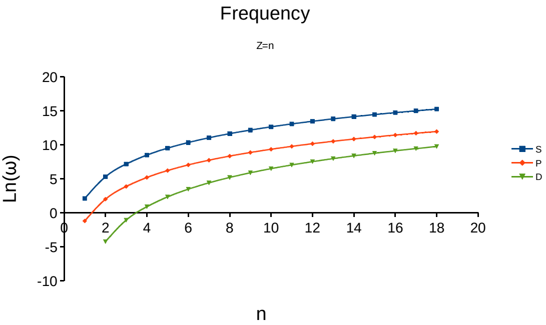
The Energies



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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