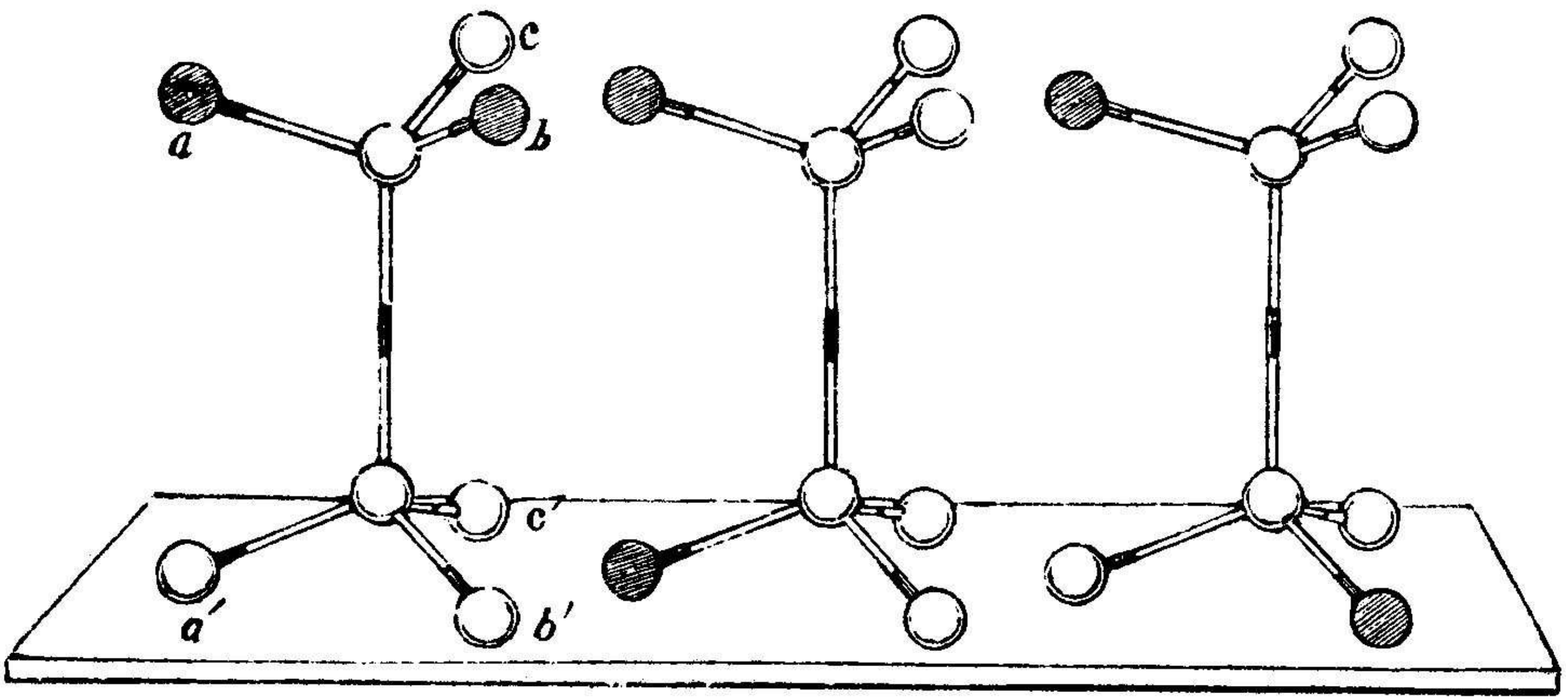
Born, Kirkwood, Lord Kelvin, Kepler
– spotkanie idei

Tomasz Grycuk

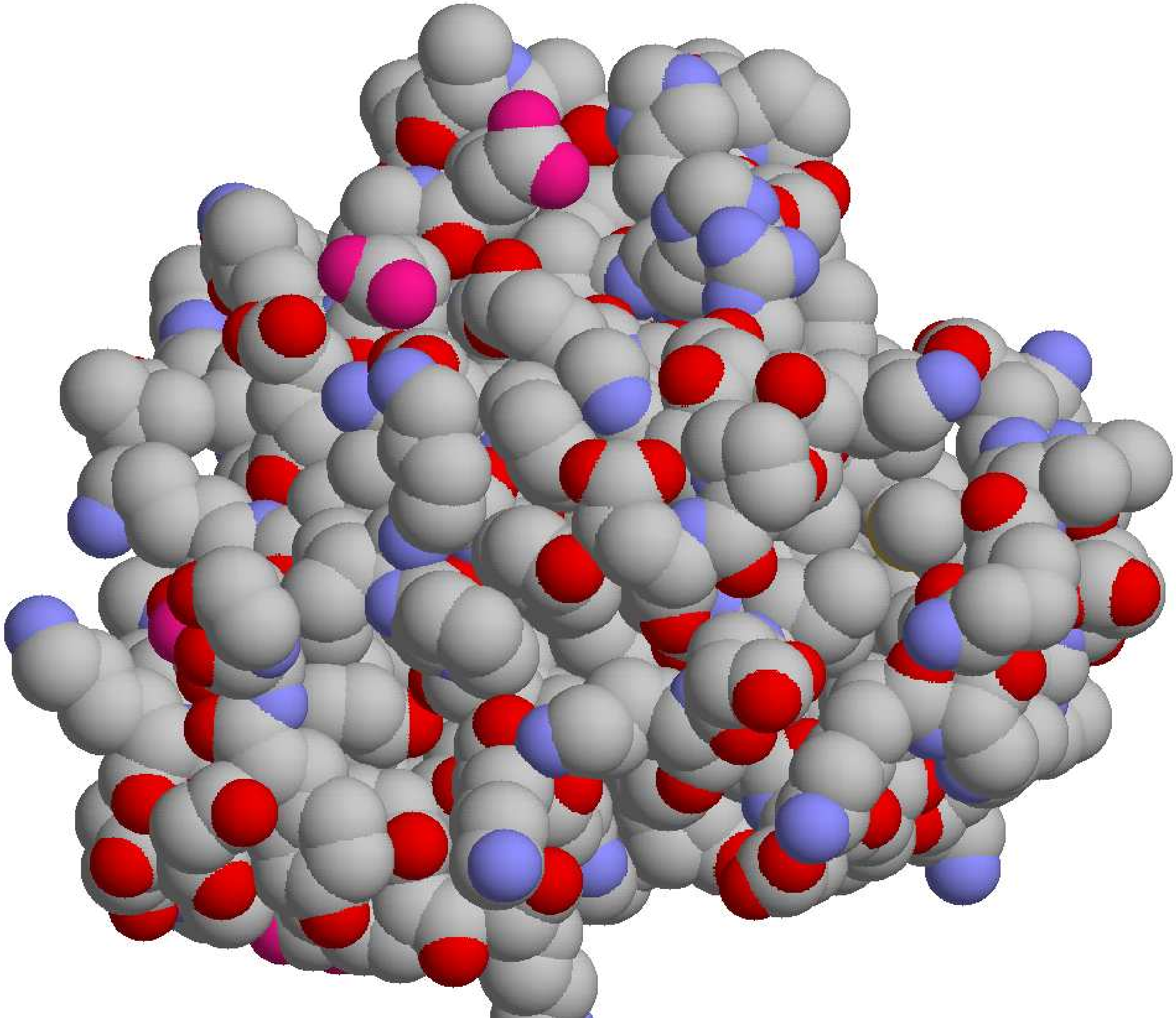
Sympozjum IFD
grudzień 2004

Paterno E. (1869) Giornale di Scienze Naturali ed Economiche di Palermo, 5, 117-122

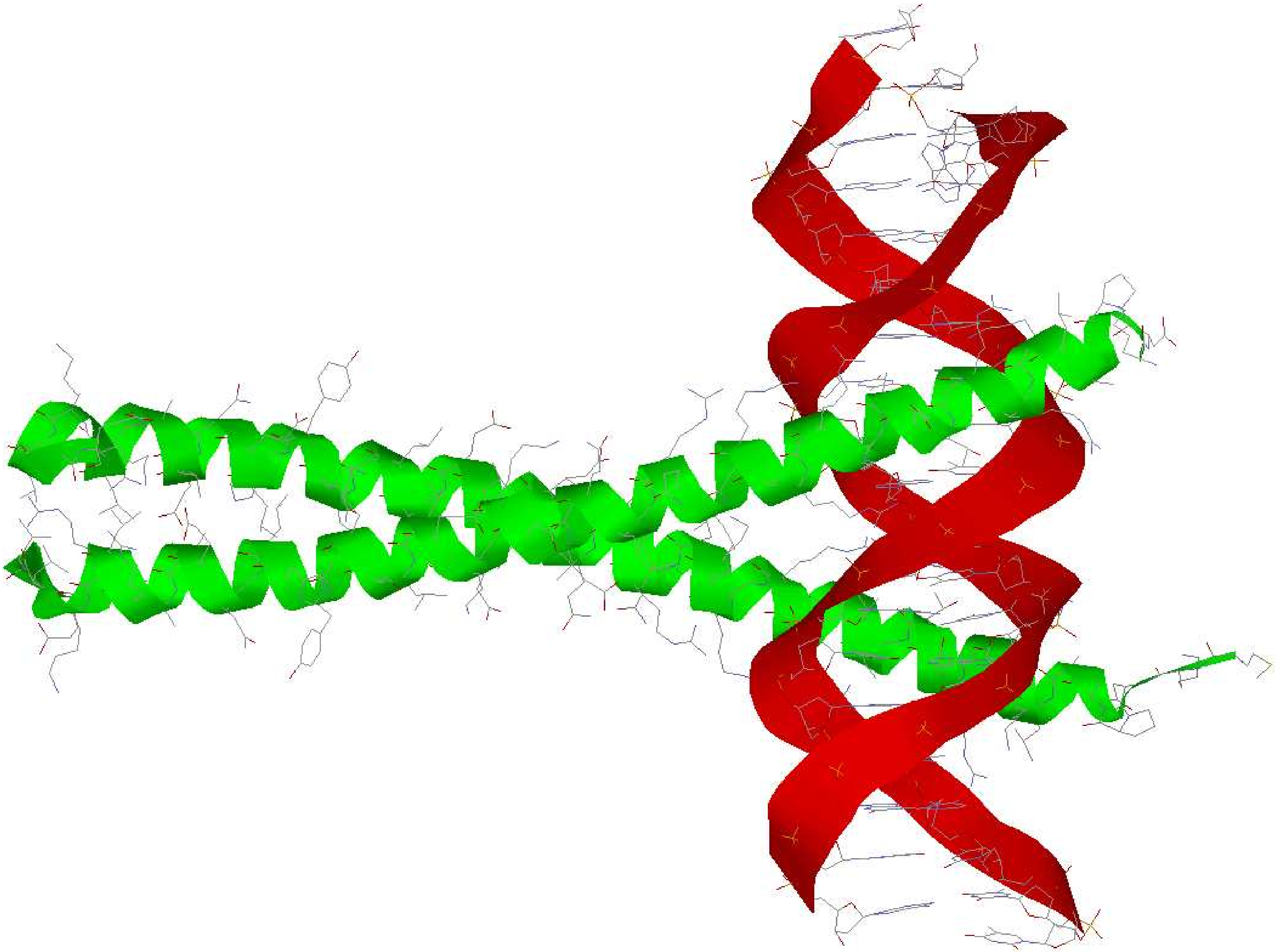


È superfluo dire che questo non è altro che un modo di rappresentare i fatti, e che tutte queste idee hanno bisogno di prove sperimentali.

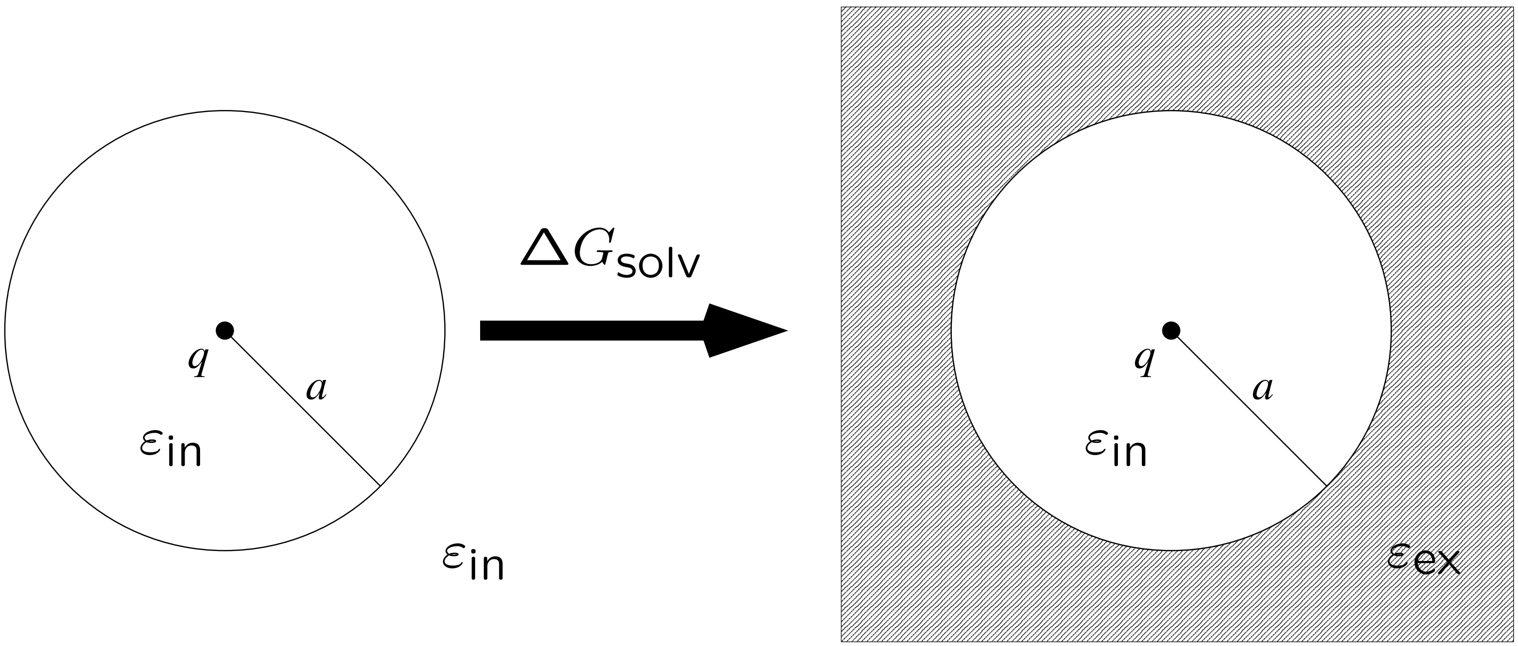
Kendrew JC at al. (1958) Nature 181, 662-6



Natura oddziaływań molekularnych



Born M. (1920) Z. Phys. 1, 45-48



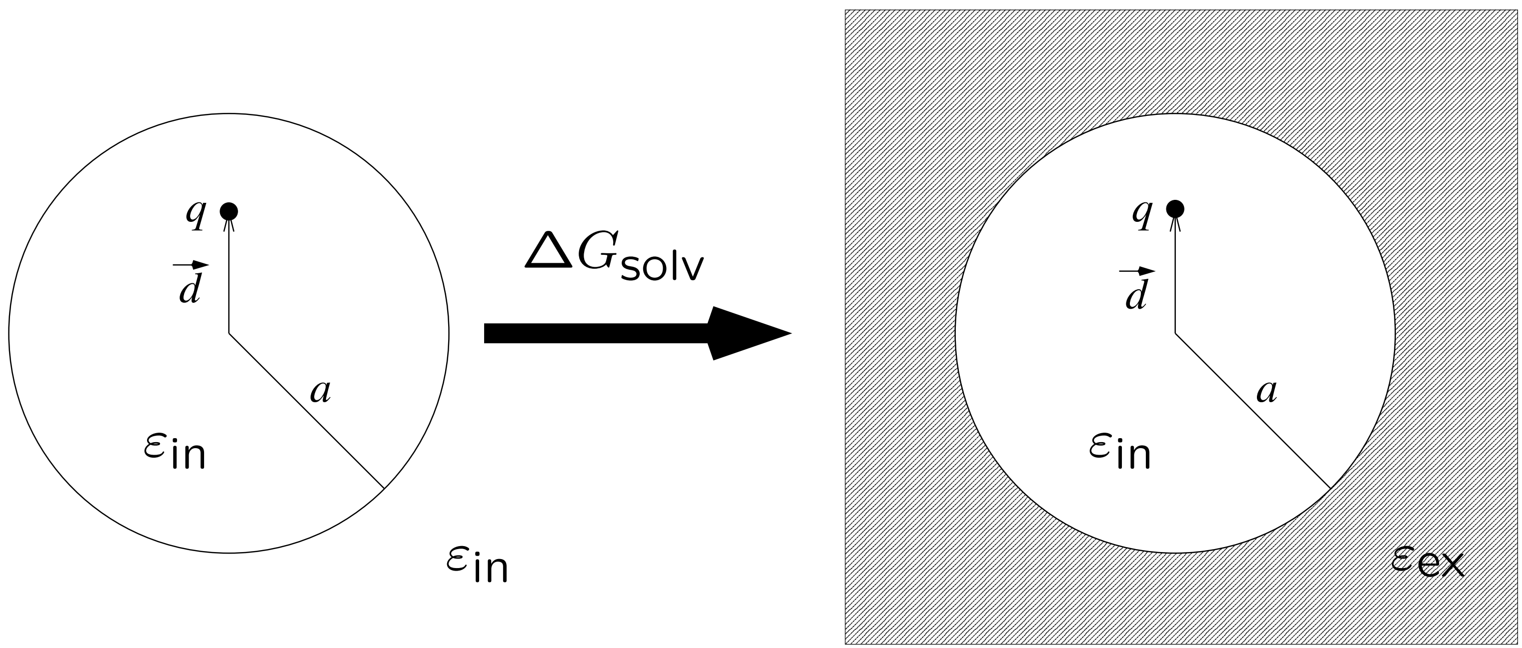
Energia solwatacji:

$$\Delta G_{\text{solv}} = \frac{-q^2}{8\pi\varepsilon_0}\left(\frac{1}{\varepsilon_{\text{in}}} - \frac{1}{\varepsilon_{\text{ex}}}\right)\frac{1}{a}$$

Promień Borna:

$$R = a$$

Kirkwood J. G. (1934) J. Chem. Phys. 2, 351- 361

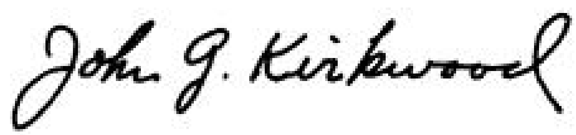


Energia solwatacji:

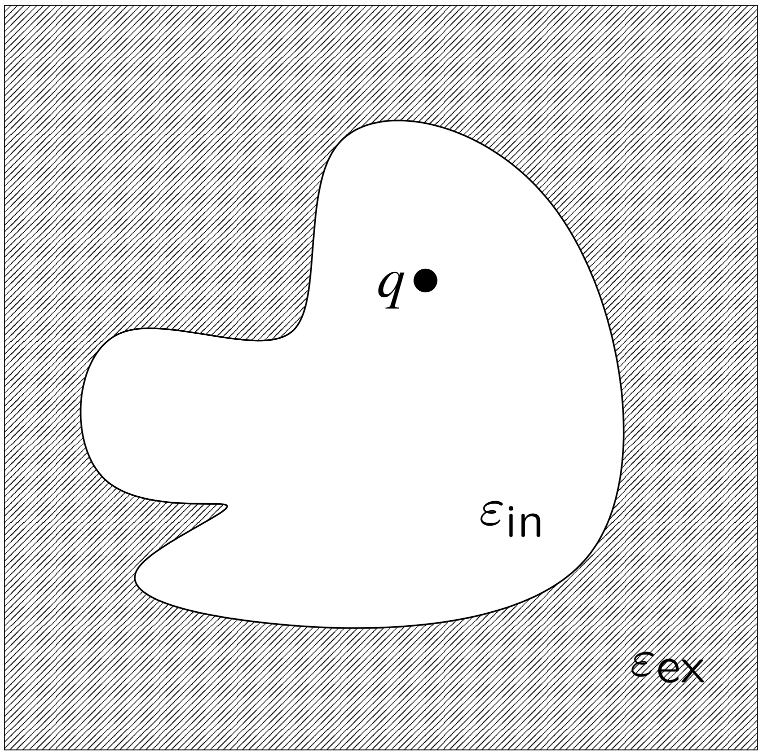
$$\Delta G_{\text{solv}} = \frac{-q^2}{8\pi\varepsilon_0}\left(\frac{1}{\varepsilon_{\text{in}}} - \frac{1}{\varepsilon_{\text{ex}}}\right)\frac{1}{a}\sum_{l=0}^{\infty}\frac{1}{1+\frac{l}{l+1}\frac{\varepsilon_{\text{in}}}{\varepsilon_{\text{ex}}}}\left(\frac{d}{a}\right)^{2l}$$

John Gamble Kirkwood

May 30, 1907 – August 9, 1959



Constanciel R., Contreras R. (1984) Theor. Chim. Acta 65, 1



Energia solwatacji:

$$\Delta G_{\text{solv}} = \frac{1}{2}\int (\mathbf{E}\cdot\mathbf{D} - \mathbf{E}_{\text{in}}\cdot\mathbf{D}_{\text{in}})\,\mathrm{d}V$$

Przybliżenie pola coulombowskiego:

$$\mathbf{D}(\mathbf{r}) \approx \frac{q}{4\pi}\frac{\mathbf{r}}{r^3}$$

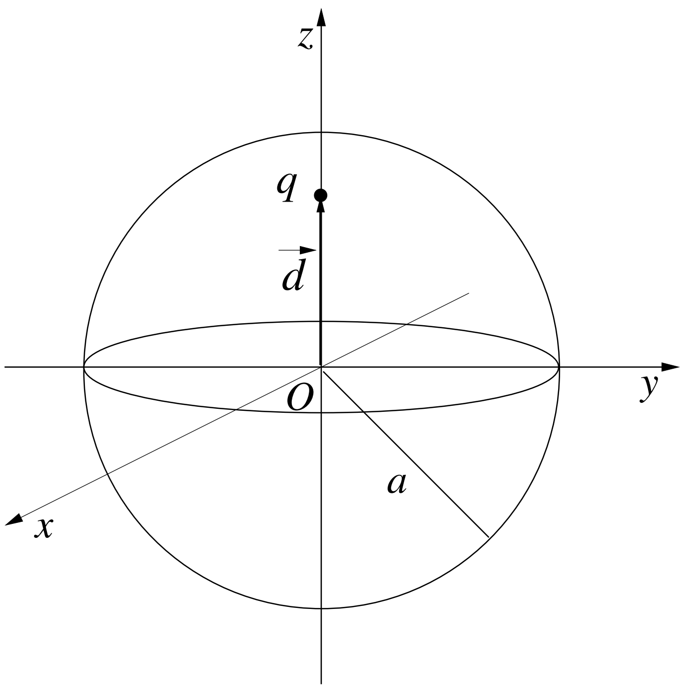
Uogólniony model Borna:

$$\Delta G_{\text{solv}} \approx \frac{-q^2}{8\pi\varepsilon_0}\left(\frac{1}{\varepsilon_{\text{in}}} - \frac{1}{\varepsilon_{\text{ex}}}\right)\underbrace{\frac{1}{4\pi}\int_{\text{ex}}\frac{1}{r^4}\,\mathrm{d}V}_{1/R}$$

Odwrotność **promienia Borna**:

$$\frac{1}{R} = \frac{1}{4\pi}\int_{\text{ex}}\frac{1}{r^4}\,\mathrm{d}V$$

Grycuk T. (2003) J. Chem. Phys. 119, 4817-4826



Energia solwatacji:

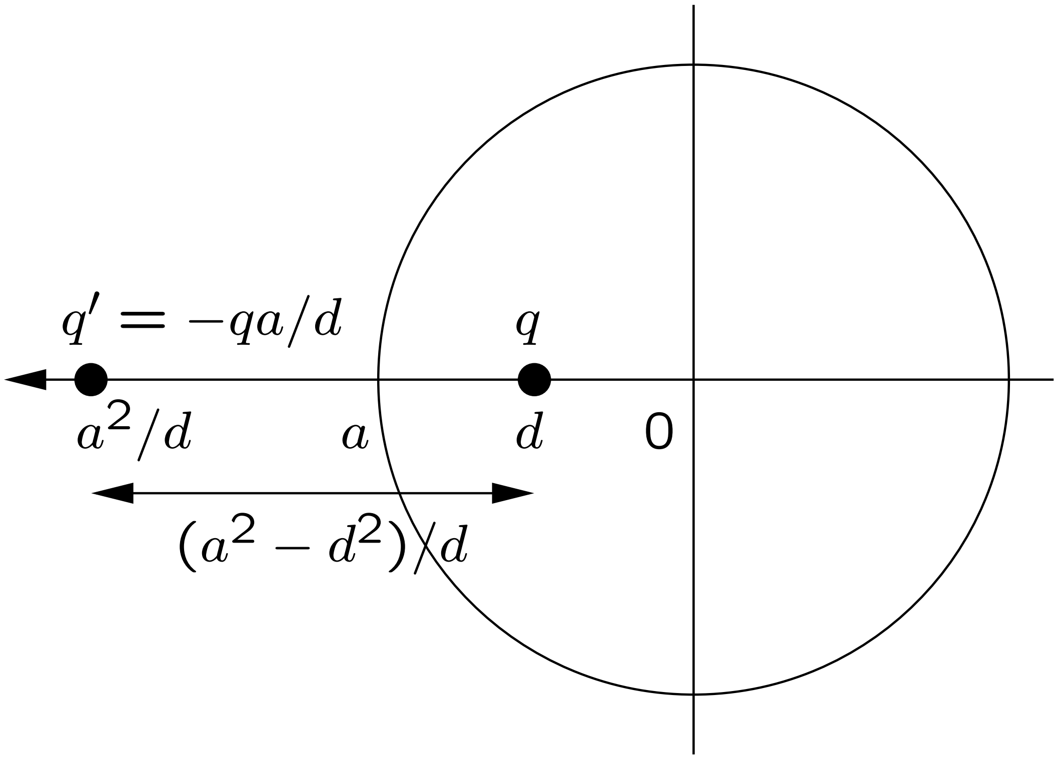
$$\Delta G_{\mathrm{solv}} = \frac{-q^2}{8\pi\varepsilon_0}\left(\frac{1}{\varepsilon_{\mathrm{in}}} - \frac{1}{\varepsilon_{\mathrm{ex}}}\right)\frac{1}{a}\sum_{l=0}^{\infty}\frac{1}{1+\frac{l}{l+1}\frac{\varepsilon_{\mathrm{in}}}{\varepsilon_{\mathrm{ex}}}}\left(\frac{d}{a}\right)^{2l}$$

$$\approx \frac{-q^2}{8\pi\varepsilon_0}\left(\frac{1}{\varepsilon_{\mathrm{in}}} - \frac{1}{\varepsilon_{\mathrm{ex}}}\right)\underbrace{\frac{1}{a\,(1-(d/a)^2)}}_{1/R}$$

Odwrotność **promienia Borna**:

$$\frac{1}{R} \approx \frac{1}{a\left(1-(d/a)^2\right)} = \left(\frac{3}{4\pi}\int_{\mathrm{ex}}\frac{1}{|\mathbf{r}-\mathbf{d}|^6}\,\mathrm{d}V\right)^{1/3}$$

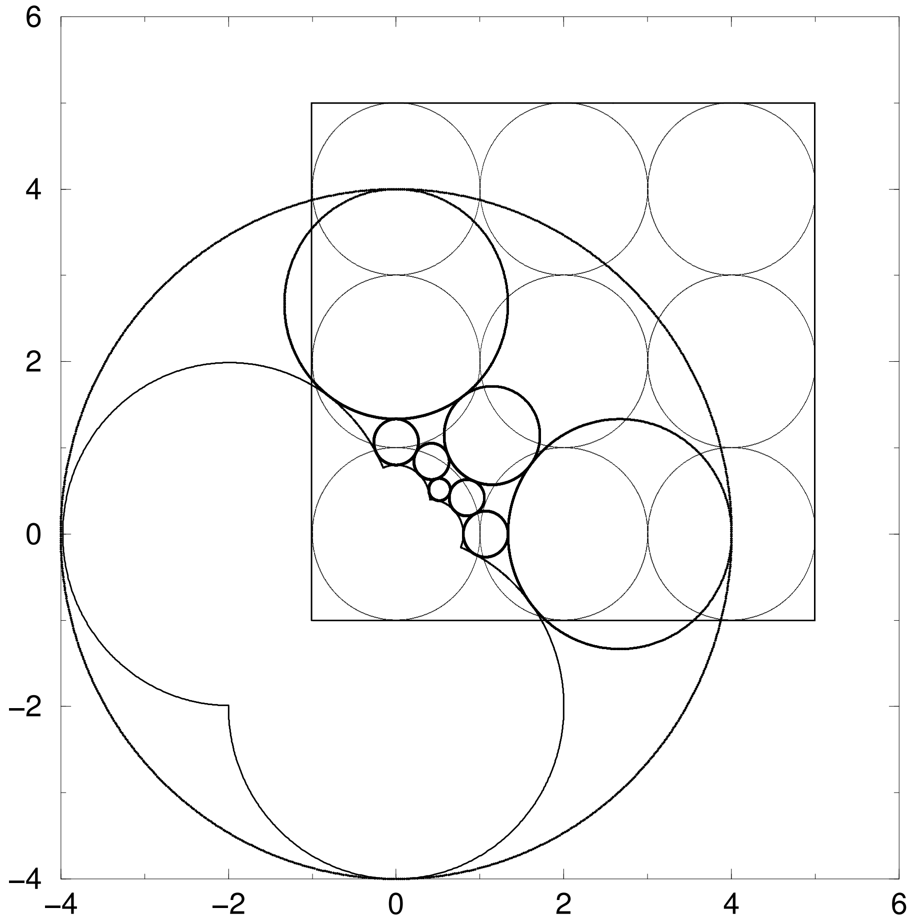
Metoda obrazów



Energia solwatacji:

$$\Delta G_{\mathsf{solv}} \sim qq' \frac{d}{a^2 - d^2} = \frac{-q^2}{a\left(1 - (d/a)^2\right)}$$

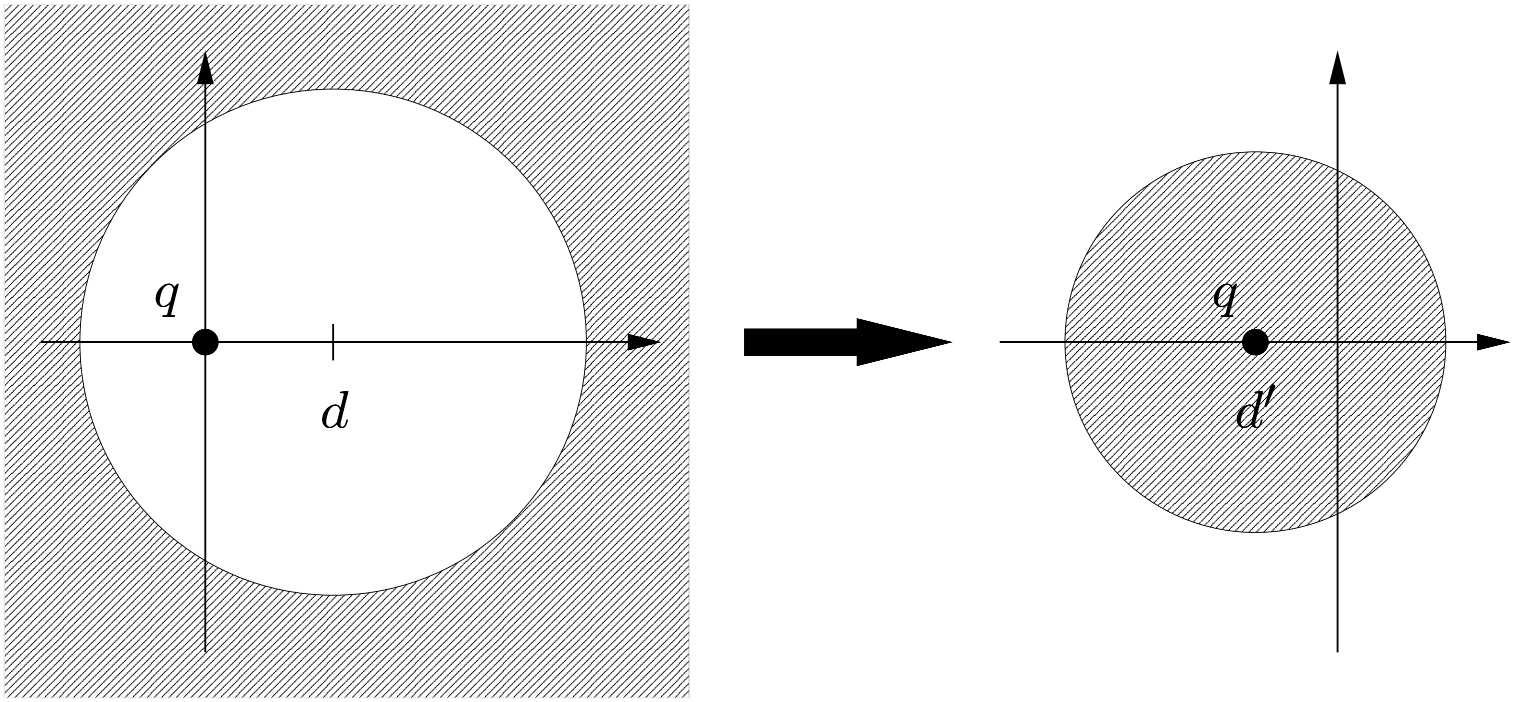
Transformacja Kelvina ($\mathbf{r} \to \frac{R^2}{r^2}\mathbf{r}$) i geometria



Sfera przechodzi w sferę:

$$\mathbf{d} \to \frac{R^2}{d^2 - a^2}\,\mathbf{d}, \qquad a \to \frac{R^2}{|a^2 - d^2|}\,a$$

Transformacja Kelvina i równania elektrostatyki



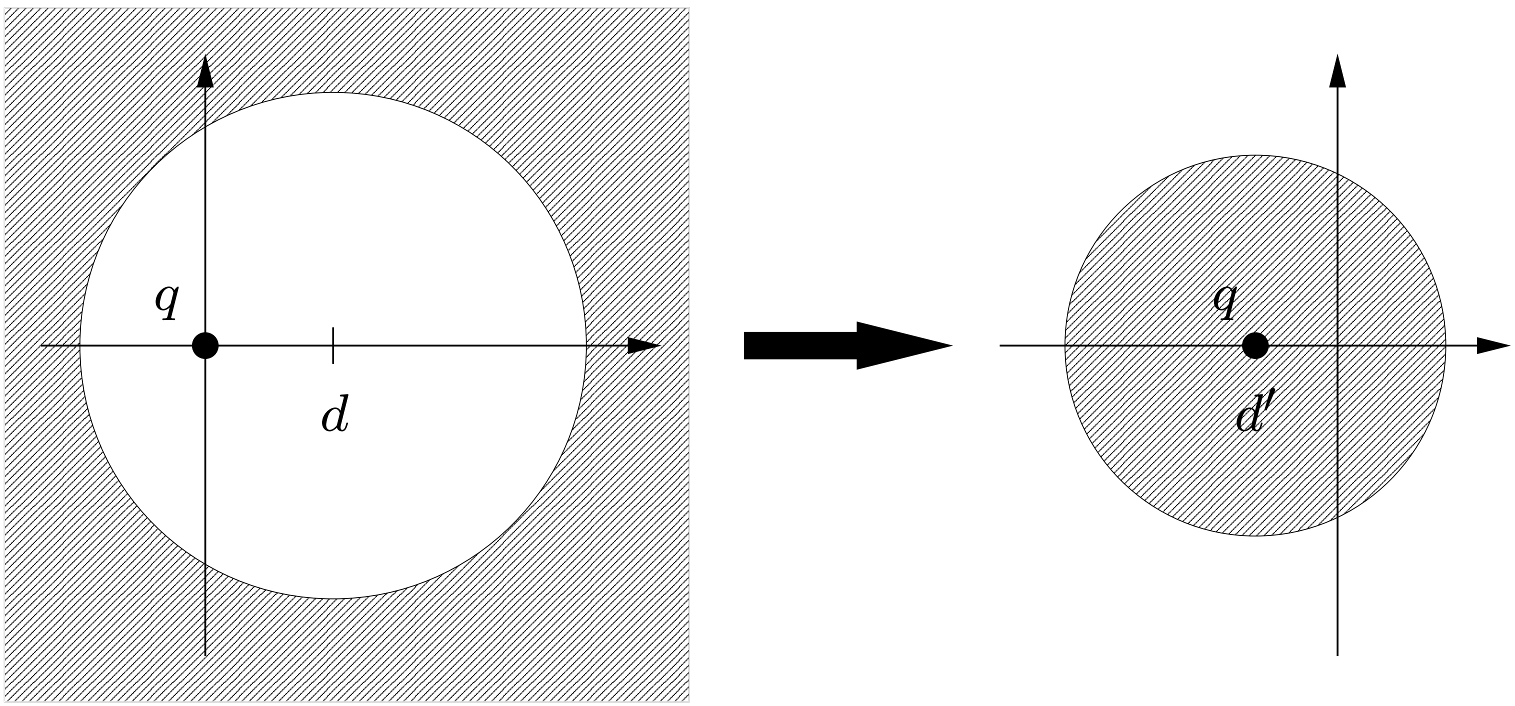
Energia solwatacji:

$$\Delta G_{\mathsf{solv}} \sim \frac{-q^2}{(a^2 - d^2)/a} \qquad\qquad a' = \frac{R^2 a}{a^2 - d^2}$$

Promień inwersji:

$$R = a' = \frac{a^2 - d^2}{a}.$$

Transformacja Kelvina i promień Borna

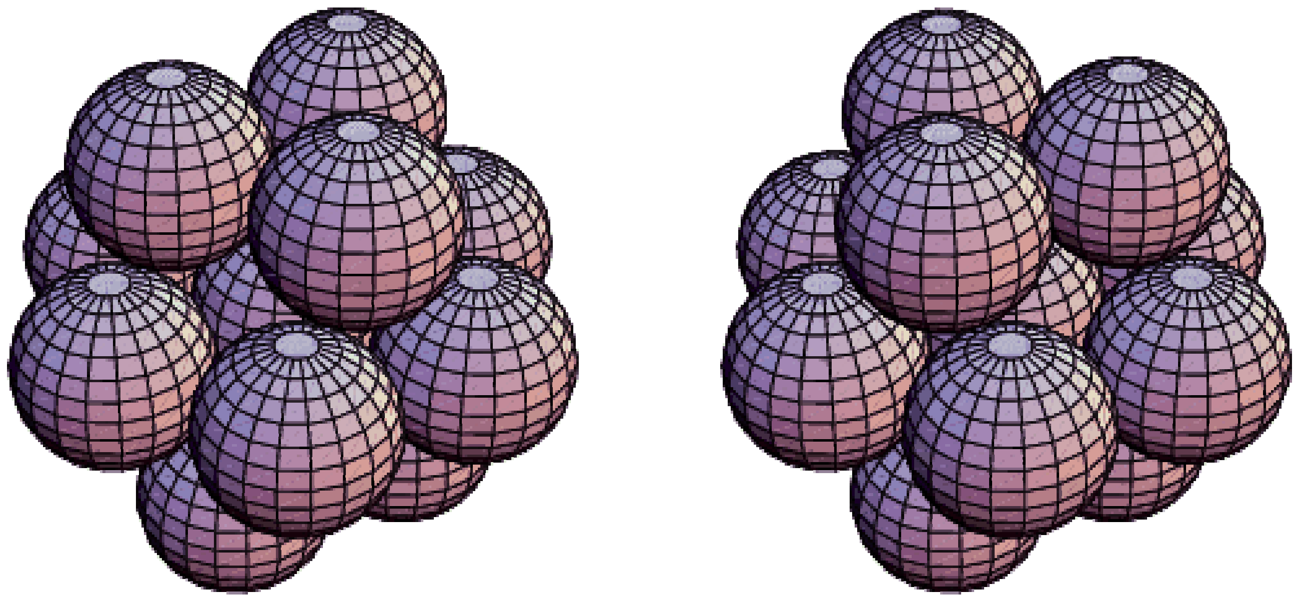


$$\int_{\text{ex}} \frac{1}{r^6}\,\mathrm{d}V = \int_{\text{in}'} \frac{1}{R^6}\,\mathrm{d}V' = \frac{4\pi}{3}\frac{1}{R^3}$$

i odwrotność **promienia Borna**:

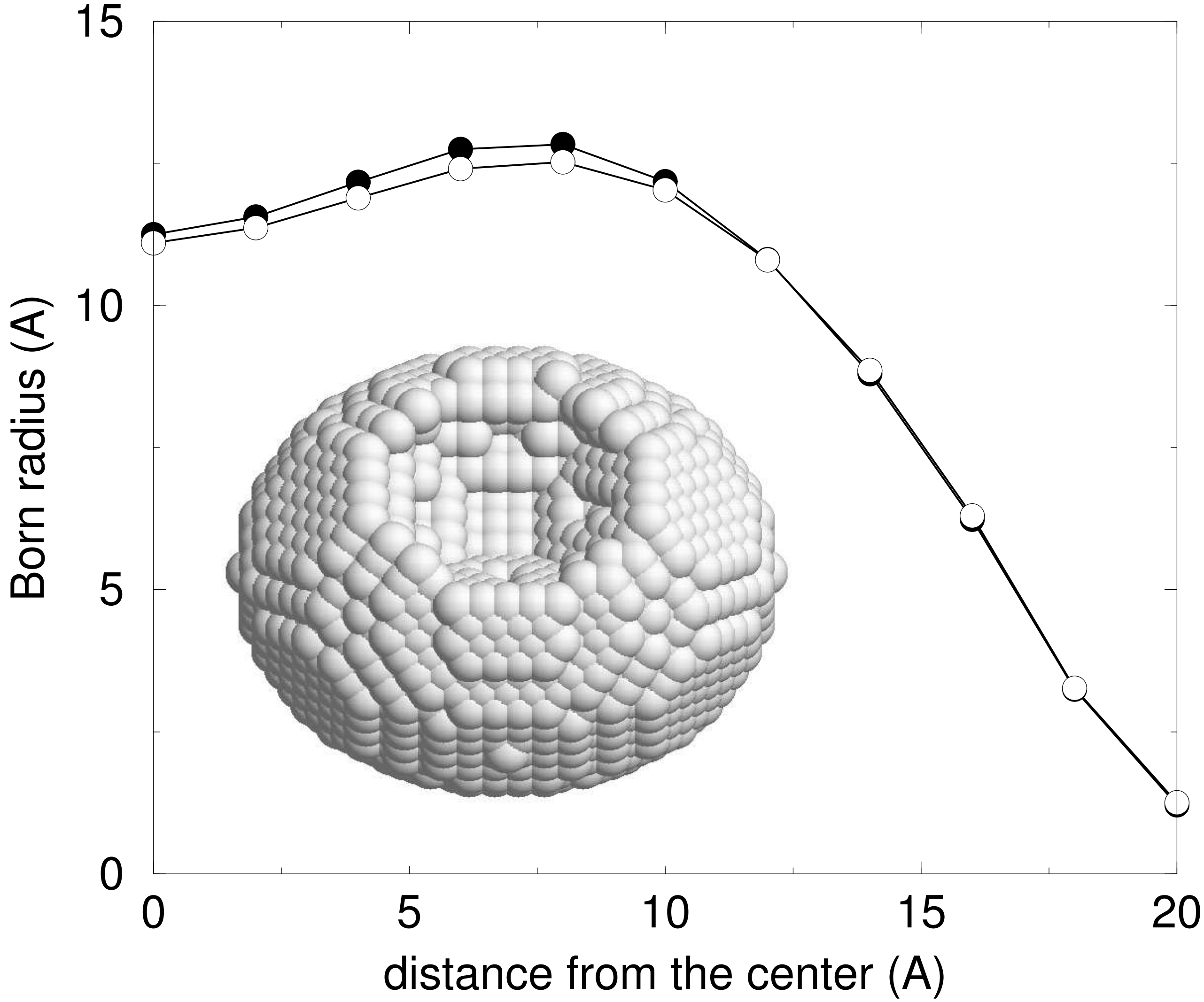
$$\frac{1}{R} = \left(\frac{3}{4\pi}\int_{\text{ex}} \frac{1}{r^6}\,\mathrm{d}V\right)^{1/3}$$

Kelper J. (1611)



$\pi/(3\sqrt{2})$

spotkanie idei



The Nobel Prize in Physics 1954

"for his fundamental research in quantum mechanics, especially for his statistical interpretation of the wavefunction"

"for the coincidence method and his discoveries made therewith"

Max Born

1/2 of the prize

United Kingdom

Edinburgh University
Edinburgh, United Kingdom

b. 1882
(in Breslau, then Germany)
d. 1970

Walther Bothe

1/2 of the prize

Federal Republic of Germany

University of Heidelberg;
Max-Planck-Institut für medizinische Forschung
Heidelberg, Federal Republic of Germany

b. 1891
d. 1957

The Nobel Prize in Physics 1954
Presentation Speech

Max Born
Biography
Nobel Lecture
Banquet Speech

Walther Bothe
Biography
Nobel Lecture
Other Resources

1953 1955

The 1954 Prize in:
Physics
Chemistry
Physiology or Medicine
Literature
Peace

Find a Laureate:
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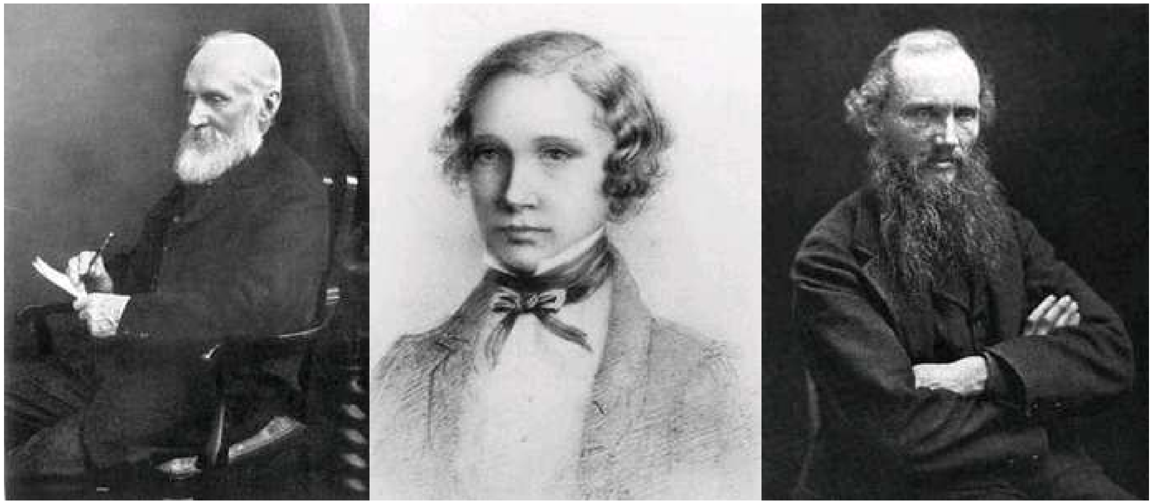
Last modified June 16, 2000

William Thomson (Lord Kelvin)

(1824 – 1907)

William Thomson
(Lord Kelvin)



1824 až 1907

termodynamika

Thomson vytvořil roku 1853 matematickou teorii, která se týkala elektrických vln.

William Thomson splečně s Jamesem Joulem objevili roku 1852, že dostatečně ochlazený plyn, který proudí tryskou z prostoru vysokého tlaku do prostoru s tlakem nižším, se mírně ochladí.

V roce 1853 podal William Thomson definici zákona zachování energie: Jako energii nějaké hmotné soustavy v určitém stavu označujeme souhrn účinků měřených jednotkami práce, a to vyvolaných mimi tuto soustavu, kdykoliv soustava přechází ze svého stavu jakýmkoiv způsobem do libovolně zvoleného základního stavu.

Nemalý podíl měl Thomson na formulování druhého termodynamického zákona.

V roce 1878 vytvořil William Thomson teorii pyroelektřiny.

Branch of Science ▸ Astronomers ▾
Nationality ▸ German ▾

Kepler, Johannes (1571-1630)

Austrian mathematician and astronomer who got himself taken on as an assistant to Brahe in order to get access to his planetary tables. Kepler had been trained as a Platonist and Neopythagorean, and was given to rather mystical views, as exemplified in his work *Mysterium Cosmographicum.* Nevertheless, Kepler was also a confirmed Copernican. In fact, he wanted to use Tycho's data to prove the validity of the Copernican theory. He analyzed the vast amount of data upon Brahe's death. From this data, he prepared new planetary tables (called the Rudolphine Tables). At first, he determined the shape of planetary orbits to be ovoid, but rejected this result for aesthetic reasons. Going back over his calculations, he found and corrected an error. The new shape turned out to be an ellipse, which fit well into Kepler's Pythagorean views on nature.

Kepler tried all sorts of mystical notions to describe planetary orbits, using the Platonic solids and musical analogies. Spread out through his voluminous calculations in *Astronomia Nova,* however, were three gems: Kepler's laws of planetary motion. For the formulation of these laws, Kepler is considered the founder of physical astronomy. The first law states that the planets move in elliptical orbits with the Sun at one focus. The second law states that the planets sweep out equal areas in equal times (which is equivalent to the statement of conservation of angular momentum.) The third law states that the period squared in proportional to the semimajor axis cubed. Kepler believed that the planets were kept in their orbits by a "anima motrix" (motive soul), but later modified it to "vis motrix" (life force). He also studied optics as an aspect of astronomy in *Astronomiae Pars Optica* (1604), and developed the concept of a ray.