Elementary atoms in spaces of constant curvature by the Nikiforov-Uvarov method

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Physics and geometry

There is currently no clear-cut answer to the question of what geometry is because "the meaning of the word geometry changes with time and with the speaker" (S.-S. Chern, From triangles to manifolds.)

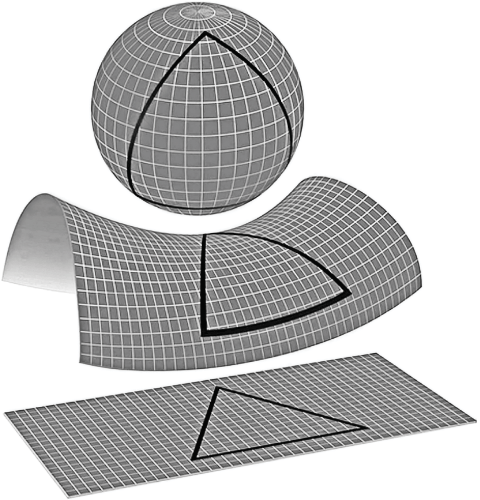
- Classical mechanics was closely connected with geometry from the very beginning (Newton, Huygens, Hamilton, Poincaré, Birkhoff).
- However, the geometries underlying Hamiltonian mechanics were a new type of geometry, namely symplectic geometry and its odd-dimensional cousin, contact geometry.
- Before Lobachevsky, the question "Does another geometry exist besides Euclidean geometry?" did not even arise.
- The recognition of non-Euclidean geometry was not easy. Chernyshevsky wrote to his sons from exile that all of Kazan laughed at Lobachevsky: "What is «ray curvature» or «curved space»? What is geometry without the axiom of parallel lines?" (S. G. Gindikin, Stories about physicists and mathematicians.)

Physics and geometry

- None of the serious scientists paid attention to Lobachevsky's publications in Russian.
- None of the French mathematicians paid attention to his latest work either.
- There were no German readers for his book in German. With one, but important, exception.
- Gauss read his short book in German and was so impressed that he began to study Russian.
- He succeeded in getting Lobachevsky elected as a corresponding member of the Royal Scientific Society of Göttingen.
- However, despite Gauss's support, Lobachevsky died without having achieved recognition of his ideas.

(V.V. Prasolov, A.B. Skopenkov, Reflections on the recognition of Lobachevsky geometry. V.G. Boltyansky, A.P. Savin Conversations about mathematics.)

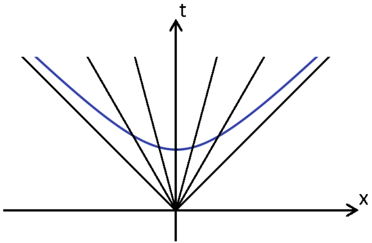
$$\alpha+\beta+\gamma-\pi=\kappa A.$$



The Friedmann-Lemaitre-Robertson-Walker metric used to describe cosmic spacetime is based on the cosmological principle that assumes homogeneity and isotropy throughout the Universe.

$$ds^2 = c^2 dt^2 - a^2(t)\left[\frac{dr^2}{1-\kappa r^2} + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)\right]$$

The concepts of a curved or flat three-dimensional space are largely conditional, depending on the method of choosing the time coordinate (Ya.B. Zeldovich, The theory of the expanding Universe, created by A.A. Friedman).



The Milne model demonstrates the relativity of space in the most striking way: a spatial slice of the same quarter of Minkowski spacetime has Euclidean geometry for the usual foliation and negatively curved hyperbolic geometry for the Milne foliation.

- An analogue of the Newton force for hyperbolic space was proposed by Lobachevsky.
- An analytical expression for the Newtonian potential in $\mathbb{H}^3$ was obtained in 1870 by Schering.
- In 1873, Lipschitz considered the motion of one body in a central potential on the sphere $\mathbb{S}^2$.
- In 1885, Killing found a generalization of all three Kepler laws to the case of the sphere $\mathbb{S}^3$. In 1886, similar results were published by Neumann.
- An extension of these results to the hyperbolic case was carried out by Liebmann in 1902. In 1903, he also proved a generalization of Bertrand's theorem for the spaces $\mathbb{S}^2$ and $\mathbb{H}^2$.
- Classical mechanics in spaces of constant curvature can be considered the predecessor of special and general relativity. After the emergence of these theories, the above-mentioned works of Schering, Killing and Liebmann were almost completely forgotten.

A.V. Shchepetilov, Comment on "Central potentials on spaces of constant curvature: The Kepler problem on the two-dimensional sphere $\mathbb{S}^2$ and the hyperbolic plane $\mathbb{H}^2$"

New parameterization of the length element

$$S_\kappa(x) = \begin{cases} \frac{1}{\sqrt{\kappa}} \sin\left(\sqrt{\kappa}x\right), \text{ if } \kappa > 0, \\ x, \text{ if } \kappa = 0, \\ \frac{1}{\sqrt{-\kappa}} \sinh\left(\sqrt{-\kappa}x\right), \text{ if } \kappa < 0. \end{cases} \quad C_\kappa(x) = \begin{cases} \cos\left(\sqrt{\kappa}x\right), \text{ if } \kappa > 0, \\ 1, \text{ if } \kappa = 0, \\ \cosh\left(\sqrt{-\kappa}x\right), \text{ if } \kappa < 0. \end{cases}$$

$$C_\kappa^2 + \kappa S_\kappa^2 = 1,\ S_\kappa' = C_\kappa,\ C_\kappa' = -\kappa S_\kappa,\ T_\kappa = \frac{S_\kappa}{C_\kappa},\ 1 + \kappa T_\kappa^2 = \frac{1}{C_\kappa^2},\ \kappa + \frac{1}{T_\kappa^2} = \frac{1}{S_\kappa^2}.$$

Old parameterization $dl^2 = \frac{dr^2}{1-\kappa r^2} + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)$.

$$r = S_\kappa(\rho).$$

New parameterization $dl^2 = d\rho^2 + S_\kappa^2(\rho)(d\theta^2 + \sin^2\theta\, d\varphi^2)$.

In what follows $\rho \to r$.

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Coulomb potential in spaces of constant curvature

Poisson's equation: $\Delta\phi(r) = -4\pi q\delta(\vec{r})$.
Laplace-Beltrami operator:

$$\Delta = \frac{1}{\sqrt{|g|}}\frac{\partial}{\partial x^i}\left(\sqrt{|g|}g^{ij}\frac{\partial}{\partial x^j}\right).$$

Metric tensor: $g_{ij} = \mathrm{diag}(1, S_\kappa^2(r), S_\kappa^2(r)\sin^2\theta)$.
Laplace equation for the central potential of a point charge in spaces of constant curvature:

$$\frac{1}{S_\kappa^2(r)}\frac{d}{dr}\left(S_\kappa^2(r)\frac{d\phi}{dr}\right) = 0.$$

Coulomb potential energy in spaces of constant curvature for the hydrogen atom:

$$V(r) = -\frac{e^2}{T_\kappa(r)}.$$

$$\left[-\Delta + \frac{2m}{\hbar^2}V\right]\Psi = \frac{2m}{\hbar^2}E\Psi.$$

Laplace-Beltrami operator:

$$\Delta = \frac{1}{\sqrt{|g|}}\frac{\partial}{\partial x^i}\left(\sqrt{|g|}g^{ij}\frac{\partial}{\partial x^j}\right).$$

Metric tensor: $g_{ij} = \mathrm{diag}(1, S_\kappa^2(r), S_\kappa^2(r)\sin^2\theta)$.

$$\Psi = Y_{lm}(\theta,\varphi)G(r).$$

Radial equation:

$$\left[-\frac{1}{S_\kappa^2(r)}\frac{d}{dr}\left(S_\kappa^2(r)\frac{d}{dr}\right)+\frac{l(l+1)}{S_\kappa^2 r)}+\frac{2m}{\hbar^2}V-\frac{2m}{\hbar^2}E\right]G(r)=0.$$

Dimensionless variable:

$$z=\frac{1}{\sqrt{\kappa}\,T_\kappa(r)}.$$

The equation to be solved is:

$$\frac{d^2G}{dz^2}+\frac{\lambda_E+\beta_R z-l(l+1)(1+z^2)}{(1+z^2)^2}G=0,\ \lambda_E=\frac{2mE}{\hbar^2\kappa},\ \beta_R=\frac{2me^2}{\hbar^2\sqrt{\kappa}}.$$

L.M. Nieto, H.C. Rosu, M. Santander, Hydrogen atom as an eigenvalue problem in 3D spaces of constant curvature and minimal length.

The spectrum of the hydrogen atom in $\mathbb{S}^3$ space was obtained by Schrödinger in 1940 using the factorization method he invented.

$$E_n = \frac{me^4}{2\hbar^2}\left(-\frac{1}{n^2} + (n^2-1)\,\frac{a_B^2}{R^2}\right), \quad a_B = \frac{\hbar^2}{me^2}, \kappa = \frac{1}{R}.$$

Schrödinger declared that he found the problem "difficult to solve in any other way." But a year later Stevenson showed that the spectrum and wave function could be obtained without too much difficulty by the usual methods of solving differential equations.

We want to solve this problem using the Nikiforov-Uvarov method. Surprisingly, in the extensive literature on this topic, we have so far found only two papers V.N. Mel'nikov, G.N. Shikin, Hydrogen-like atom in the gravitational field of the universe and V.D. Ivashchuk, V. N. Mel'nikov, Dually-charged mesoatom on the space of constant negative curvature where this method is mentioned in connection with similar problems, but in our opinion it is not used in the most optimal way.

Nikiforov-Uvarov method

The Nikiforov-Uvarov method can be applied to second-order differential equations of generalized hypergeometric type, which have the following form

$$u'' + \frac{\pi_1(z)}{\sigma(z)}u' + \frac{\sigma_1(z)}{\sigma^2(z)}u = 0,$$

where the prime denotes differentiation with respect to the independent variable z (which may be complex), $\pi_1(z)$ is a polynomial of degree no higher than the first, and $\sigma(z)$, $\sigma_1(z)$ are polynomials of degree no higher than the second.

Gauge transformations of functions of generalized hypergeometric type

The set of such functions is invariant under "gauge" transformations $u(z) \to y(z)$:

$$u(z) = e^{\varphi(z)} y(z),$$

If the calibration function satisfies the equation

$$\varphi' = \frac{\pi(z)}{\sigma(z)},$$

where $\pi(z)$ is some polynomial of degree no higher than one. Then

$$y'' + \frac{\pi_2(z)}{\sigma(z)} y' + \frac{\sigma_2(z)}{\sigma^2(z)} y = 0,$$

where

$$\pi_2(z) = \pi_1(z) + 2\pi(z)$$

is a polynomial of degree no higher than one, and

$$\sigma_2(z) = \sigma_1(z) + \pi^2(z) + \pi(z) \left[\pi_1(z) - \sigma'(z)\right] + \pi'(z)\sigma(z)$$

is a polynomial of degree no higher than two.

Reduction to an equation of hypergeometric type

We can take advantage of the freedom in choosing the polynomial $\pi(z)$ and simplify the original equation. Namely, we choose $\pi(z)$ such that

$$\sigma_2(z) = \lambda\sigma(z),$$

where λ is a constant. Then the original equation is simplified to a hypergeometric equation:

$$\sigma(z)y'' + \pi_2(z)y' + \lambda y = 0.$$

This choice means

$$\pi^2 + \pi[\pi_1 - \sigma'] + \sigma_1 - k\sigma = 0,$$

where

$$k = \lambda - \pi'$$

is another constant.

The quadratic equation for $\pi(z)$ has a solution

$$\pi = \frac{\sigma' - \pi_1}{2} \pm \sqrt{\left(\frac{\sigma' - \pi_1}{2}\right)^2 - \sigma_1 + k\sigma}.$$

Since π is a polynomial,

$$\sigma_3(z) = \left(\frac{\sigma' - \pi_1}{2}\right)^2 - \sigma_1 + k\sigma$$

must be the square of a first-order polynomial. Therefore, it has a double root and its discriminant is zero:

$$\Delta(\sigma_3) = 0.$$

This equation defines the constant k and, therefore, the polynomial $\pi(z)$ and the constant λ.

In a bound state problem, the hypergeometric type equation must have a polynomial solution.

For $v_n(z) = y^{(n)}(z)$ we also obtain an equation of hypergeometric type:

$$\sigma v_n'' + \tau_n(z) v_n' + \mu_n v_n = 0,$$

and recurrence relations

$$\tau_n(z) = \sigma'(z) + \tau_{n-1}(z), \quad \mu_n = \mu_{n-1} + \tau_{n-1}',$$

with initial values

$$\tau_0(z) = \pi_2(z), \quad \mu_0 = \lambda.$$

If $y(z) = y_n(z)$ is a polynomial of order n, then $v_n = \mathrm{const}$ and the equation for v_n will be satisfied only if $\mu_n = 0$.

Repeated applications of recurrence relations will give

$$\tau_n(z) = n\sigma'(z) + \tau(z), \quad \mu_n = \lambda + n\tau' + \frac{1}{2}n(n-1)\sigma'',$$

Therefore, in order for $y(z) = y_n(z)$, as a solution of a hypergeometric equation, to be a polynomial of order n, the following "quantization condition" must be satisfied:

$$\lambda = \lambda_n = -n\tau' - \frac{1}{2}n(n-1)\sigma''.$$

Rodriguez formula

$$y_n(z) = \frac{B_n}{\rho(z)} \left[\sigma^n(z)\rho(z)\right]^{(n)},$$

where B_n is some (normalization) constant, and the weight function $\rho(z)$ satisfies the Pearson equation

$$(\sigma\rho)' = \rho\pi_2.$$

The equation to be solved is:

$$\frac{d^2G}{dz^2} + \frac{\lambda_E + \beta_R z - l(l+1)(1+z^2)}{(1+z^2)^2}\,G = 0.$$

$$\sigma = 1 + z^2,\;\; \pi_1 = 0,\;\; \sigma_1 = \lambda_E + \beta_R z - l(l+1)(1+z^2).$$

$$\sigma_3 = z^2[1 + k + l(l+1)] - \beta_R z + k + l(l+1) - \lambda_E.$$

$$\Delta(\sigma_3) = \beta_R^2 - 4[1 + k + l(l+1)][k + l(l+1) - \lambda_E] = 0.$$

Application of the formalism to our problem

$$x = 1 + k + l(l+1).$$

$$\frac{\beta_R^2}{4} = x(x - 1 - \lambda_E).$$

Of the two possible π, we choose the one with $\pi' < 0$:

$$\pi = (1 - \sqrt{x})z + \sqrt{x - 1 - \lambda_E}, \quad \pi_2 = 2\pi.$$

Quantization condition:

$$\lambda = -n_r\tau' - \frac{1}{2}n_r(n_r - 1)\sigma'' = -2n_r(1 - \sqrt{x}) - n_r(n_r - 1).$$

$k = \lambda - \pi' = \lambda - 1 + \sqrt{x}$. We express k through x, $k = x - 1 - l(l+1)$, and arrive at a quadratic equation:

$$x - (2n_r + 1)\sqrt{x} + n_r(n_r + 1) - l(l+1) = 0.$$

$$\sqrt{x} = n_r + \frac{1}{2} \pm \left(l + \frac{1}{2} \right), \quad \sqrt{x} = n_r + l + 1 = n.$$

Therefore,

$$\frac{\beta_R^2}{4} = n^2(n^2 - 1 - \lambda_E), \quad \lambda_E = n^2 - 1 - \frac{\beta_R^2}{4n^2}$$

$$E_n = Ry \left(-\frac{1}{n^2} + (n^2 - 1)\, \kappa a_B^2 \right), \quad Ry = \frac{\hbar^2}{2ma_B^2} = \frac{me^4}{2\hbar^2}.$$

Finding the calibration function

$$\frac{d\varphi}{dz}=\frac{\pi}{\sigma}=\frac{-(n-1)z+\sqrt{n^2-1-\lambda_E}}{1+z^2}=\frac{-(n-1)z+\frac{\beta_R}{2n}}{1+z^2}.$$

$$\varphi=-\frac{1}{2}(n-1)\ln\left(1+z^2\right)+\frac{\beta_R}{2n}\arctan z.$$

$$1+z^2=\frac{1}{\kappa S_\kappa^2(r)},\quad \arctan z=\frac{i}{2}\ln\frac{1-iz}{1+iz},\quad \frac{\beta_R}{2n}\arctan z=\frac{\pi}{2n\sqrt{\kappa}a_B}-\frac{1}{n}\frac{r}{a_B}.$$

$$G_{n,l}(r)=B_{n,n_r}\,[\sqrt{\kappa}S_\kappa(r)]^{n-1}e^{-\frac{1}{n}\frac{r}{a_B}}y_{n-l-1}^{n}(z).$$

Finding the weight function

$$\frac{d}{dz}(\rho\sigma) = \rho\pi_2, \quad \frac{(\rho\sigma)'}{\rho\sigma} = \frac{\pi_2}{\sigma} = 2\varphi', \quad \rho(z) = \frac{1}{1+z^2}\, e^{2\varphi}.$$

$$\rho_n(z) = (1+z^2)^{-n} e^{\frac{\beta_R}{n}\arctan z}.$$

$$y_{n_r}^n = \frac{1}{\rho(z)}\left[(1+z^2)^{n_r}\rho(z)\right]^{(n_r)}.$$

To determine the normalization factor one can calculate the corresponding normalization integrals directly: S.I. Vinitsky et al., A Hydrogen atom in the curved space. Expansion over free solutions on the three-dimensional sphere.

Since this is a rather laborious approach, we prefer the indirect way using raising and lowering operators H.I. Leemon, Dynamical symmetries in a spherical geometry. II, P.W. Higgs, Dynamical symmetries in a spherical geometry. I.

$$\hat{A}_+(l) = \frac{2}{\sqrt{\kappa}}\,\frac{l}{n+l}\left[-\frac{l+1}{T_\kappa(r)} + \frac{1}{l a_B} - \frac{d}{dr}\right],$$

$$\hat{A}_-(l) = \frac{\sqrt{\kappa}}{2}\,\frac{n^2 a_B^2}{1+n^2(l+1)^2 a_B^2\kappa}\,\frac{l+1}{n-l-1}\left[-\frac{l}{T_\kappa(r)} + \frac{1}{(l+1)a_B} + \frac{d}{dr}\right].$$

$$B_{n,n_r} = \frac{\sqrt{\kappa}}{2}\sqrt{\frac{n^2 a_B^2}{1+n^2(l+1)^2\kappa a_B^2}\,\frac{n+l+1}{n-l-1}}\,B_{n,n_r-1}.$$

This relation allows us to calculate the normalization coefficients recursively, starting from $B_{n,0}$. For the latter, we have

$$B_{n,0}^{-2} = \int S_\kappa^2(r)[\sqrt{\kappa}S_\kappa(r)]^{2(n-1)}e^{-\frac{2r}{na_B}}\,dr.$$

If $\kappa < 0$, then the last integral in converges only for $n\sqrt{-\kappa} < \frac{1}{na_B}$, or $n^2 < \frac{R}{a_B}$, where $R = \frac{1}{\sqrt{-k}}$. Therefore, in a space of constant negative curvature, hydrogen-like elementary atoms have only a finite, albeit very large $n \sim \sqrt{\frac{R}{a_B}}$, number of bound states] L. Infeld, A. Schild, A note on the Kepler problem in a space of constant negative curvature.

In the flat limit $\kappa \to 0$, $S_\kappa(r) \to r$,

$$B_{n,0}^{-2} \;\to\; \kappa^{n-1} \int\limits_0^\infty r^{2n} e^{-\frac{2r}{na_B}}\, dr = \kappa^{n-1} \left(\frac{na_B}{2}\right)^{2n+1} (2n)!,$$

and, as a result,

$$B_{n,n_r} \;\to\; (\sqrt{\kappa})^{n_r+1-n} \left(\frac{2}{na_B}\right)^{n+\frac{1}{2}-n_r} \sqrt{\frac{1}{2n(n-l-1)!(n+l)!}}.$$

Normalization and flat limit

On the other hand, when $\kappa \to 0$, then

$$z \to \frac{1}{\sqrt{\kappa}\, r}, \quad 1+z^2 \to \frac{1}{\kappa\, r^2}, \quad \rho \to \kappa^n\, r^{2n}\, e^{\frac{\pi}{n\sqrt{\kappa}\,a_B}}\, e^{-\frac{2r}{na_B}},$$

and

$$y^n_{n_r} \to \kappa^{-n_r}\, r^{-2n}\, e^{\frac{2r}{na_B}}\, \frac{d^{n_r}}{dz^{n_r}}\left[r^{2(n-n_r)}\, e^{-\frac{2r}{na_B}}\right]$$
$$= (-1)^{n_r}\, (\sqrt{\kappa})^{-n_r}\, r^{-2n}\left(\frac{na_B}{2}\right)^{2n-n_r} e^{-1/t}\, \frac{d^{n_r}}{dt^{n_r}}\left[t^{-2(n-n_r)} e^{1/t}\right],$$

where $t = -\frac{na_B}{2r}$. Next we use the following Duff identity

$$\frac{d^n}{dt^n}\left[t^{-k}\, e^{1/t}\right] = (-1)^n\, n!\, t^{-(n+k)}\, e^{1/t}\, L^{k-1}_n\left(-\frac{1}{t}\right),$$

where $L^m_n(x)$ is the associated Laguerre polynomial. As a result, we get

$$|n, n_r\rangle \to (-1)^{n_r}\, (n-l-1)!\, (\sqrt{\kappa})^{n-1-n_r}\, r^{n-1-n_r}\, e^{-\frac{r}{na_B}}\, L^{2l+1}_{n-l-1}\left(\frac{2r}{na_B}\right).$$

Finally,

$$B_{n,n_r}|n,n_r\rangle \to (-1)^{n-l-1}\,\frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{a_B^3(n+l)!}}\left(\frac{2r}{na_B}\right)^l e^{-\frac{r}{na_B}}\,L_{n-l-1}^{2l+1}\left(\frac{2r}{na_B}\right).$$

Up to a possible irrelevant sign, the right-hand side of is exactly the wave function of the hydrogen atom in flat space. Note that many different conventions are used for ordinary and associated Laguerre polynomials in the physics literature. We follow conventions of Arfken and Weber, Mathematical methods for physicists.

Concluding remarks

- The Nikiforov-Uvarov method has been used in many quantum mechanical problems.
- Hydrogen-like atoms in spaces of constant curvature represent another quantum mechanical problem where this method can be successfully applied.
- Moreover, in our opinion, in this case the Nikiforov-Uvarov method provides the most natural and simple way to solve the problem.