Practical Quantum Mechanics-
from exactly solvable Schrödinger equations, shape invariant potentials, and supersymmetry

Reinhart Kühne

Brownian motion and Schrödinger equation

Langevin equation as starting point

$$m\ddot{x} = \underbrace{-\gamma\dot{x}}_{\text{friction}} + \underbrace{F}_{\substack{\text{systematic}\\ \text{force}}} + \underbrace{\Gamma}_{\substack{\text{fluctuating}\\ \text{force}}}$$

with $\delta-$correlated fluctuations

$$<\Gamma>=0 \qquad <\Gamma(t)\Gamma(t')>=2D\delta(t-t')$$

and

$$F=-\partial_x\Phi$$ (force derived from potential)

summary

$$(m\ddot{x})+\gamma\dot{x}=-\partial_x\Phi+\Gamma$$

$$\dot{x} = -\partial_x\Phi+\Gamma$$ (Langevin equation)

Paul Langevin

* January 23. 1872
† December19. 1946

- french physicist

- studied at the Ecole Supériere de Physique et de Chimie Industrielles de la Ville de Paris

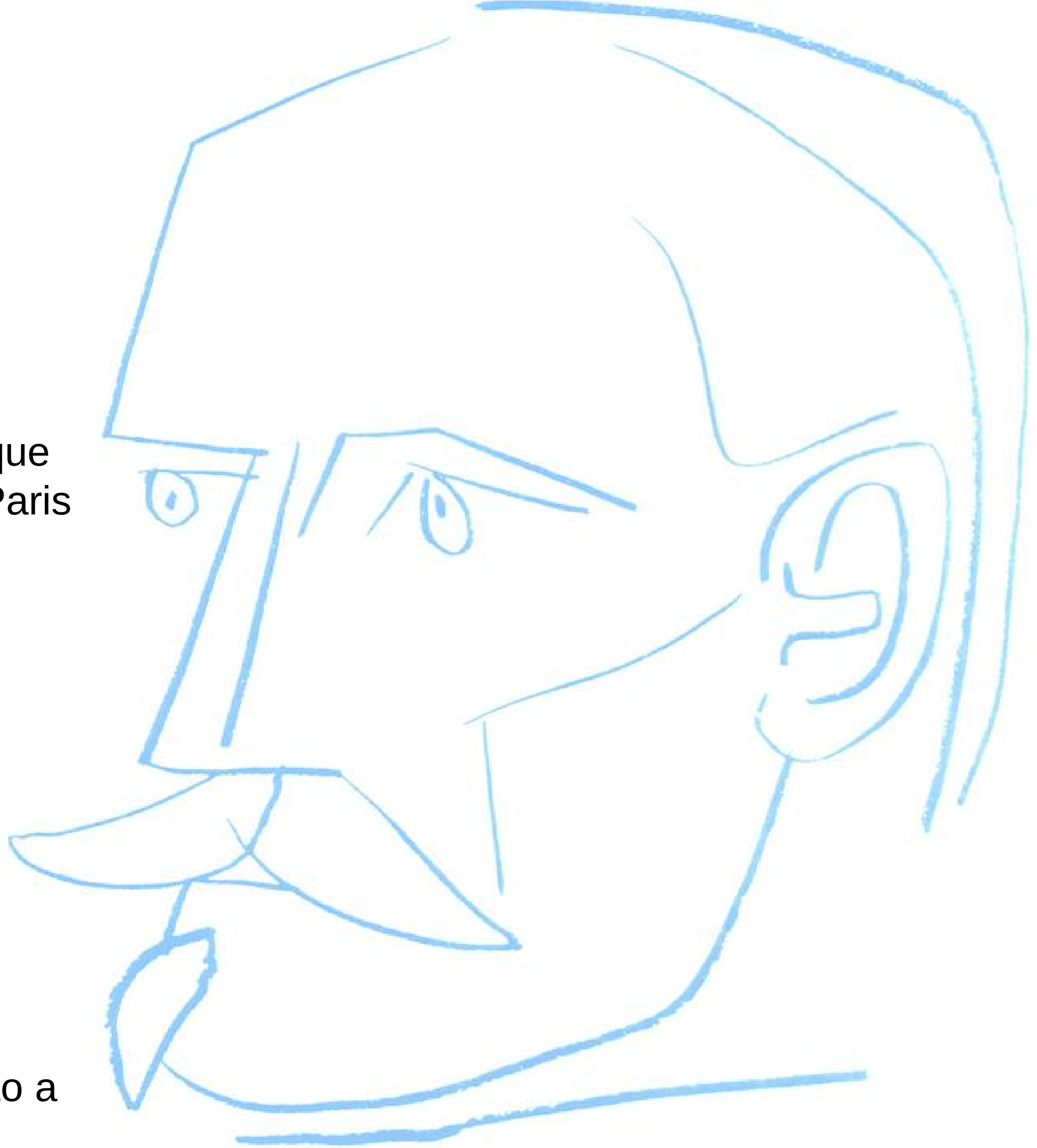
- career at this school, director at last

- since 1909 professor for physics at the Collège de France

- student of Pierre (†1906) and Marie Curie (†1934). He was a friend of the family and he had 1910 an affaire with Marie Curie.

- in the 30‘s and 40´s years he belonged to a bohemian in Paris with Picasso.

- applied firstly in 1916 the Piezo electricity of quartz crystals by constructing the first ultrasonic object detector (Sonar)



Paul Langevin painted by Pablo Picasso, 1938

source: http:// amp2005.blog.lemonde.fr/files/langevin_by_picasso.jpg
und www.wikipedia.org/wiki/Paul_Langevin

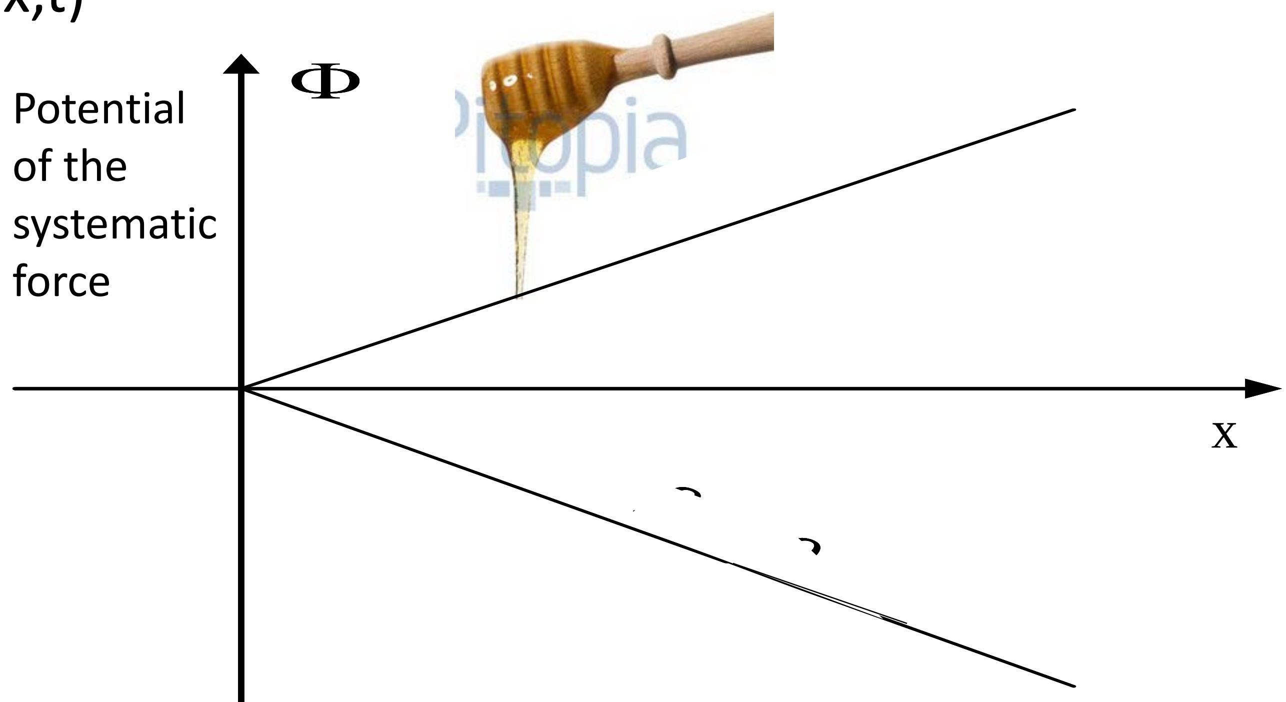
Langevin equation

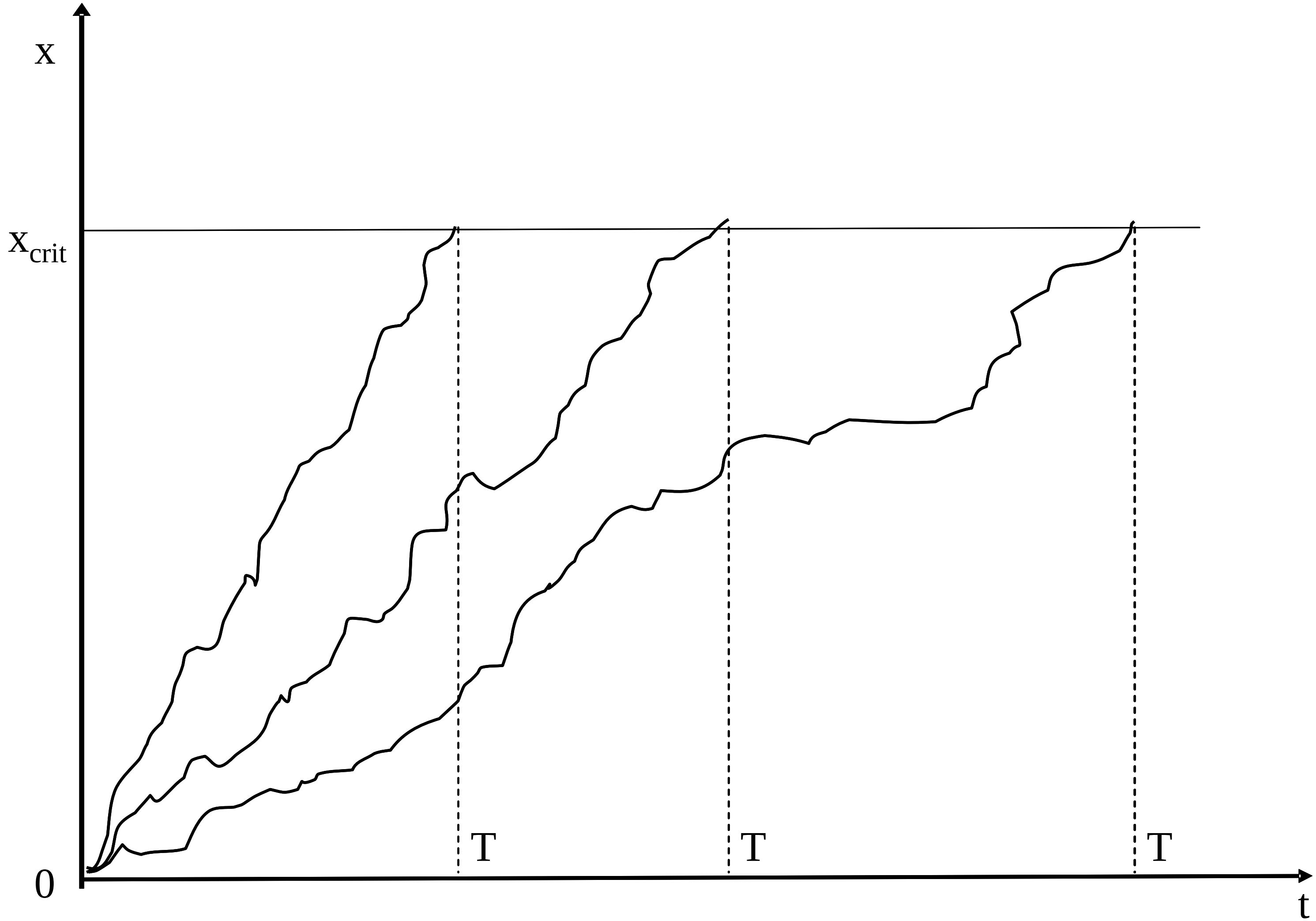
$$\dot{x} = -\Phi' + \Gamma$$

drift   diffusion

stochastic equivalent equation of motion for prob. distribution function P(x,t)

$$\dot{P}(x,t) = \partial_x \Phi' P(x,t) + D\partial_x^2 P(x,t)$$





Trajectories of the system status with common start at x=0

T= point in time, when firstly hitting a certain critical value x_{crit}

Special cases to interprete the Fokker-Planck equation

$$\dot{P}(x,t) = \left\{\partial_x \Phi' + D\partial_x^2\right\} P(x,t)$$

a) Pure drift (D=0) $\quad \dot{P}(x,t) - \partial_x \Phi' P(x,t) = 0$

Solution by method of characteristics

$$P(x,t) \equiv P(x(t))$$

$$\dot{x} = -\Phi'$$

= sharp movement along the trajectory $x=x(t)$

b) Pure diffusion ($\Phi' =0$) $\quad \dot{P}(x,t) = D\partial_x^2 P(x,t)$

$$P(x,t) = \frac{1}{\sqrt{2\pi D t}} e^{-\frac{(x-x_0)^2}{4Dt}}$$

= dissolving Gaussian distribution

General Solution for P(x,t) by Separation

Starting equation (Fokker-Planck equation)

$$\dot{P}(x,t) = \left(\partial_x \Phi'(x) + \partial_x^2\right) P(x,t)$$

∂_t=0 gives stationary solution

$$P^{st}(x) = N e^{-\Phi(x)}$$

separation ansatz for complete solution

$$P(x,t) = \sqrt{P^{st}(x)}\,\varphi(x)\,e^{-\lambda t} = e^{-\frac{1}{2}\Phi(x)}\varphi(x)\,e^{-\lambda t}$$

gives

$$-\lambda\varphi = e^{\frac{1}{2}\Phi}(\partial_x\Phi' + \partial_x^2)e^{-\frac{1}{2}\Phi}\varphi$$

or

$$\lambda\varphi = (-\partial_x + \frac{1}{2}\Phi')(\partial_x + \frac{1}{2}\Phi')\varphi$$

$$= (-\partial_x^2 + \frac{1}{4}\Phi'^2 - \frac{1}{2}\Phi'')\varphi$$

The equation of motion for the probability distribution of the Brownian motion (Fokker-Planck equation) thus has the form of a Schrödinger-equation

$$H\varphi = \lambda\varphi \quad ; \quad H = (-\partial_x^2 + V_S)$$

with the Schrödinger-potential

$$V_S = \frac{1}{4}\Phi'^2 - \frac{1}{2}\Phi''$$

and the correspondence

$$\text{energy eigenvalue } E \Leftrightarrow \text{decaying time constant } \lambda$$

$$\text{particle density } \psi^*\psi \Leftrightarrow \text{probability density } P$$

$$\text{wave function } \psi \Leftrightarrow \text{eigen function } \varphi = P/\sqrt{P^{st}}$$

Elementary application examples

- Square well potential
- δ-potential

Square-Well Potential and Ladder Operators

The Schrödiger equation for a single particle moving in a one-dimensional infinitely deep square-well potential

$$V(x) = \begin{cases} 0 & \text{for} \left|x\right| \le \dfrac{L}{2} \\ \infty & \text{else} \end{cases}$$

in dimensionless variables ($x' = \pi x/L$, $V' = V/(\hbar^2\pi^2/2mL^2)$, $\varepsilon = E/(\hbar^2\pi^2/2mL^2)$, $\psi' = \psi\sqrt{(\pi/L)}$, ' suppressed) reads

$$\left\{-\partial_x^2 + V(x)\right\}\psi_\nu(x) = \varepsilon_\nu \psi_\nu(x) \qquad V(x) = \begin{cases} 0 & \left|x\right| \le \pi/2 \\ \infty & \left|x\right| > \pi/2 \end{cases}$$

with the solutions

$$\psi_\nu = \begin{cases} N \sin k_\nu^{as} x \\ N \cos k_\nu^{s} x \end{cases} \qquad \left|x\right| \le \frac{\pi}{2} \qquad \psi_\nu = 0 \quad \text{else}$$

and

$$\varepsilon_\nu = (k_\nu^{as,s})^2$$

Fitting the boundary conditions gives

$$\psi_\nu(\pi/2) = 0 \rightarrow k_\nu^{as} = 2\nu \quad \nu = 1,2,3\ldots; \quad k_\nu^{s} = 2\nu + 1 \quad \nu = 0,1,2\ldots$$

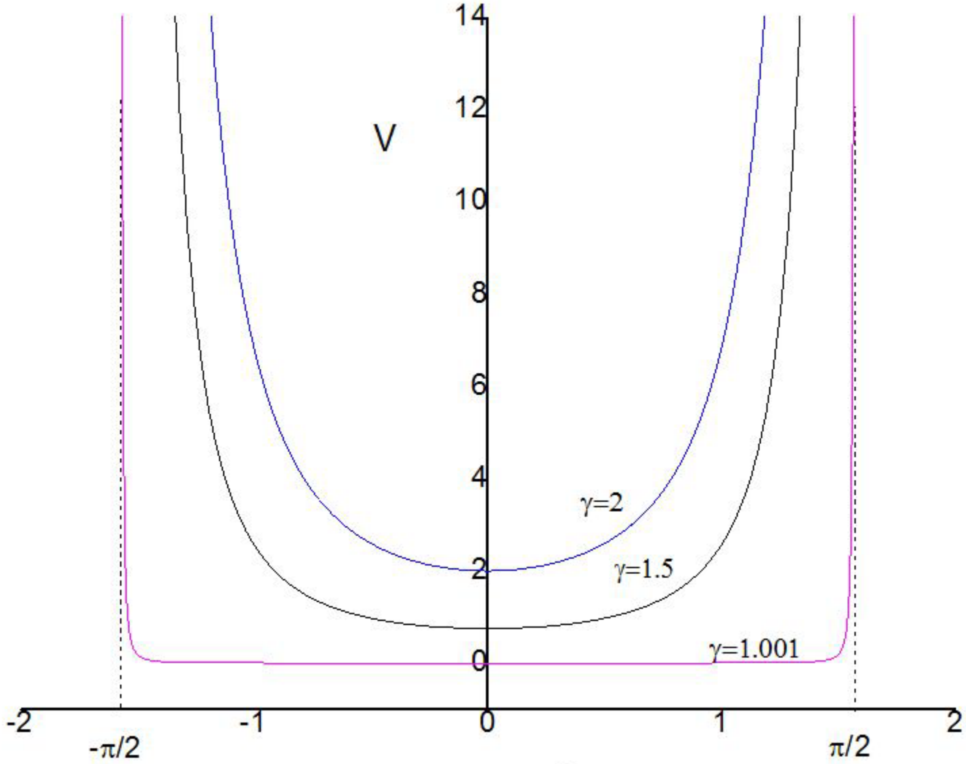
factorization $$-\partial_x^2 + V(x) - \varepsilon_0 = (-\partial_x + \tan x)(\partial_x + \tan x)$$
$$= -\partial_x^2 + \tan^2 x - \tan' x = -\partial_x^2 - 1 = L^- L^+$$

Generalization of the decomposition gives

$$(-\partial_x + \gamma \tan x)(\partial_x + \gamma \tan x) = -\partial_x^2 - \gamma \tan' x + \gamma^2 \tan^2 x$$
$$= -\partial_x^2 + \frac{\gamma(\gamma - 1)}{\cos^2 x} - \gamma^2 \equiv H(\gamma) - \gamma^2$$

with the generalized Hamiltonian

$$H(\gamma) = -\partial_x^2 + V(x)$$
$$\equiv -\partial_x^2 + \frac{\gamma(\gamma - 1)}{\cos^2 x}$$



Ladder operators

The commutation relation

$$b_\gamma b_\gamma^+ = (\partial_x + \gamma \tan x)(-\partial_x + \gamma \tan x) = -\partial_x^2 + \gamma \tan' x + \gamma^2 \tan^2 x = -\partial_x^2 + \frac{\gamma(\gamma+1)}{\cos^2 x} - \gamma^2$$

$$b_{\gamma+1}^+ b_{\gamma+1} = (-\partial_x + (\gamma+1)\tan x)(\partial_x + (\gamma+1)\tan x) = -\partial_x^2 - (\gamma+1)\tan' x + (\gamma+1)^2 \tan^2 x$$

$$= -\partial_x^2 + \frac{\gamma(\gamma+1)}{\cos^2 x} - (\gamma+1)^2 = b_\gamma b_\gamma^+ - 2\gamma - 1$$

introduced into the Schrödinger equation for γ→γ+1 gives

$$(H(\gamma+1) - (\gamma+1)^2)\psi_\nu(\gamma+1) = (\varepsilon_\nu(\gamma+1) - (\gamma+1)^2)\psi_\nu(\gamma+1) \qquad \Big| \, b_\gamma^+$$

$$b_\gamma^+ \underbrace{b_{\gamma+1}^+ b_{\gamma+1}}_{b_\gamma b_\gamma^+ - \underline{2\gamma-1}} \psi_\nu(\gamma+1) = (\varepsilon_\nu(\gamma+1) \underbrace{-(\gamma+1)^2}_{-\gamma^2 - \underline{2\gamma-1}}) b_\gamma^+ \psi_\nu(\gamma+1)$$

$$(H(\gamma) - \gamma^2) b_\gamma^+ \psi_\nu(\gamma+1) = (\varepsilon_\nu(\gamma+1) - \gamma^2) b_\gamma^+ \psi_\nu(\gamma+1)$$

comparison with $(H(\gamma) - \gamma^2)\psi_{\nu+1}(\gamma) = (\varepsilon_{\nu+1}(\gamma) - \gamma^2)\psi_{\nu+1}(\gamma)$

gives $\varepsilon_\nu(\gamma+1) = \varepsilon_{\nu+1}(\gamma)$ and $\psi_{\nu+1}(\gamma) \propto b_\gamma^+ \psi_\nu(\gamma+1)$

starting with the ground state

$$b_\gamma \psi_0(\gamma) = 0 \quad \text{resp.} \quad \varepsilon_0(\gamma) = \gamma^2$$

gives

$$\varepsilon_1(\gamma) = \varepsilon_0(\gamma+1) = (\gamma+1)^2$$

$$\varepsilon_2(\gamma) = \varepsilon_1(\gamma+1) = (\gamma+2)^2$$

$$....$$

$$\varepsilon_\nu(\gamma) = (\gamma+\nu)^2$$

or for γ=1

$$\varepsilon_\nu(1) = (\nu+1)^2$$

and the ladder operator representation reads

$$\psi_1(\gamma) \propto b_\gamma^+ \psi_0(\gamma+1)$$

$$\psi_2(\gamma) \propto b_\gamma^+ \psi_1(\gamma+1)$$

$$\propto b_\gamma^+ b_{\gamma+1}^+ \psi_0(\gamma+2)$$

$$....$$

$$\psi_\nu(\gamma) \propto b_\gamma^+ b_{\gamma+1}^+ \cdot ... \cdot b_{\gamma+\nu-1}^+ \psi_0(\gamma+\nu)$$

Eigenfunction expansion of the Schrödinger equation with a δ-potential and natural boundary conditions

The Schrödinger equation with a δ-potential reads

$$H\varphi \equiv (-\partial_x^2 - 2\gamma\,\delta(x))\,\varphi = \varepsilon\,\varphi \qquad\qquad \gamma > 0$$

with natural boundary condition $(\varphi\,(x \to \pm\infty) = 0)$

we get

ground state $\quad \varphi_0 = \sqrt{\gamma}e^{-\gamma|x|} \qquad\qquad \varepsilon_0 = -\gamma^2$

symmetric scattering states

$$\varphi_k^s = \frac{1}{\sqrt{\pi}}\sin(k|x| - \alpha_k) \qquad \varepsilon_k = k^2 \qquad \tan\alpha_k = k/\gamma$$

antisymmetric scattering states

$$\varphi_k^{as} = \frac{1}{\sqrt{\pi}}\sin kx \qquad\qquad \varepsilon_k = k^2 \qquad\qquad k > 0$$

Factorization

Decomposition

$$b = \partial_x + \gamma \operatorname{sign} x \qquad b^+ = -\partial_x + \gamma \operatorname{sign} x$$

$$b^+ b = -\partial_x^2 - \gamma(\operatorname{sign} x)' + (\gamma \operatorname{sign} x)^2$$

$$= \underbrace{-\partial_x^2 - 2\gamma\,\delta(x)}_{H} + \gamma^2$$

gives

$$H = b^+ b - \gamma^2$$

From this it follows

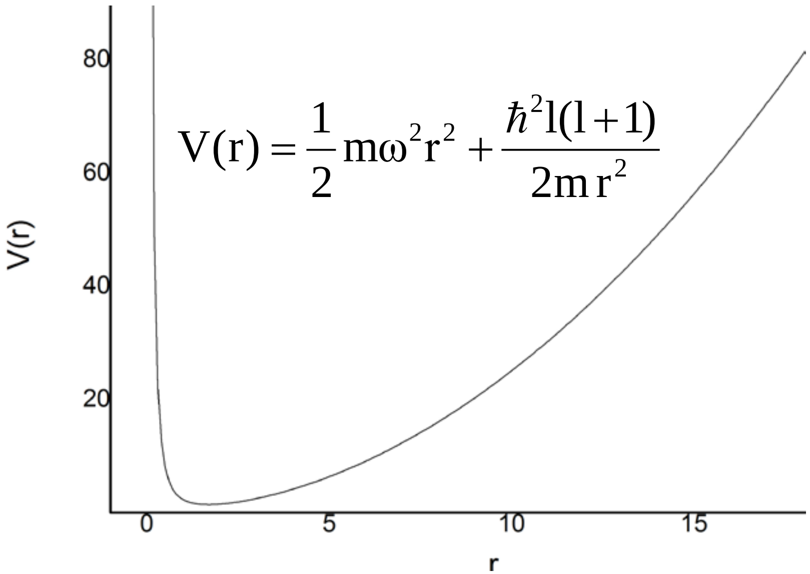
$$\varepsilon \geq -\gamma^2$$

and for the ground state

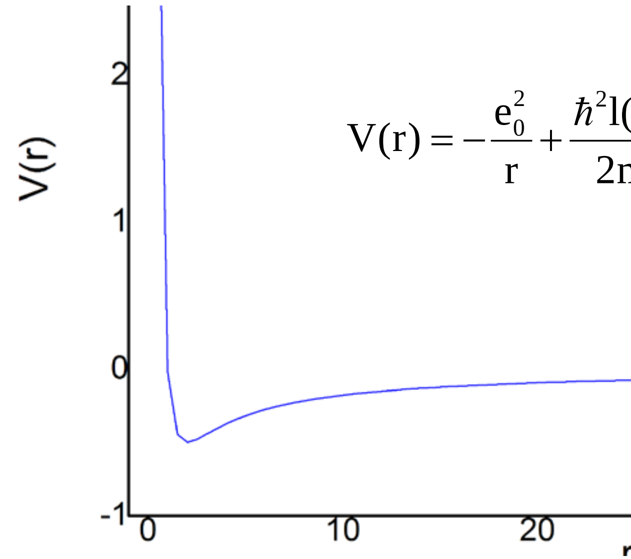
$$\varepsilon_0 = -\gamma^2 \quad b\,\varphi_0 = 0 \;\Rightarrow\; \varphi_0 = N e^{-\gamma|x|}$$

Shape invariant potentials (I)

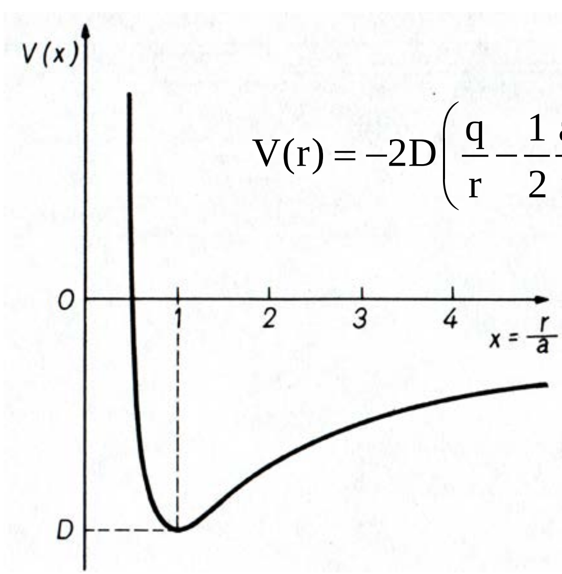
- Harmonic oscillator
- Coulomb potential
- Kratzer potential
- Morse potential



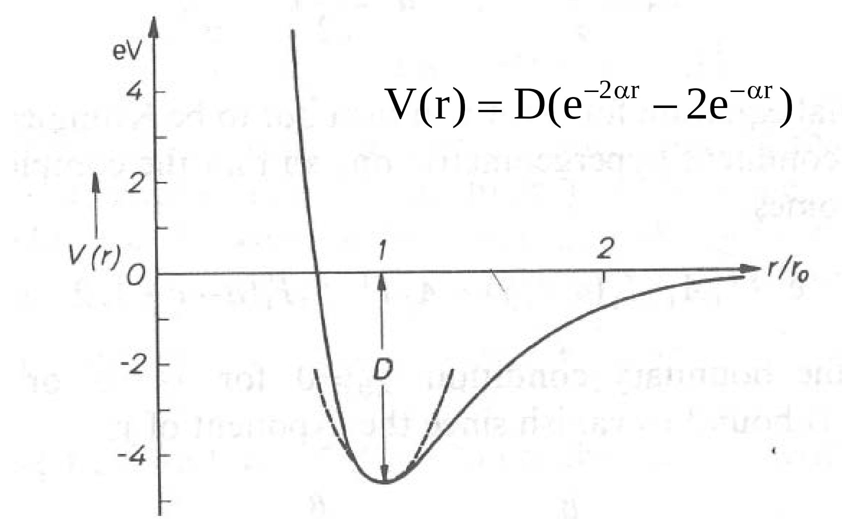
3D harm. oscillator



Coulomb potential



Kratzer potential



Morse potential

Schrödinger equation for a particle in the 3D harm. oscillator potential V ~ r^2

The Schrödinger equation for a particle in the 3D harm. oscillator V= 1/2 $m\omega^2 r^2$ reads

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2} m\,\omega^2\, r^2\right)\psi = E\psi$$

Scaling with $a_0^2 = \hbar/(2m\omega)$ gives

$$E = \frac{\hbar^2}{2m\,a_0^2}\,\varepsilon \qquad r' = \frac{r}{a_0} \qquad \psi'(x', y', z') = \sqrt{a_0^3}\,\psi(x, y, z)$$

and transforms the Schrödinger equation into (‘suppressed)

$$\left(-\nabla^2 + \frac{1}{4} r^2\right)\psi = \varepsilon\,\psi$$

Introducing spherical polar coordinates

$$\nabla^2 = \frac{1}{r^2}\partial_r r^2 \partial_r + \frac{1}{r^2}\underbrace{\frac{1}{\sin^2\vartheta}\partial_\varphi^2 + \cot\vartheta\,\partial_\vartheta + \partial_\vartheta^2}_{-\frac{1}{\hbar^2}L^2}$$

and splitting off the wave function into radial and angular par

$$\psi(r,\varphi,\vartheta) = \underbrace{R(r)}_{\frac{1}{r}\chi(r)}\psi_{l,m}(\varphi,\vartheta)$$

gives with $L^2\psi_{l,m}(\varphi,\vartheta) = \hbar^2 l(l+1)\psi_{l,m}(\varphi,\vartheta)$ for $l=0,1,2,\ldots$ as Schrödinger equation

$$H(l)\chi = \left(-\partial_r^2 + \frac{1}{4}r^2 + \frac{l(l+1)}{r^2}\right)\chi = \varepsilon(l)\chi \qquad l = 0,1,2,\ldots.$$

Factorization gives

$$H(\mathrm{l}) - (\mathrm{l} + \frac{3}{2}) \equiv \underbrace{\left(-\partial_{\mathrm{r}} + \frac{1}{2}\mathrm{r} - \frac{\mathrm{l}+1}{\mathrm{r}} \right)}_{\mathrm{b}^{+}(\mathrm{l})} \underbrace{\left(\partial_{\mathrm{r}} + \frac{1}{2}\mathrm{r} - \frac{\mathrm{l}+1}{\mathrm{r}} \right)}_{\mathrm{b}(\mathrm{l})} = \mathrm{b}^{+}(\mathrm{l})\mathrm{b}(\mathrm{l})$$

from this follows

$$\varepsilon(\mathrm{l}) - (\mathrm{l} + \frac{3}{2}) \geq 0$$

and for the ground state

$$\varepsilon_0(\mathrm{l}) = \mathrm{l} + \frac{3}{2}$$

$$\mathrm{b}(\mathrm{l})\,\chi_0 = 0 \quad \text{or} \quad \chi_0 = N\,\mathrm{r}^{\mathrm{l}+1} e^{-\frac{1}{4}\mathrm{r}^2}$$

The commutation relation

$$b(l)b^{+}(l)=(\partial_r+\frac{1}{2}r-\frac{l+1}{r})(-\partial_r+\frac{1}{2}r-\frac{l+1}{r})$$

$$=-\partial_r^2+\frac{1}{4}r^2+\frac{(l+1)(l+2)}{r^2}-l-\frac{1}{2}=b^{+}(l+1)b(l+1)+2$$

transforms the product $b^{+}(l)H(l+1)$ into

$$b^{+}(l)H(l+1)=\left(H(l)-1\right)b^{+}(l)$$

Starting with the ground state

$$H(l)\chi_0(l)=\varepsilon_0(l)\chi_0(l)=(l+\frac{3}{2})\chi_0(l)$$

the substitution $l\rightarrow l+1$gives

$$H(l+1)\chi_0(l+1)=(l+\frac{5}{2})\chi_0(l+1)$$

multiplying from left with $b^+(l)$

$$\underbrace{b^+(l)H(l+1)}_{(H(l)-1)\,b^+(l)}\chi_0(l+1) = (l+\frac{5}{2})b^+(l)\,\chi_0(l+1)$$

yields to

$$H(l)\underbrace{b^+(l)\chi_0(l+1)}_{\propto\,\chi_1(l)} = \underbrace{(l+\frac{7}{2})}_{=\,\varepsilon_1(l)}\underbrace{b^+(l)\chi_0(l+1)}_{\propto\,\chi_1(l)}$$

continuation allows the ladder array

$$\chi_n(l) \sim b^+(l)b^+(l+1)\cdot\ldots\cdot b^+(l+n)\,\chi_0(l+n)$$

with the eigenvalues

$$\varepsilon_n(l) = 2n + l + \frac{3}{2} \quad , \quad n = 0,1,2,\ldots$$

Generalization to a particle in a harmonic potential with a potential barrier at x=0

The considered potential reads

$$V(x) = \frac{1}{2} m\omega^2 x^2 + \frac{\alpha}{x^2}$$

leading to the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \partial_x^2 + \frac{1}{2} m\omega^2 x^2 + \frac{\alpha}{x^2} \right) \varphi = E\,\varphi$$

Scaling space coordinate and energy

$$x' = \frac{x}{a_0} \qquad \varepsilon = \frac{E}{\frac{\hbar^2}{2m\,a_0^2}} \qquad a_0^2 = \frac{\hbar}{2m\omega} \qquad \frac{2m\,\alpha}{\hbar^2} = \gamma(\gamma+1)$$

gives for the Schrödinger equation

$$\left(-\partial_x^2+\frac{1}{4}x^2+\frac{\gamma(\gamma+1)}{x^2}\right)\varphi=\varepsilon\,\varphi$$

with the eigenfunctions as ladder array

$$\varphi_n(\gamma)\sim b^+(\gamma)b^+(\gamma+1)\cdot\ldots\cdot b^+(\gamma+n)\varphi_0(\gamma+n)$$

with

$$b(\gamma)=\partial_x+\frac{1}{2}x-\frac{\gamma+1}{x}$$

and the eigenvalues

$$\varepsilon_n(\gamma)=2n+\gamma+\frac{3}{2}\quad,\quad n=0,1,2,\ldots$$

Schrödinger equation for a particle in the Coulomb potential V = -e²/r

The Schrödinger equation for a particle in the Coulomb potential V= -e^2/r reads

$$(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r})\psi = E\psi$$

Scaling with $a_0 = \hbar^2/(e^2 m)$ gives

$$E = \frac{\hbar^2}{2m\, a_0^2}\varepsilon \qquad r' = \frac{r}{a_0} \qquad \psi'(x', y', z') = \sqrt{a_0^3}\,\psi(x, y, z)$$

and transforms the Schrödinger equation into (‘suppressed)

$$(-\nabla^2 - \frac{2}{r})\psi = \Big((-\nabla + \vec{r}^{\,0})(\nabla + \vec{r}^{\,0}) - 1\Big)\psi = \varepsilon\,\psi$$

The factorization allows an estimate of the energy levels ($\int dV\,|\psi|^2 = 1$)

$$\varepsilon = -1 + \int dV \left|(\nabla + \vec{r}^{\,0})\psi\right|^2 \geq 0 \qquad \text{or} \qquad \varepsilon \geq -1$$

with the ground state

$$\varepsilon_0 = -1 \qquad (\nabla + \vec{r}^{\,0})\psi_0 = 0 \qquad \psi_0 = N e^{-r}$$

Introducing spherical polar coordinates

$$\nabla^2 = \frac{1}{r^2}\partial_r r^2 \partial_r + \frac{1}{r^2}\underbrace{\frac{1}{\sin^2\vartheta}\partial_\varphi^2 + \cot\vartheta\,\partial_\vartheta + \partial_\vartheta^2}_{-\frac{1}{\hbar^2}L^2}$$

and splitting off the wave function into radial and angular part

$$\psi(r,\vartheta,\varphi) = \underbrace{R(r)}_{\frac{1}{r}\chi(r)}\,\psi_{l,m}(\vartheta,\varphi)$$

gives with $L^2\psi_{l,m}(\varphi,\vartheta) = \hbar^2 l(l+1)\psi_{l,m}(\varphi,\vartheta)$ as Schrödinger equation

$$H\chi = \left(-\partial_r^2 - \frac{2}{r} + \frac{l(l+1)}{r^2}\right)\chi(r) = \varepsilon\chi \qquad l = 0,1,2,\ldots.$$

Factorization gives

$$H + \frac{1}{(l+1)^2} \equiv \underbrace{\left(-\partial_r - \frac{l+1}{r} + \frac{1}{l+1}\right)}_{b^+(l)}\underbrace{\left(\partial_r - \frac{l+1}{r} + \frac{1}{l+1}\right)}_{b(l)} = b^+(l)b(l)$$

from this follows $\quad \varepsilon + \dfrac{1}{(l+1)^2} \geq 0$

and for the ground state $\quad \varepsilon_0(l) = -\dfrac{1}{(l+1)^2}$

$$b(l)\chi_0(l) = 0 \ \text{ or } \ \chi_0(l) = N\, r^{l+1} e^{-\frac{r}{l+1}}$$

The commutation relation

$$b^+(l)H(l+1)-H(l)b^+(l)=0$$

allows a ladder array

$$\chi_n(l) \sim \underbrace{b^+(l)b^+(l+1)\cdot\ldots\cdot b^+(l+n-1)}_{\text{n factors}}\chi_0(l+n)$$

with the eigenvalues

$$\varepsilon_n(l) = -\frac{1}{(n+l+1)^2} \qquad n=0,1,2,...$$

from this follows for the ground state

$$\varepsilon_0 = -\frac{1}{(n+l+1)^2}\bigg|_{n=0,l=0} = -1 \text{ resp. } -13.6\text{eV}$$

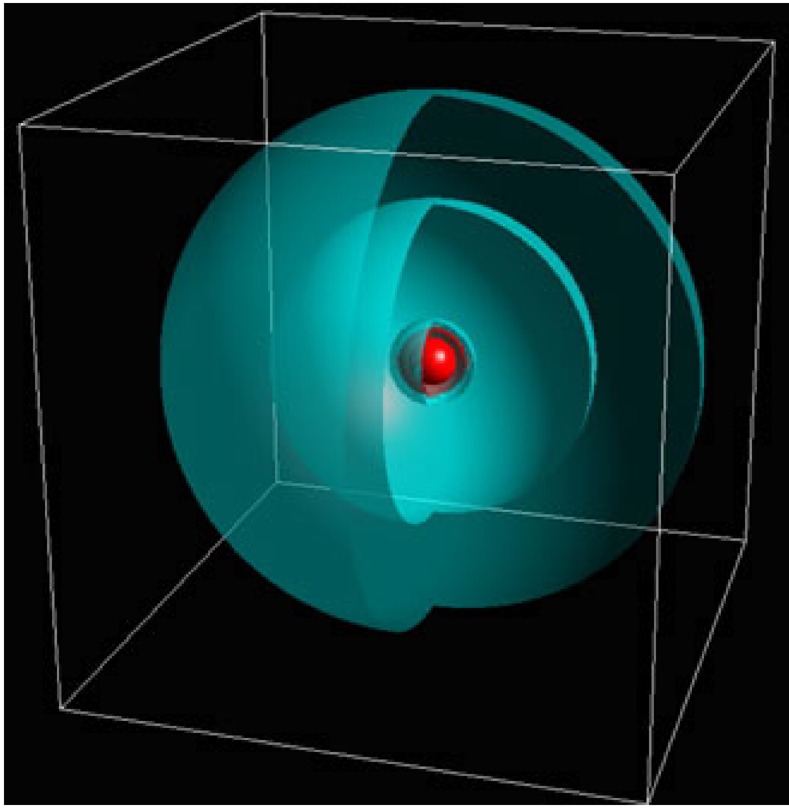
Once you have understood the Hydrogen atom, it is easy to extend the principles to atoms with higher atom numbers:

e.g.the Li-atom (atom number Z=3):

- two electrons in the most inner shell
- last electron is located in the next inner shell.

only partly similar to the Hydrogen atom:

- for Hydrogen the most outer electron can directly occupy the ground state
- for the Li-atom, the s-shell is occupied with the two inner electrons, the most outer electron can occupy as its ground state only the next shell n=1 l=0



Electron shells for l=0 (sherical symmetry) for the Coulomb potential

$$\varepsilon_0^{H} = \varepsilon_{\text{ionization}}^{H\to H^+} = -\left.\frac{1}{(n+l+1)}\right|_{n=0,l=0} = -1 \text{ resp. } -13.6\,\text{eV}$$

$$\varepsilon_0^{Li} = \varepsilon_{\text{ionization}}^{Li\to Li^+} = -\left.\frac{1}{(n+l+1)^2}\right|_{n=1,l=0} = -\frac{1}{4} \text{ resp. } -3.4\,\text{eV}$$

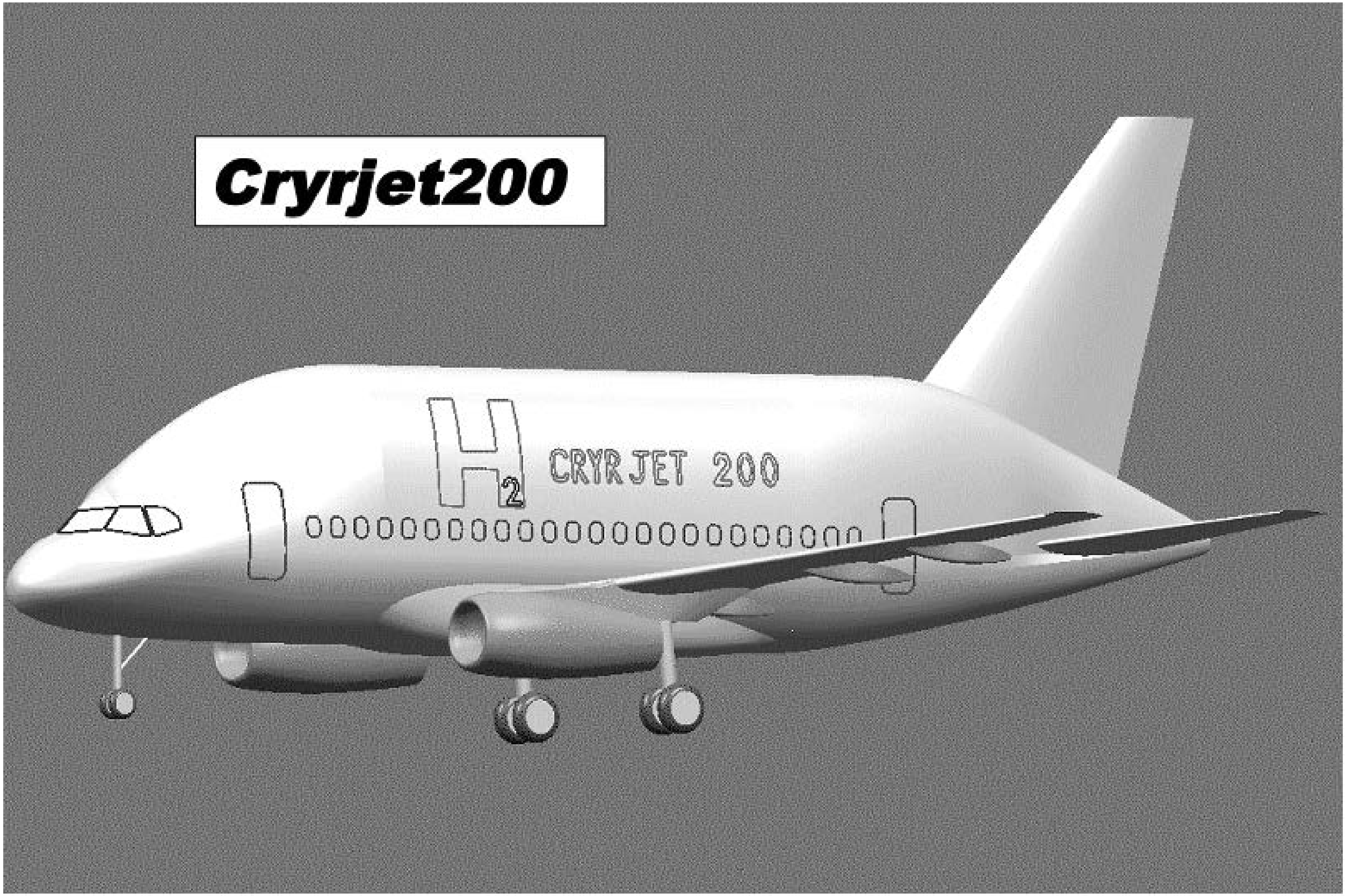
The ionization energy to get a Li^{+}-ion is thus an order of magnitude smaler compared to the H^{+}-ion This corresponds to a much lower reactivity of the Li^{+}-Ion and explains at once the adjacent table of energy densities specially for Hydrogen and Lithium

Energy density sorted by gravimetric density

Material	**gravimetric density [Wh/kg]**
Diesel	13 800
Gasoline	12 200
LNG	12 100
Propane (liquid)	13 900
Ethanol	7 850
Methane	15 400
Liquid H2	39 000
150 Bar H2	39 000
Lithium	110
Dry ice subl.	160

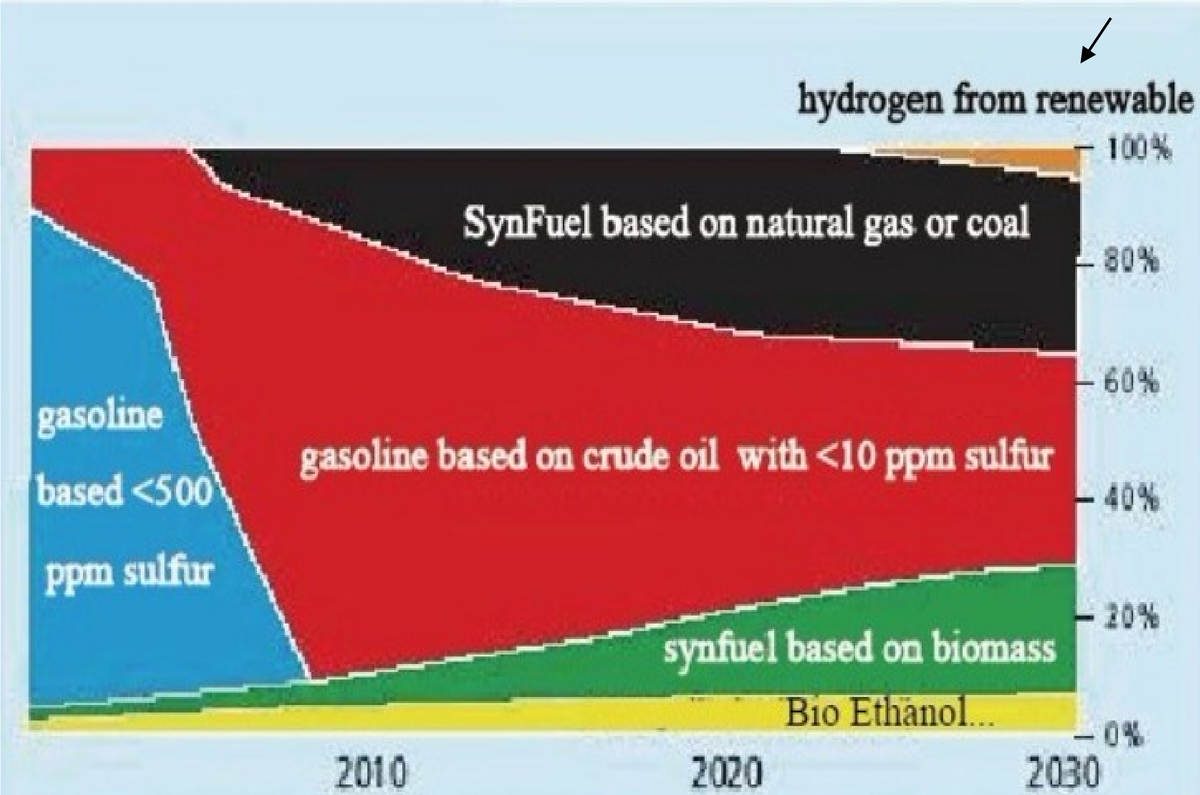
Ariane rocket drive test field Lampoldshausen, Germany (200 000 horse power, 250 t total rocket weight)

Standard regional aircraft- 70 pax



Source: Westerberger, A.: Cyroplane – Hydrogen Aircraft, H2 Expo Hamburg, 11.10.03

Fuels in Europe



Source: VDI Nachrichten, Nr. 50, 16.12.05,S. 24

Material	Volumetric density [Wh/l]
Diesel	10 900
Gasoline	9 700
LNG	7 216
Propane (liquid)	7 000
Ethanol	6 100
Methanol	4 600
Liquid H2	2600
150 Bar H2	405
Lithium	250
Dry ice subl.	250

Energy Density sorted by volumetric density

source: Energy Density
http://xtronics.com/reference/energy_density.htm

Vehicle sales drop 8% due to rising fuel prices, end of stimulus policy

Analysts said the use of electric vehicles is being hampered by their high cost and a lack of charging stations.

VINCENT THIAN / AP

A model stands next to China's BYD F3 at 2012 Beijing International Automotive Exhibition in Beijing on Tuesday. The Chinese battery and car maker's profit for the first quarter of the year fell as much as 90 percent.

April 27, 2012

CHINA DAILY

Battery maker registers lower profit in first quarter

The Vito E-CELL – The first pure battery-powered utility vehicle of the Daimler AG

Technical Data	
Vehicle	Vito E-CELL
Engine	Power: max. 90 kW (122 PS) Max. Torque: 280 Nm
Speed	80 km/h (limited)
Range	130 km (NEFZ)
Durability	4 years
Battery	Capacity: 16 Ah, 32 kWh

Since 2010 there are 100 Mercedes-Benz Vito E-CELL in use by selected customers.

Explanation of the differences in energy densities

- from a tank full of Diesel each component of the tank content, namely Carbon and Hydrogen, can be burned up in the compactness of a solid state
- to guarantee the reversible battery process in a Li+-Ion battery a comprehensive logistics consisting of anode, cathode and diaphragma has to be housed in the accumulator
- as a consequence the energy density always differs by 2 orders of magnitudes between the accumulator „Diesel tank“ and the accumulator „Li+-Ion battery“!

all electric shuttle buses on the EXPO in Shanghai

Quelle: Foto X. Bei

Vehicle Concept of modern Trolley Busses with details of vehicle equipment

2. **Trolley Poles**
5. **Roof Structures**
7. **Engine (170 KW)**
11. **Diesel electric power unit**
14. **Compressor**

Source: Troullier, C.: Willkommen in der O-Bus Stadt; O-Bus Fachtagung, 10./11. Mai 2007, Solingen

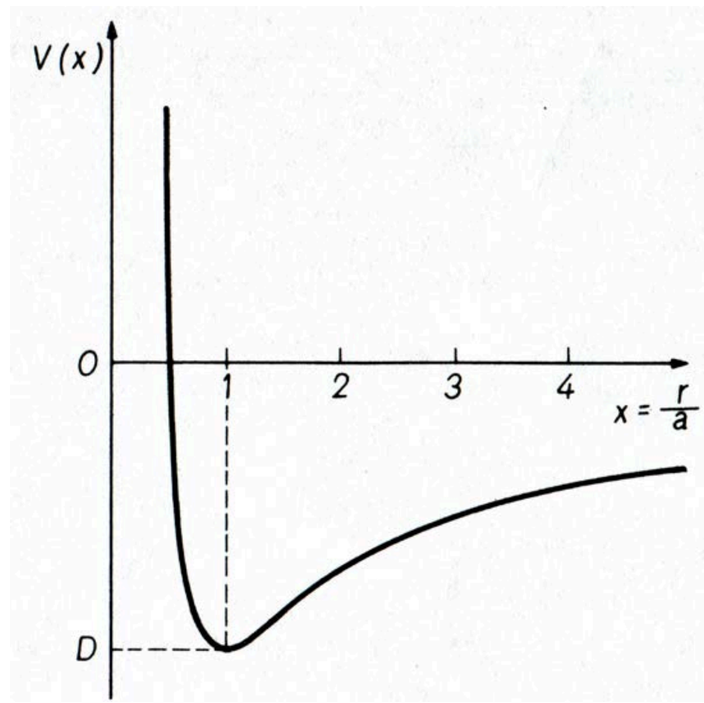
Double articulated trolley bus and light rail
- no difference in capacity and service but 80% cost savings
- the Zürich example

Quelle: Trolley Motion: Der Trolleybus als Alternative
zur Stadtbahn; Fachtagung KTBB 2008

Generalization to a diatomic molecular potential (Kratzer potential)

The considered Kratzer potential is a generalization of the central force ~ -1/r and a centrifugal barrier as model for a molecule's center of mass movement and reads

$$V(r) = -2D\left(\frac{a}{r} - \frac{1}{2}\frac{a^2}{r^2}\right)$$



leading to the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - D\left(\frac{2a}{r} - \frac{a^2}{r^2}\right)\right)\psi = E\,\psi$$

Scaling space coordinate and energy

$$x = \frac{r}{a} \qquad \varepsilon = \frac{2m\,a^2 E}{\hbar^2} \qquad\qquad \frac{2m\,a^2}{\hbar^2} D = \gamma^2$$

gives the Schrödinger equation for the radial part

$$H\varphi \equiv \left(-\partial_x^2 - \frac{2\gamma^2}{x} + \frac{\gamma^2 + l(l+1))}{x^2} \right)\varphi = \varepsilon\,\varphi$$

Factorization with $\lambda(\lambda\text{-}1) = \gamma^2 + l(l+1)$

$$H + \frac{\gamma^4}{\lambda^2} = \underbrace{(-\partial_x + \frac{\gamma^2}{\lambda} - \frac{\lambda}{x})}_{b^+(\lambda)}\underbrace{(\partial_x + \frac{\gamma^2}{\lambda} - \frac{\lambda}{x})}_{b(\lambda)}$$

gives because of the decomposition into hermitian conjugate factors

$$\varepsilon + \frac{\gamma^4}{\lambda^2} \geq 0 \quad \text{or} \quad \varepsilon \geq -\frac{\gamma^4}{\lambda^2}$$

$$\varepsilon_0 = -\frac{\gamma^4}{\lambda^2} \quad \text{and} \quad b(\lambda)\varphi_0 = 0 \;\rightarrow\; \varphi_0 = N\,x^\lambda e^{-\frac{\gamma^2}{\lambda}x} \;,\; \lambda > 0$$

The commutation relation

$$b^{+}\left(\lambda\right)H\left(\lambda+1\right)-H\left(\lambda\right)b^{+}\left(\lambda\right)=0$$

allows a ladder array

$$\varphi_{\nu}(\lambda)\sim\underbrace{b^{+}(\lambda)b^{+}(\lambda+1)\cdot\ldots\cdot b^{+}(\lambda+\nu-1)}_{\nu\ \text{factors}}\varphi_{0}(\lambda+\nu)$$

with the eigenvalues of the bound states

$$\varepsilon_{\nu}(\lambda)=-\frac{\gamma^{4}}{(\nu+\lambda)^{2}}\qquad\nu=0,1,2,\ldots$$

The scattering states belong to the range $\varepsilon\geq 0$.

Schrödinger equation for the Morse potential

$$V(r) = D(e^{-2\alpha\frac{r-r_0}{r_0}} - 2e^{-\alpha\frac{r-r_0}{r_0}})$$

The considered Morse potential leads to the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + D(e^{-2\alpha\frac{r-r_0}{r_0}} - 2e^{-\alpha\frac{r-r_0}{r_0}}\right)\psi = E\,\psi \qquad r > 0$$

Introduction of dimension less variables

$$\varepsilon = \frac{2mr_0^2 E}{\hbar^2\alpha^2} \qquad \gamma^2 = \frac{2mr_0^2 D}{\hbar^2\alpha^2} \qquad x = \alpha\frac{r-r_0}{r_0} - \ln\gamma$$

gives for the radial part with l=0

$$(-\partial_x^2 + e^{-2x} - 2\gamma\, e^{-x})\varphi = \varepsilon\,\varphi$$

Introducing the factors

$$b(\gamma) = \partial_x - e^{-x} + \gamma - 1/2 \qquad b^+(\gamma) = -\partial_x - e^{-x} + \gamma - 1/2$$

gives

$$b^+(\gamma)b(\gamma) = -\partial_x^2 + e^{-2x} - 2\gamma e^{-x} + (\gamma - 1/2)^2$$

and converts the Schrödinger equation with the Morse potential into

$$H\varphi = \left(b^+(\gamma)b(\gamma) - (\gamma - 1/2)^2\right)\varphi = \varepsilon\,\varphi$$

Because of the decomposition into hermitian conjugate factors, the estimation

$$\varepsilon \geq -(\gamma - 1/2)^2$$

holds, which gives for the ground state

$$\varepsilon_0 = -(\gamma - 1/2)^2 \qquad b\,\varphi_0 = 0 \qquad \varphi_0 = N\,e^{-(\gamma-\frac{1}{2})x - e^{-x}}$$

Changing γ→γ–1 in the Schrödinger equation gives

$$H(\gamma-1)\varphi_\nu(\gamma-1)=\varepsilon_\nu(\gamma-1)\varphi_\nu(\gamma-1) \qquad \Big|\, b^+(\gamma)\cdot$$

$$b^+(\gamma)\left(\underbrace{b^+(\gamma-1)b(\gamma-1)}_{b(\gamma)b^+(\gamma)-2\gamma+2}-(\gamma-\frac{3}{2})^2\right)\varphi_\nu(\gamma-1)=\varepsilon_\nu(\gamma-1)b^+(\gamma)\varphi_\nu(\gamma-1)$$

$$\underbrace{\left(b^+(\gamma)b(\gamma)-(\gamma-\frac{1}{2})^2\right)}_{H(\gamma)}b^+(\gamma)\varphi_\nu(\gamma-1)=\varepsilon_\nu(\gamma-1)b^+(\gamma)\varphi_\nu(\gamma-1)$$

$$H(\gamma)b^+(\gamma)\varphi_\nu(\gamma-1)=\varepsilon_\nu(\gamma-1)b^+(\gamma)\varphi_\nu(\gamma-1)$$

comparison with

$$H(\gamma)\varphi_{\nu+1}(\gamma)=\varepsilon_{\nu+1}(\gamma)\varphi_{\nu+1}(\gamma)$$

gives

$$\varepsilon_\nu(\gamma-1)=\varepsilon_{\nu+1}(\gamma)$$

and

$$\varphi_{\nu+1}(\gamma)\ \square\ b^+(\gamma)\varphi_\nu(\gamma-1)$$

starting with the ground state

$$b(\gamma)\varphi_0 = 0 \;\; \text{resp.} \;\; \varepsilon_0(\gamma) = -(\gamma - \frac{1}{2})^2$$

gives

$$\varepsilon_1(\gamma) = \varepsilon_0(\gamma - 1) = -(\gamma - \frac{3}{2})^2$$

$$\varepsilon_2(\gamma) = \varepsilon_1(\gamma - 1) = -(\gamma - \frac{5}{2})^2$$

....

$$\varepsilon_\nu(\gamma) = -(\gamma - \frac{1}{2} - \nu)^2 \qquad \nu = 0, 1, 2, \ldots, \nu_{\max}$$

and the ladder operator representation reads

$$\varphi_\nu(\gamma) \propto b^+(\gamma) b^+(\gamma - 1) \cdot \ldots \cdot b^+(\gamma - \nu + 1) \varphi_0(\gamma - \nu)$$

The bound states the energy eigenvalues must be negative and cannot lie below the potential minimum

$$-\gamma^2 < \varepsilon < 0 \qquad \varepsilon_{\min} = \varepsilon(\nu = \gamma - \frac{1}{2}) \quad \rightarrow \quad \nu_{\max} = \left[\gamma - \frac{1}{2} \right]$$

Connection to the Kratzer potential Schrödinger equation

The substitution

$$y = e^{-x}$$

gives for the Schrödinger equation with the Morse potential

$$0 = (-y\partial_y y\partial_y + y^2 - 2\gamma y - \varepsilon)\varphi$$

$$= y^{3/2}(-\frac{1}{\sqrt{y}}\partial_y y\partial_y + \sqrt{y} - 2\gamma\frac{1}{\sqrt{y}} - \varepsilon\frac{1}{y\sqrt{y}})\varphi$$

$$= y^{3/2}(-\frac{1}{\sqrt{y}}\partial_y y\partial_y\frac{1}{\sqrt{y}} + 1 - \frac{2\gamma}{y} - \frac{\varepsilon}{y^2})\underbrace{\sqrt{y}\,\varphi}_{\chi}$$

$$= y^{3/2}((-\partial_y - \frac{1/2}{y})(\partial_y - \frac{1/2}{y}) + 1 - \frac{2\gamma}{y} - \frac{\varepsilon}{y^2})\chi$$

$$= y^{3/2}(-\partial_y^2 + 1 - \frac{2\gamma}{y} + \frac{-\varepsilon - 1/4}{y^2})\chi$$

The abbreviation

$$\varepsilon = -s^2$$

transforms the Schrödinger equation for the bound states

$(-(\gamma-1/2)^2 \leq \varepsilon = -s^2 < 0)$ into

$$0 = (-\partial_y^2 + 1 - \frac{2\gamma}{y} + \frac{s^2 - 1/4}{y^2})\chi$$

Decomposition into hermitian conjugate factors yields

$$-\partial_y^2 + 1 - \frac{2\gamma}{y} + \frac{s^2 - 1/4}{y^2} =$$

$$\underbrace{(-\partial_y + \frac{\gamma}{s+1/2} - \frac{s+1/2}{y})}_{\tilde{b}^+(s)}\underbrace{(\partial_y + \frac{\gamma}{s+1/2} - \frac{s+1/2}{y})}_{\tilde{b}(s)} + 1 - (\frac{\gamma}{s+1/2})^2$$

The Schrödinger equation can be summarized as

$$\tilde{H}\chi \equiv (-\partial_y^2 + 1 - \frac{2\gamma}{y} + \frac{s^2 - 1/4}{y^2})\chi = 0$$

$$= \left(\tilde{b}^+(s)\tilde{b}(s) + 1 - (\frac{\gamma}{s+1/2})^2 \right)\chi$$

The commutation relation

$$\tilde{b}^+(s)\tilde{H}(s+1) - \tilde{H}(s)\tilde{b}^+(s) = 0$$

allows a ladder array

$$\chi_\nu(s) \sim \underbrace{\tilde{b}^+(s)\tilde{b}^+(s+1)\cdot \ldots \cdot \tilde{b}^+(s+\nu-1)}_{\nu \text{ factors}}\chi_0(s+\nu)$$

with the eigenvalues of the bound states

$$\varepsilon_\nu = -(\gamma - \frac{1}{2} - \nu)^2 \qquad \nu = 0, 1, 2, \ldots$$

The scattering states belong to the range $\varepsilon \geq 0$.

Literature:

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