

Practical Quantum Mechanics -
from Exactly Solvable Schrödinger Equations,
Shape Invariant Potentials, and Supersymmetry
with Applications in Stochastics and Nonlinear
Evolution Equations for Disaster Description
and Traffic Breakdown Propagation

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contents

- Elementary application examples
 - square well potential, δ -potential, and combinations
- Factorization of the Schrödinger equation
 - creation and annihilation operators, ladder operators
- Transformation to shape invariant potentials
 - algebraic approach, mapping by canonical transformation, Lie algebraic methods
- Application examples
 - disaster description
 - wide moving jams

General concepts in quantum mechanics

Starting point: Newton's law for point mechanics:

$$\dot{\vec{x}} = \frac{\vec{p}}{m} \quad \left| \quad \begin{array}{l} m \ddot{\vec{x}} = \vec{F} \\ \dot{\vec{p}} = -\nabla V \end{array} \right. \Rightarrow \text{trajectory } \vec{x} = \vec{x}(t)$$
$$\frac{1}{m} \vec{p} \dot{\vec{p}} = - \dot{\vec{x}} \nabla V \quad \text{or} \quad \frac{d}{dt} \left(\underbrace{\frac{1}{2m} \vec{p}^2 + V}_H \right) = 0$$

equivalent to the conservation law

$$\frac{d}{dt} H = 0 \quad H = \underbrace{\frac{1}{2m} \vec{p}^2}_{\text{kin. energy}} + \underbrace{V}_{\text{potential}} = E = \text{const.} \quad \text{Hamiltonian}$$

Alternative to Newton's law for point mechanics: The Hamilton-Jacobi equation

Sought is a canonical transformation

$$P_k = P_k(\vec{p}, \vec{x}, t) \quad Q_k = Q_k(\vec{p}, \vec{x}, t)$$

such that

$$\tilde{H}(\{P_k\}, \{Q_k\}, t) = H(\vec{p}, \vec{x}, t) + \frac{\partial S}{\partial t} = 0 \quad (1)$$

holds

This solves the mechanical problem completely and the P_k and Q_k are integrals of the equation of motion

$$\dot{P}_k = -\frac{\partial \tilde{H}}{\partial Q_k} = 0 \Rightarrow P_k = \text{const.} \quad \dot{Q}_k = \frac{\partial \tilde{H}}{\partial P_k} = 0 \Rightarrow Q_k = \text{const.}$$

The generating function S for the transformation (1) is the action spectrum with dimension

$[S] = \text{energy} \cdot \text{time}$
or $\text{mass} \cdot \text{velocity} \cdot \text{distance}$

which has the vivid meaning of a parcel postage rate depending on weight & transport speed & distance



If we insert $(\vec{p})_k = \frac{\partial S}{\partial \mathbf{x}_k}$ $P_k = \frac{\partial S}{\partial Q_k}$

into equ. (1) we get the **Hamilton-Jacobi differential equation** for the action spectrum S

$$H\left(\mathbf{p}_k = \frac{\partial S}{\partial \mathbf{x}_k}, \mathbf{x}_k, t\right) + \frac{\partial S(\mathbf{x}_k, P_k, t)}{\partial t} = 0$$

For a conservative system for which a potential exists the Hamilton function reads

$$H(\{p_k\}, \{x_k\}, t) = \frac{\vec{p}^2}{2m} + V(\vec{x})$$

and the Hamilton-Jacobi differential equation is given by

$$-\frac{\partial S}{\partial t} = \frac{1}{2m} \sum \left(\frac{\partial S}{\partial x_k} \right)^2 + V(\{x_k\})$$

The Hamilton-Jacobische differential equation is a partial differential equation for the $f+1$ variables x_k and t (f = number of degrees of freedom). The P_k are constants according to the definition of the action spectrum.

The differential equation is nonlinear and there is no chance to find a general solution (which depends on arbitrary functions).

In quantum mechanics we start with the Schrödinger equation, an equation of motion for the wave function ψ with a Hamiltonian formed by a translation rule

Schrödinger equation for the wave function ψ

$$i\hbar\dot{\psi} = H\psi \quad H = \frac{\vec{p}^2}{2m} + V \quad \vec{p} \rightarrow \frac{\hbar}{i}\nabla \quad V \rightarrow V.$$

Instead of sharp trajectories $\Omega(t)$, we have now expectation values $\int \psi^* \Omega \psi d^3x$ formed with the wave function ψ for finding Ω with a certain probability.

Erwin Schrödinger

born 1887 in Vienna, Austria

1921 1 year at Univ. Stuttgart!!

Excerpt of the Univ. calendar 1921
“Erwin Schrödinger- dyn. Systems”



1926 Schrödinger equation

1933 Nobel prize

1936 emigration to Dublin
Ireland

1944 “What is life”

1956 Return to Vienna

1961 died in Vienna



Bust of
Erwin
Schrödinger
at the Univ.
of Vienna

Classical Limit of Quantum Mechanics: Quasi Classical Approximation.

For sufficient large momentum of a particle (small de-Broglie-wavelength) the behavior does not differ from classical mechanics. The limiting process from quantum mechanics to classical mechanics is demonstrated easiest if a wavefunction in the form

$$\psi(\vec{x}, t) = e^{\frac{i}{\hbar}S(\vec{x}, t)}$$

is inserted into the Schrödinger equation

$$i\hbar\dot{\psi} = H\psi \equiv \underbrace{\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)}_{\frac{\vec{p}^2}{2m} \equiv E_{\text{kin}}}\psi$$

leading for $S(x,t)$ to

$$-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V(\vec{x}) - \frac{i\hbar}{2m}\Delta S$$

The comparison with the Hamilton-Jakobi differential equation of classical mechanics

$$-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V(\vec{x})$$

with the classical action spectrum S shows similarity in the limit $\hbar \rightarrow 0$.

(reminder: the trajectories of a classical particle are orthogonal to the plane $S=\text{const.}$)

Elementary application examples

- Rectangular potential hole
- Square well potential
- δ -potential
- Potential hole with superimposed δ -wall/hole

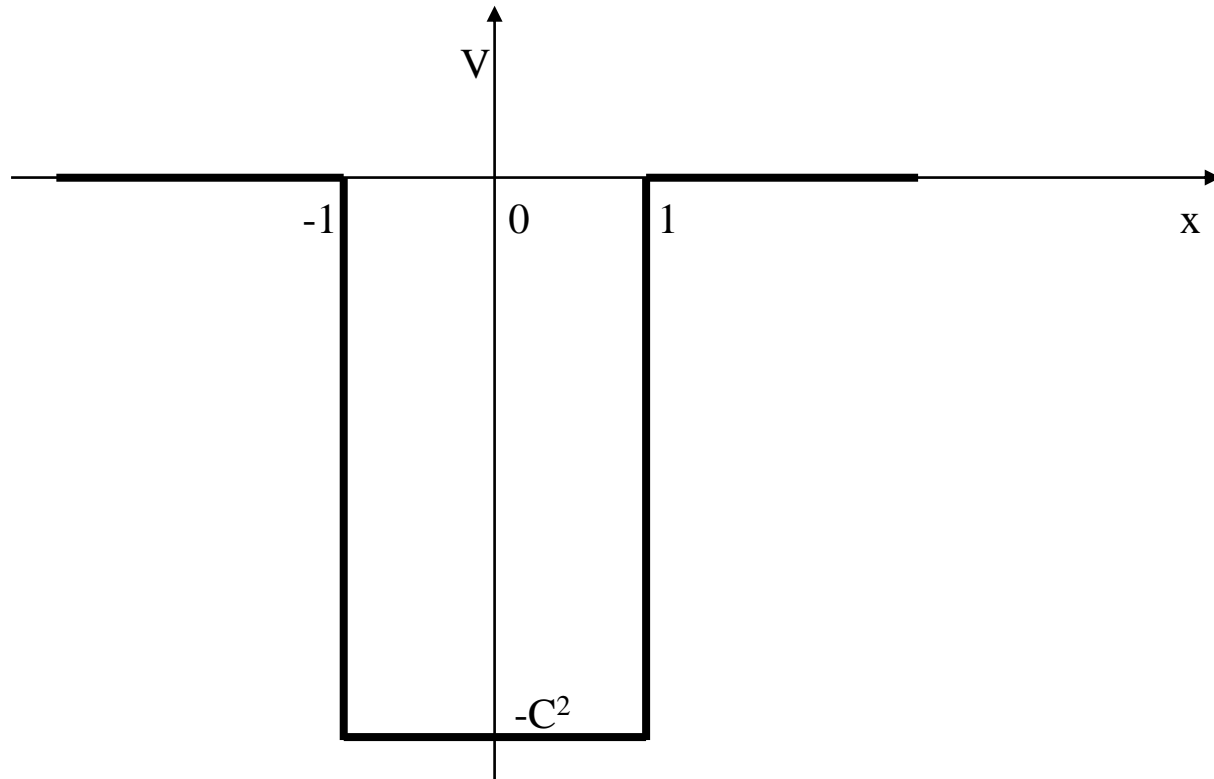
Rectangular Potential Hole

The Schrödinger equation for a single particle moving in a one-dimensional rectangular potential hole with

normalized width $V(x) = \begin{cases} -C^2 & \text{for } |x| < 1 \\ 0 & \text{for } |x| > 1 \end{cases}$

reads

$$\left\{ -\partial_x^2 + V(x) \right\} \varphi_v(x) = \varepsilon_v \varphi_v(x)$$



Ground state

The ground state of the Schrödinger equation for a single particle moving in a one-dimensional rectangular potential hole is given by

$$\varepsilon_0 = k_0^2 - C^2 \quad \varphi_0 = \begin{cases} N_0 \cos k_0 x & |x| < 1 \\ N_0 \cos k_0 e^{-\kappa_0(|x|-1)} & |x| > 1 \end{cases} \quad \kappa_0 = \sqrt{C^2 - k_0^2}$$

under continuity conditions at $x=\pm 1$. Fitting the continuity conditions at $x=\pm 1$ for the derivative of φ_0 gives

$$k_0 \tan k_0 = \kappa_0 \quad \kappa_0 = \sqrt{C^2 - k_0^2}$$

or

$$k_0 = C \cos k_0$$

$$k_0^2 \leq k_0 \tan k_0 \leq \frac{k_0}{\pi/2 - k_0} \text{ gives}$$

as lower limit

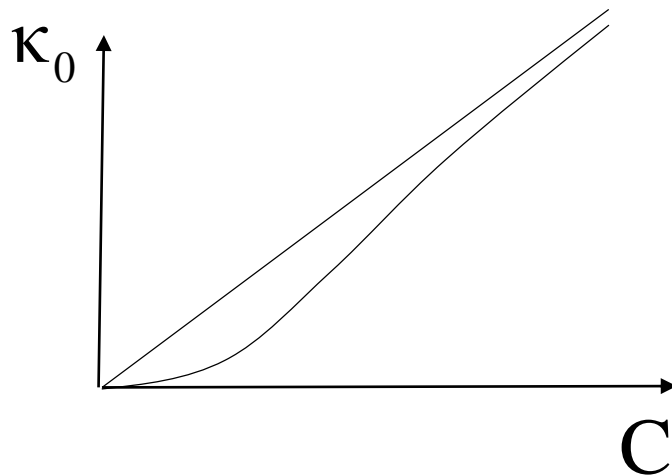
$$k_0^2 \leq \kappa_0 \text{ or } \kappa_0 \geq -\frac{1}{2} + \sqrt{\frac{1}{4} + C^2} \approx C^2 - C^4$$

as upper limit

$$k_0 \leq \pi/2 \text{ or } \kappa_0 \leq \sqrt{C^2 - (\pi/2)^2} \approx |C| - \frac{\pi^2}{8|C|}$$

Summary($C > 0$)

$$C^2 \leq \kappa_0 \leq C$$



Exited states

symmetric eigenfunctions

$$\varepsilon_v = k_v^2 - C^2 \quad \varphi_v^s = N_v \begin{cases} \cos k_v x & |x| < 1 \\ \cos k_v e^{-\kappa_v(|x|-1)} & |x| > 1 \end{cases} \quad \kappa_v = \sqrt{C^2 - k_v^2} \quad v = 1, 2, 3, \dots$$

asymmetric eigenfunctions

$$\varepsilon_v = k_v^2 - C^2 \quad \varphi_v^{as} = N_v \begin{cases} \sin k_v x & |x| < 1 \\ +\sin k_v e^{-\kappa_v(|x|-1)} & x > 1 \\ -\sin k_v e^{-\kappa_v(|x|-1)} & x < -1 \end{cases} \quad \kappa_v = \sqrt{C^2 - k_v^2} \quad v = 1, 2, 3, \dots$$

Continuity of φ' at $x=1$ gives
for the symmetric eigenfunctions

$$\tan k_v = \frac{\sqrt{C^2 - k_v^2}}{k_v} \quad k_v = \arctan \frac{\sqrt{C^2 - k_v^2}}{k_v} \quad v = 1, 2, 3, \dots$$

and for the asymmetric eigenfunctions

$$\tan k_v = -\frac{k_v}{\sqrt{C^2 - k_v^2}} \quad k_v = -\arctan \frac{k_v}{\sqrt{C^2 - k_v^2}} \quad v = 1, 2, 3, \dots$$

Evaluation of the relations $\tan k_v = \frac{\sqrt{C^2 - k_v^2}}{k_v}$ and $\tan k_v = -\frac{k_v}{\sqrt{C^2 - k_v^2}}$

The wave numbers k_v in the energy eigenvalues $\varepsilon_v = k_v^2 - C^2$ obey the relations for the symmetric eigenfunctions

$$\tan k_v = \frac{\sqrt{C^2 - k_v^2}}{k_v} \quad k_v = \arctan \frac{\sqrt{C^2 - k_v^2}}{k_v} = v\pi + \text{Arctan} \frac{\sqrt{C^2 - k_v^2}}{k_v} \quad v = 1, 2, 3, \dots$$

and for the asymmetric eigenfunctions

$$\tan k_v = -\frac{k_v}{\sqrt{C^2 - k_v^2}} \quad k_v = -\text{arccot} \frac{\sqrt{C^2 - k_v^2}}{k_v} = (v+1)\pi + \text{Arctan} \frac{\sqrt{C^2 - k_v^2}}{k_v} \quad v = 1, 2, 3, \dots$$

with the transformation to the principal value. Both results can be summarized as

$$k_v = v \frac{\pi}{2} + \text{Arctan} \frac{\sqrt{C^2 - k_v^2}}{k_v} \quad \text{or} \quad k_v = C \cos \left(k_v - v \frac{\pi}{2} \right) \quad v = 0, 1, 2, \dots, v_{\max}$$

including the groundstate wavenumber k_0 . Since $k_v < |C|$ and $\text{Arctan} \frac{\sqrt{C^2 - k_v^2}}{k_v} < \frac{\pi}{2}$

$$v_{\max} = \left[\frac{|C|}{(\pi/2)} \right], \quad [\dots] = \text{largest integer from } \dots$$

For $C \gtrsim v\pi/2$ the conditional equation

$$k_v = v \frac{\pi}{2} + \text{Arccos} \frac{k_v}{|C|}$$

simplifies with

$$C = v \frac{\pi}{2} + \delta, \quad \delta \ll 1$$

to

$$k_v = v \frac{\pi}{2} + \delta - v \frac{\pi}{4} \delta^2 + \dots = C - v \frac{\pi}{4} \delta^2 + \dots$$

which gives for the energy eigenvalues

$$\varepsilon_v = k_v^2 - C^2 \approx -\left(v \frac{\pi}{2}\right)^2 \delta^2$$

For an infinitely deep potential hole ($C^2 \rightarrow \infty$) the conditional equation has the limit

$$\text{Arctan} \frac{\sqrt{C^2 - k_v^2}}{k_v} \rightarrow \frac{\pi}{2} \quad \text{and} \quad k_v \rightarrow (v+1) \frac{\pi}{2} \quad v = 0, 1, 2, \dots$$

which leads to the eigenvalues

$$\varepsilon_v \rightarrow (v+1)^2 \left(\frac{\pi}{2}\right)^2 - C^2 \quad v = 0, 1, 2, \dots$$

in accordance with the eigenvalues of the square well potential

The conditional equation for the wavenumbers

$$\cos(k_v - v \frac{\pi}{2}) = k_v / |C|$$

can be transformed into

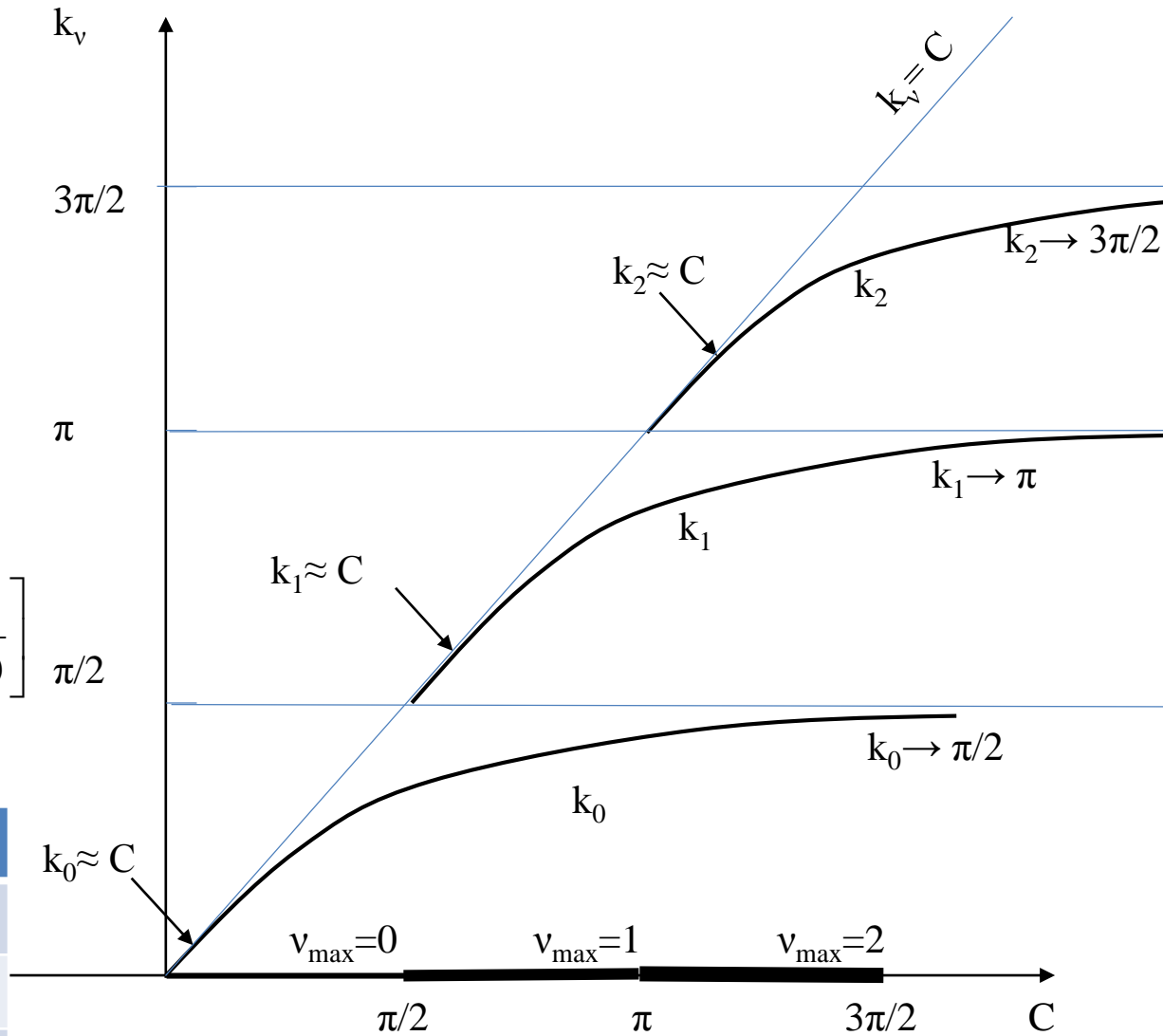
$$k_v = \begin{cases} |C| \cos k_v & v = 0, 4, 8, \dots \\ |C| \sin k_v & v = 1, 5, 9, \dots \\ -|C| \cos k_v & v = 2, 6, 10, \dots \\ -|C| \sin k_v & v = 3, 7, 11, \dots \end{cases}$$

with

$$v \frac{\pi}{2} \leq k_v < (v+1) \frac{\pi}{2} \quad v \leq v_{\max} \equiv \left[\frac{|C|}{(\pi/2)} \right] \pi/2$$

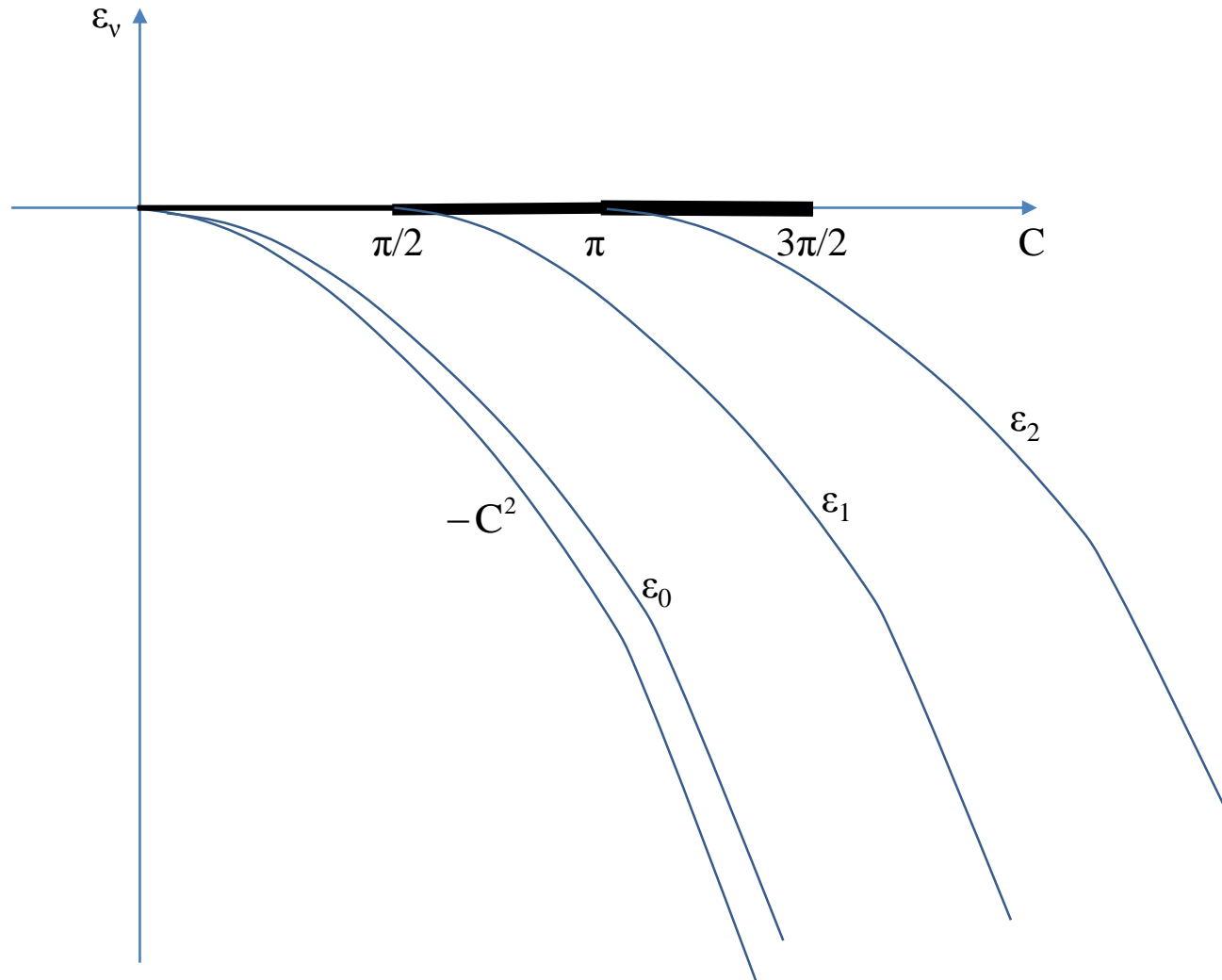
Results for $C^2=25$

v	$v\pi/2$	k_v	$(v+1)\pi/2$
0	0.0	1.306	1.571
1	1.571	2.596	3.142
2	3.142	3.837	4.712
3	4.712	4.937	6.283



Energy eigenvalues

$$\varepsilon_v = k_v^2 - C^2$$



Results for $C^2=25$

v	ε_v
0	-23.29
1	-18.26
2	-10.27
3	- 0.92

Scattering states

After analyzing the bound states (ground state, excited states) we investigate the scattering states ($\varepsilon = k^2 > 0$)

The Schrödinger equation

$$\left\{ -\partial_x^2 + V(x) \right\} \varphi_k(x) = k^2 \varphi_k(x) \quad V(x) = \begin{cases} -C^2 & \text{for } |x| < 1 \\ 0 & \text{for } |x| > 1 \end{cases}$$

is solved in 3 regions: (1) $x < -1$, (2) $-1 < x < 1$, and (3) $x > 1$.

(1) $x < -1$:

$$\varphi_k(x) = I e^{ikx} + R e^{-ikx}$$

(2) $-1 < x < 1$:

$$\varphi_k(x) = A e^{i\mu x} + B e^{-i\mu x} \quad \mu = \sqrt{C^2 + k^2}$$

(3) $x > 1$:

$$\varphi_k(x) = T e^{ikx} \quad \text{only outgoing wave}$$

Since the potential is finite everywhere, both the wave function and its derivative must be continuous everywhere.

At $x = -1$ these two conditions yield

$$I e^{-ik} + R e^{ik} = A e^{-i\mu} + B e^{i\mu}$$

$$ik(I e^{-ik} - R e^{ik}) = i\mu(A e^{-i\mu} - B e^{i\mu})$$

at $x = 1$ we have

$$A e^{i\mu} + B e^{-i\mu} = T e^{ik}$$

$$i\mu(A e^{i\mu} - B e^{-i\mu}) = ik T e^{ik}$$

which can be summarized in matrixform

$$\begin{pmatrix} e^{-i\mu} & e^{i\mu} & -e^{ik} & 0 \\ e^{-i\mu} & -e^{i\mu} & \frac{k}{\mu} e^{ik} & 0 \\ e^{i\mu} & e^{-i\mu} & 0 & -e^{ik} \\ e^{i\mu} & -e^{-i\mu} & 0 & -\frac{k}{\mu} e^{ik} \end{pmatrix} \begin{pmatrix} A \\ B \\ R \\ T \end{pmatrix} = \begin{pmatrix} I e^{-ik} \\ \frac{k}{\mu} I e^{-ik} \\ 0 \\ 0 \end{pmatrix}$$

We have 4 linear equations for the unknowns R, T, A, and B, so we can express these constants in terms of the amplitude I of the incident wave, which is put to 1 ($C \neq \infty$) for simplicity.

Inserting yields

$$|T|^2 = \frac{1}{1 + (\mu^2 - k^2)^2 \sin^2 2\mu / 4k^2 \mu^2}$$

$$|R|^2 + |T|^2 = 1$$

In the limit $C^2 \rightarrow \infty$ T, R, and $I \rightarrow 0$, and there is no scattering solution. In this limit and only the bound states exist

We can write this in original parameters and get

$$|T|^2 = \frac{1}{1 + \frac{C^4}{4k^2(C^2 + k^2)} \sin^2 2\sqrt{C^2 + k^2}}$$

The transmission becomes 1 (i.e. no reflection) under the condition

$$2\sqrt{C^2 + k^2} = n\pi \quad n = 0, 1, 2, \dots$$

This phenomenon occurs in the Ramsauer-Townsend effect*), which involves the scattering of electrons off atoms of inert gases. Classical physics predicts that the number of electrons scattered should increase monotonically with their energy, but in fact a minimum is observed for certain electron energies. A model in which the inert gas atom is treated as a finite square well provides a simplified explanation of the effect.

*) Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education

Factorization

The definition $\mathbf{b}_{k_0} = \partial_x + \begin{cases} k_0 \tan k_0 x & \text{for } |x| < 1 \\ \kappa_0 & \text{for } |x| > 1 \end{cases}$ $\kappa_0 = \sqrt{C^2 - k_0^2}$ gives

$$\begin{aligned}
 \mathbf{b}_{k_0}^+ \mathbf{b}_{k_0} &= \\
 & \left(-\partial_x + k_0 \tan k_0 x \Theta(1 - |x|) + \kappa_0 \Theta(|x| - 1) \right) \left(\partial_x + k_0 \tan k_0 x \Theta(1 - |x|) + \kappa_0 \Theta(|x| - 1) \right) \\
 &= -\partial_x^2 - \left(k_0 \tan k_0 x \Theta(1 - |x|) + \kappa_0 \Theta(|x| - 1) \right)' + \left(k_0 \tan k_0 x \Theta(1 - |x|) + \kappa_0 \Theta(|x| - 1) \right)^2 \\
 &= -\partial_x^2 - \frac{k_0^2}{\cos^2 k_0 x} \Theta(1 - |x|) + \underbrace{(-k_0 \tan k_0 x + \kappa_0) \delta(|x| - 1) \text{sign } x}_{\stackrel{!}{=} 0} \\
 & \quad + k_0^2 \underbrace{\tan^2 k_0 x \Theta(1 - |x|)}_{\frac{1}{\cos^2 k_0 x} - 1} + \kappa_0^2 \underbrace{\Theta(|x| - 1)}_{1 - \Theta(1 - |x|)} \\
 &= -\partial_x^2 - \underbrace{(k_0^2 + \kappa_0^2) \Theta(1 - |x|) + \kappa_0^2}_{\equiv V - \varepsilon_0} \quad \text{with} \quad -k_0 \tan k_0 + \kappa_0 = 0
 \end{aligned}$$

and allows the decomposition

$$\mathbf{H} - \varepsilon_0 = -\partial_x^2 + V - \varepsilon_0 \equiv \mathbf{b}_{k_0}^+ \mathbf{b}_{k_0} \quad \varepsilon_0 = -\kappa_0^2 \quad V = -(k_0^2 + \kappa_0^2) \Theta(1 - |x|)$$

Square-Well Potential

The Schrödinger equation for a single particle moving in a one-dimensional rectangular potential hole shows in the limiting case $C^2 \rightarrow \infty$ no scattering states solutions. We can therefore rescale the potential by adding C^2 and get for an infinitely deep square-well potential of width ℓ

$$V(x) = \begin{cases} 0 & \text{for } |x| \leq \ell \\ \infty & \text{else} \end{cases}$$

In dimensionless variables ($x' = x/\ell$, $V' = V/(\hbar^2/2m\ell^2)$, $\varepsilon = E/(\hbar^2/2m\ell^2)$, $\psi' = \psi/\sqrt{\ell}$, 'suppressed') the associated Schrödinger equation reads

$$\left\{ -\partial_x^2 + V(x) \right\} \psi_v(x) = \varepsilon_v \psi_v(x) \quad V(x) = \begin{cases} 0 & |x| \leq 1 \\ \infty & |x| > 1 \end{cases}$$

with the solutions

$$\psi_v = \begin{cases} N_v \sin k_v^{\text{as}} x & |x| \leq 1 \\ N_v \cos k_v^{\text{s}} x & |x| \leq 1 \\ \psi_v = 0 & \text{else} \end{cases}$$

and

$$\varepsilon_v = (k_v^{\text{as,s}})^2$$

Fitting the boundary conditions gives

$$\psi_v(1) = 0 \Rightarrow k_v^{\text{as}} = v\pi \quad v = 1, 2, 3, \dots; \quad k_v^{\text{s}} = \left(v + \frac{1}{2}\right)\pi \quad v = 0, 1, 2, \dots$$

$$\varepsilon_v = (k_v^{\text{as,s}})^2 = (v+1)^2 \left(\frac{\pi}{2}\right)^2 \quad v = 0, 1, 2, \dots$$

Factorization gives $-\partial_x^2 + V(x) - \varepsilon_0 = -\partial_x^2 - \left(\frac{\pi}{2}\right)^2 = L^+L^- = \left(-\partial_x + \frac{\pi}{2} \tan \frac{\pi}{2} x\right)\left(\partial_x + \frac{\pi}{2} \tan \frac{\pi}{2} x\right)$

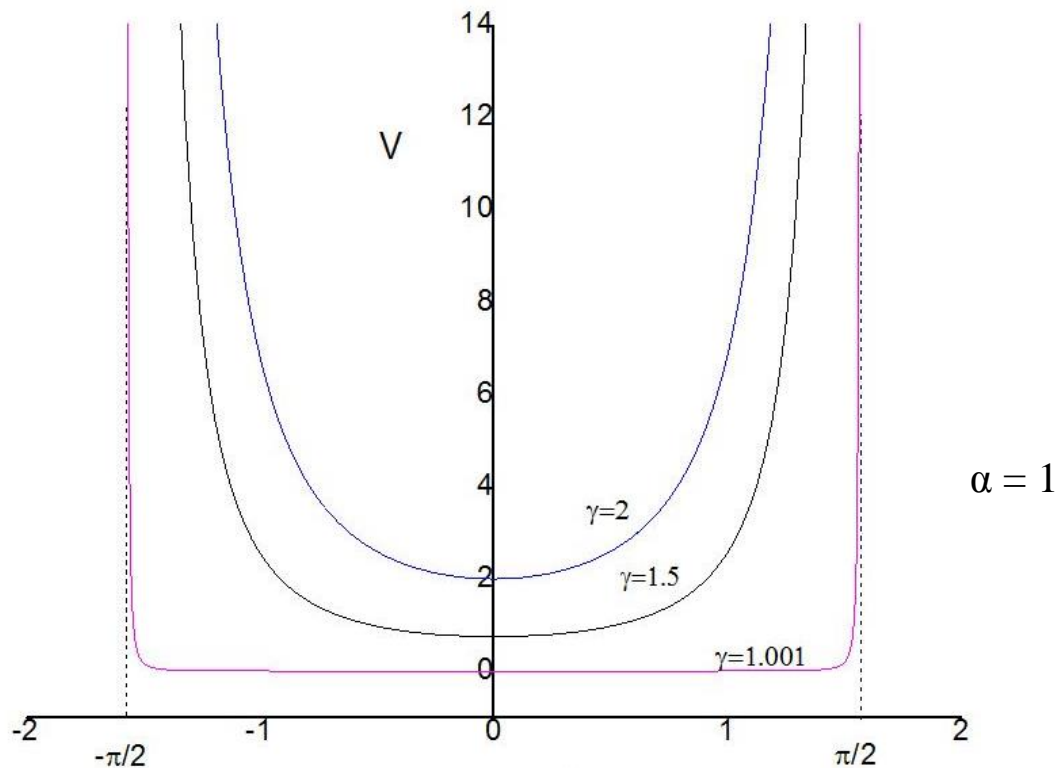
$$= -\partial_x^2 + \underbrace{\left(\frac{\pi}{2}\right)^2 \tan^2 \frac{\pi}{2} x}_{\frac{1}{\cos^2 \frac{\pi}{2} x} - 1} - \frac{\pi}{2} \underbrace{\tan' \frac{\pi}{2} x}_{\frac{\pi}{2} \frac{1}{\cos^2 \frac{\pi}{2} x}} = -\partial_x^2 - \left(\frac{\pi}{2}\right)^2$$

Generalization of the decomposition gives

$$L_\gamma^+ L_\gamma^- \equiv \left(-\partial_x + \alpha\gamma \tan \alpha x\right)\left(\partial_x + \alpha\gamma \tan \alpha x\right) = -\partial_x^2 - \alpha\gamma \tan' \alpha x + \alpha^2 \gamma^2 \tan^2 \frac{\pi}{2} x = -\partial_x^2 + \underbrace{\frac{\alpha^2 \gamma(\gamma-1)}{\cos^2 x}}_{H(\gamma)} - \alpha^2 \gamma^2$$

with the generalized Hamiltonian

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



Ladder operators

The commutation relation

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

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

introduced into the Schrödinger equation with the generalized potential gives for $\gamma \rightarrow \gamma+1$

$$(\mathbf{H}(\gamma+1) - \alpha^2(\gamma+1)^2)\psi_{\nu}(\gamma+1) = (\varepsilon_{\nu}(\gamma+1) - \alpha^2(\gamma+1)^2)\psi_{\nu}(\gamma+1) \quad \left| b_{\gamma}^{+} \right.$$

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

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

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

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

starting with the ground state

gives $\mathbf{b}_\gamma \psi_0(\gamma) = 0$ resp. $\varepsilon_0(\gamma) = \alpha^2 \gamma^2$

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

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

....

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

or for $\gamma=1$

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

and the ladder operator representation reads

$$\psi_1(\gamma) \sim \mathbf{b}_\gamma^+ \psi_0(\gamma + 1)$$

$$\psi_2(\gamma) \sim \mathbf{b}_\gamma^+ \psi_1(\gamma + 1) \sim \mathbf{b}_\gamma^+ \mathbf{b}_{\gamma+1}^+ \psi_0(\gamma + 2)$$

....

$$\psi_\nu(\gamma) \sim \mathbf{b}_\gamma^+ \mathbf{b}_{\gamma+1}^+ \cdots \mathbf{b}_{\gamma+\nu-1}^+ \psi_0(\gamma + \nu)$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

The Schrödinger equation for a particle in the hyperbolic Pöschl-Teller potential reads (first for the scattering states)

$$\varepsilon = k^2 > 0 \quad \left(-\partial_x^2 - \frac{\lambda(\lambda+1)}{\cosh^2 x} \right) \psi = k^2 \psi \quad \lambda > 0$$

$$\left(-\partial_x^2 + \underbrace{\frac{-\lambda^2}{\cosh^2 x}}_{(\lambda \operatorname{th} x)^2 - \lambda^2} + \underbrace{\frac{-\lambda}{\cosh^2 x}}_{-(\lambda \operatorname{th} x)'} \right) \psi = k^2 \psi$$

$$\left(\underbrace{(-\partial_x + \lambda \operatorname{th} x)}_{\Omega^+} \underbrace{(\partial_x + \lambda \operatorname{th} x)}_{\Omega} - \lambda^2 \right) \psi = k^2 \psi$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

For the scattering states ($\varepsilon > 0$) only the asymptotic behavior is considered. $|x| \rightarrow \infty$ gives $\text{th}x \rightarrow \text{sign}x$

$$\begin{aligned}\Omega^+ \Omega &\rightarrow (-\partial_x + \lambda \text{sign}x)(\partial_x + \lambda \text{sign}x) \\ &= -\partial_x^2 - \lambda (\text{sign}x)' + \lambda^2 = -\partial_x^2 - 2\lambda\delta(x) + \lambda^2\end{aligned}$$

and the Schrödinger equation has the asymptotic form

$$\left(-\partial_x^2 - 2\lambda\delta(x)\right)\psi = k^2\psi$$

with the solution

$$\psi = \begin{cases} \psi^s = \frac{1}{\sqrt{\pi}} \sin(k|x| - \alpha_k) \\ \psi^{\text{as}} = \frac{1}{\sqrt{\pi}} \sin kx \end{cases} \quad \tan \alpha_k = k / \lambda$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

The general solution is a linear combination

$$\psi = c\psi^s + d\psi^{as}$$

We want a solution with the asymptotic form

$$\psi = \begin{cases} e^{ikx} + Re^{-ikx} & x < 0 \\ Te^{ikx} & x > 0 \end{cases}$$

i.e.

$$e^{ikx} + Re^{-ikx} = \frac{c}{\sqrt{\pi}} \frac{e^{i(-kx-\alpha_k)} - e^{-i(-kx-\alpha_k)}}{2i} + \frac{d}{\sqrt{\pi}} \frac{e^{ikx} - e^{-ikx}}{2i}$$
$$Te^{ikx} = \frac{c}{\sqrt{\pi}} \frac{e^{i(kx-\alpha_k)} - e^{-i(kx-\alpha_k)}}{2i} + \frac{d}{\sqrt{\pi}} \frac{e^{ikx} - e^{-ikx}}{2i}$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

Comparison of the coefficients of e^{ikx} and e^{-ikx} results in

$$1 = \frac{-c}{2i\sqrt{\pi}} e^{i\alpha_k} + \frac{d}{2i\sqrt{\pi}} \quad R = \frac{c}{2i\sqrt{\pi}} e^{-i\alpha_k} - \frac{d}{2i\sqrt{\pi}}$$

$$0 = \frac{-c}{2i\sqrt{\pi}} e^{i\alpha_k} - \frac{d}{2i\sqrt{\pi}} \quad T = \frac{c}{2i\sqrt{\pi}} e^{-i\alpha_k} + \frac{d}{2i\sqrt{\pi}}$$

T and R can be computed from these equations to

$$R = e^{-i\alpha_k} \cos\alpha_k \quad T = ie^{-i\alpha_k} \sin\alpha_k$$

satisfying the conservation law

$$|T|^2 + |R|^2 = 1$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

For the bound states ($\varepsilon_n < 0$) the Schrödinger equation for the hyperbolic Pöschl-Teller potential is given by

$$H(\lambda)\psi_n \equiv \left(-\partial_x^2 - \frac{\lambda(\lambda+1)}{\cosh^2 x}\right)\psi_n = \varepsilon_n \psi_n \quad \lambda > 0$$

$$\left(-\partial_x^2 + \underbrace{\lambda^2 \left(1 - \frac{1}{\cosh^2 x}\right)}_{(\lambda \operatorname{th} x)^2} - \underbrace{\frac{\lambda}{\cosh^2 x}}_{(\lambda \operatorname{th} x)'} - \lambda^2\right)\psi_n = \varepsilon_n \psi_n$$

$$\underbrace{\left(-\partial_x + \lambda \operatorname{th} x\right)}_{\Omega^+(\lambda)} \underbrace{\left(\partial_x + \lambda \operatorname{th} x\right)}_{\Omega(\lambda)} \psi_n = \varepsilon_n \psi_n$$

The decomposition into 2 hermitian conjugate factors was done with regard to a ground state for which a norm is possible and enables the estimation

$$\lambda^2 + \varepsilon_n \geq 0$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

From the estimation follows for the ground state which can be normalized

$$\varepsilon_0 = -\lambda^2 \quad \text{or} \quad \Omega \psi_0 = 0 \rightarrow \psi_0 = N \cosh^{-\lambda} x \quad \lambda > 0$$

Changing $\lambda \rightarrow \lambda - 1$ in the Schrödinger equation gives

$$H(\lambda - 1)\psi_n(\lambda - 1) = \varepsilon_n(\lambda - 1)\psi_n(\lambda - 1) \quad \Big| \Omega^+(\lambda).$$

Multiplying with $\Omega^+(\lambda)$ from left gives

$$\Omega^+(\lambda)(\Omega^+(\lambda - 1)\Omega(\lambda - 1) - (\lambda - 1)^2)\psi_n(\lambda - 1) = \varepsilon_n(\lambda - 1)\Omega^+(\lambda)\psi_n(\lambda - 1)$$

Inserting the commutation relation

$$\begin{aligned} & \Omega^+(\lambda - 1)\Omega(\lambda - 1) - \Omega(\lambda)\Omega^+(\lambda) \\ &= (-\partial_x + (\lambda - 1) \operatorname{th}x)(\partial_x + (\lambda - 1) \operatorname{th}x) - (\partial_x + \lambda \operatorname{th}x)(-\partial_x + \lambda \operatorname{th}x) \\ &= -2\lambda + 1 \end{aligned}$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

$$\Omega^+(\lambda) \underbrace{(\Omega^+(\lambda-1)\Omega(\lambda-1) - (\lambda-1)^2)}_{\Omega(\lambda)\Omega^+(\lambda) - 2\lambda + 1} \psi_n(\lambda-1) = \varepsilon_n(\lambda-1)\Omega^+(\lambda)\psi_n(\lambda-1)$$

$$\underbrace{(\Omega^+(\lambda)\Omega(\lambda) - \lambda^2)}_{H(\lambda)} \Omega^+(\lambda)\psi_n(\lambda-1) = \varepsilon_n(\lambda-1)\Omega^+(\lambda)\psi_n(\lambda-1)$$

$$\text{gives } H(\lambda)\Omega^+(\lambda)\psi_n(\lambda-1) = \varepsilon_n(\lambda-1)\Omega^+(\lambda)\psi_n(\lambda-1)$$

Comparison with

$$H(\lambda)\psi_{n+1}(\lambda) = \varepsilon_{n+1}(\lambda)\psi_{n+1}(\lambda)$$

yields to

$$\varepsilon_n(\lambda-1) = \varepsilon_{n+1}(\lambda) \quad \psi_{n+1}(\lambda) \sim \Omega^+(\lambda)\psi_n(\lambda-1)$$

Excursus: Schrödinger equation for the hyperbolic Pöschl-Teller potential

Starting with the ground state gives

$$\varepsilon_0 = -\lambda^2$$

$$\varepsilon_1 = -(\lambda - 1)^2$$

...

$$\varepsilon_n = -(\lambda - n)^2 \quad n = 0, 1, 2, \dots, n_{\max} = [\lambda]_{\text{unambiguousness}}^{\text{for}}$$

and allows the ladder representation

$$\psi_1(\lambda) \sim \Omega^+(\lambda)\psi_0(\lambda - 1)$$

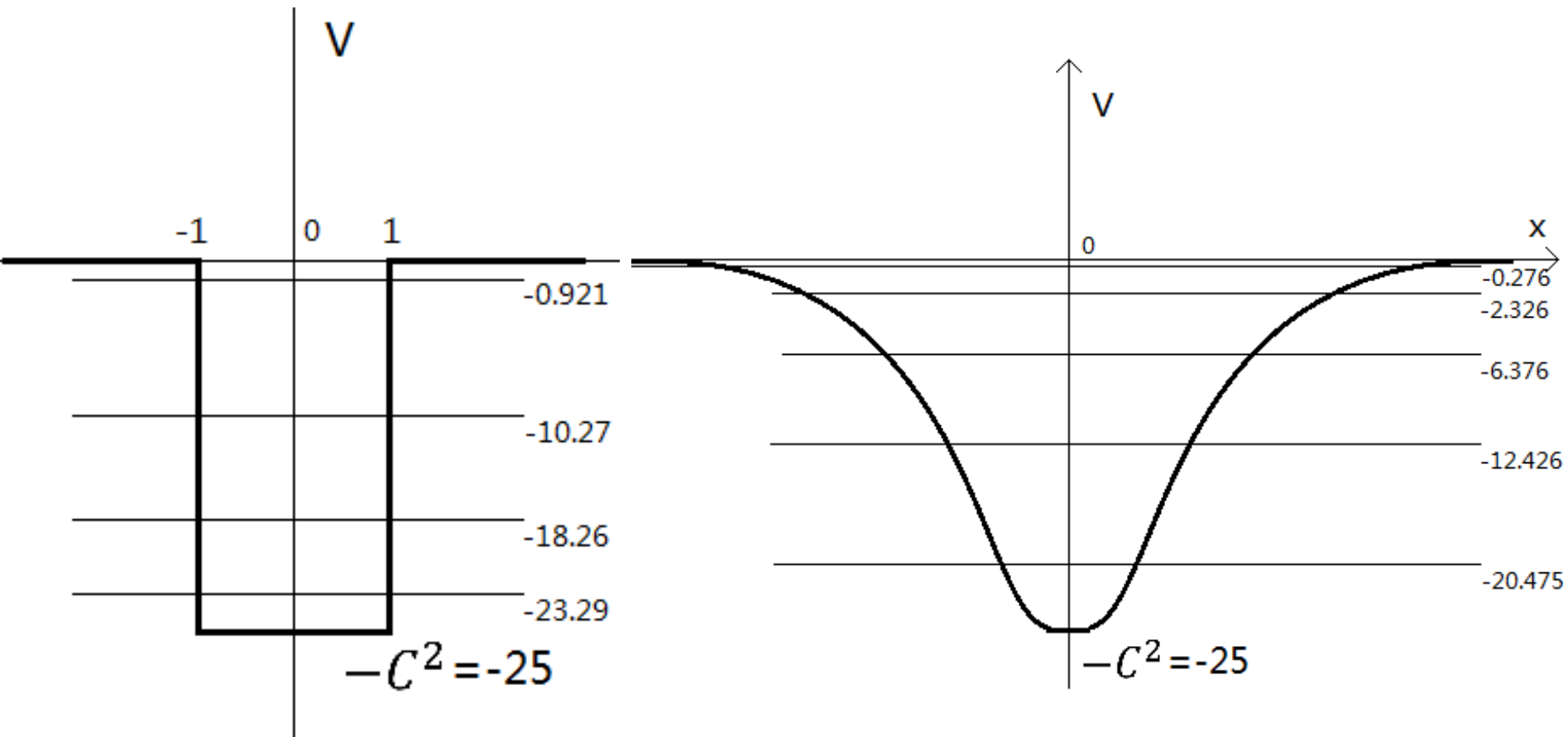
$$\psi_2(\lambda) \sim \Omega^+(\lambda)\psi_1(\lambda - 1) \sim \Omega^+(\lambda)\Omega^+(\lambda - 1)\psi_0(\lambda - 2)$$

...

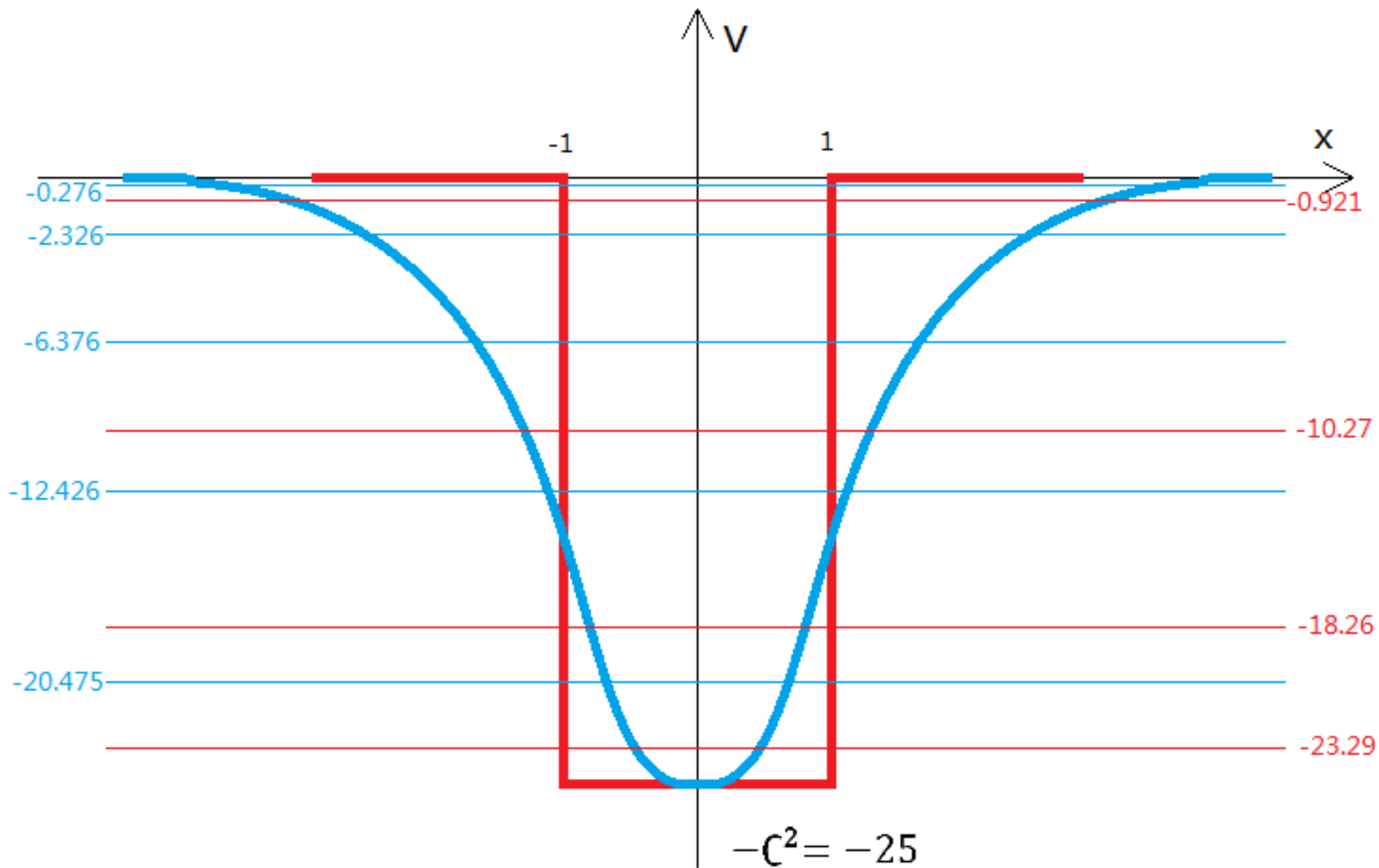
$$\psi_n(\lambda) \sim \underbrace{\Omega^+(\lambda)\tilde{\Omega}^+(\lambda - 1)\dots\tilde{\Omega}^+(\lambda - n + 1)}_{n \text{ factors}}\psi_0(\lambda - n)$$

Comparison of energy eigenvalues and potential shape for the potential well and the Pöschl-Teller potential

(example shown for $C^2 = \lambda(\lambda+1) = 25$ or $\lambda = -\frac{1}{2} + \sqrt{\frac{1}{4} + C^2} = 4.525$)



Synopsis of potential well and Pöschl-Teller potential



Potential well

Pöschl-Teller potential

Factorization

$$H \equiv b_{k_0}^+ b_{k_0} - \kappa_0^2 \quad V = - \frac{C^2}{k_0^2 + \kappa_0^2} \Theta(1 - |x|)$$

$$b_{k_0} = \partial_x + k_0 \tan k_0 x \Theta(1 - |x|) + \kappa_0 \Theta(|x| - 1)$$

$$H = \Omega^+ \Omega - \lambda^2 \quad V = - \frac{\lambda(\lambda+1)}{\cosh^2 x}$$

$$\Omega = \partial_x + \lambda \operatorname{th} x \quad \lambda > 0$$

Area under potential hump

$$A \equiv \int_{-\infty}^{+\infty} (-V(x)) dx = \int_{-1}^{+1} C^2 dx = 2C^2$$

$$A \equiv \int_{-\infty}^{+\infty} (-V(x)) dx = \int_{-\infty}^{+\infty} \frac{\lambda(\lambda+1)}{\cosh^2 x} dx = 2\lambda(\lambda+1)$$

Ground state

$$b_{k_0} \varphi_0 = 0 \Rightarrow$$

$$\varphi_0 = N \cos k_0 x \Theta(1 - |x|)$$

$$+ N \cos k_0 e^{-\sqrt{C^2 - k_0^2} (|x| - 1)} \Theta(|x| - 1)$$

$$\varepsilon_0 = -\kappa_0^2 = -(C^2 - k_0^2) = -C^2 \sin^2 k_0$$

$$\Omega \varphi_0 = 0 \Rightarrow$$

$$\varphi_0 = \frac{N}{\cosh^\lambda x}$$

$$\varepsilon_0 = -\lambda^2$$

Potential well

Pöschl-Teller potential

Conditional equation for ground state eigenvalue

$$\varepsilon_0 = k_0^2 - C^2$$

$$k_0 \tan k_0 = \sqrt{C^2 - k_0^2} \quad \text{or} \quad \cos k_0 = \frac{k_0}{C}$$

Bound states eigenvalues

$$k_v = v \frac{\pi}{2} + \text{Arctan} \frac{\sqrt{C^2 - k_v^2}}{k_v} \quad \text{or} \quad \frac{k_v}{C} = \cos(k_v - v \frac{\pi}{2})$$

$$\varepsilon_v = k_v^2 - C^2 = -C^2 \sin^2(k_v - v \frac{\pi}{2}) \quad v = 0, 1, \dots, \left[\frac{|C|}{(\pi/2)} \right] \quad \varepsilon_v = -(\lambda - v)^2 \quad v = 0, 1, 2, \dots, [\lambda]$$

Scattering states eigenfunctions and eigenvalues

$$\psi = \begin{cases} e^{ikx} + R e^{-ikx} & x < -1 \\ T e^{ikx} & x > +1 \end{cases}$$

$$|T|^2 = 1 - |R|^2 = \frac{1}{1 + \frac{C^4 \sin^2 2\sqrt{C^2 + k^2}}{4k^2 (C^2 + k^2)}} \quad \varepsilon_k = k^2$$

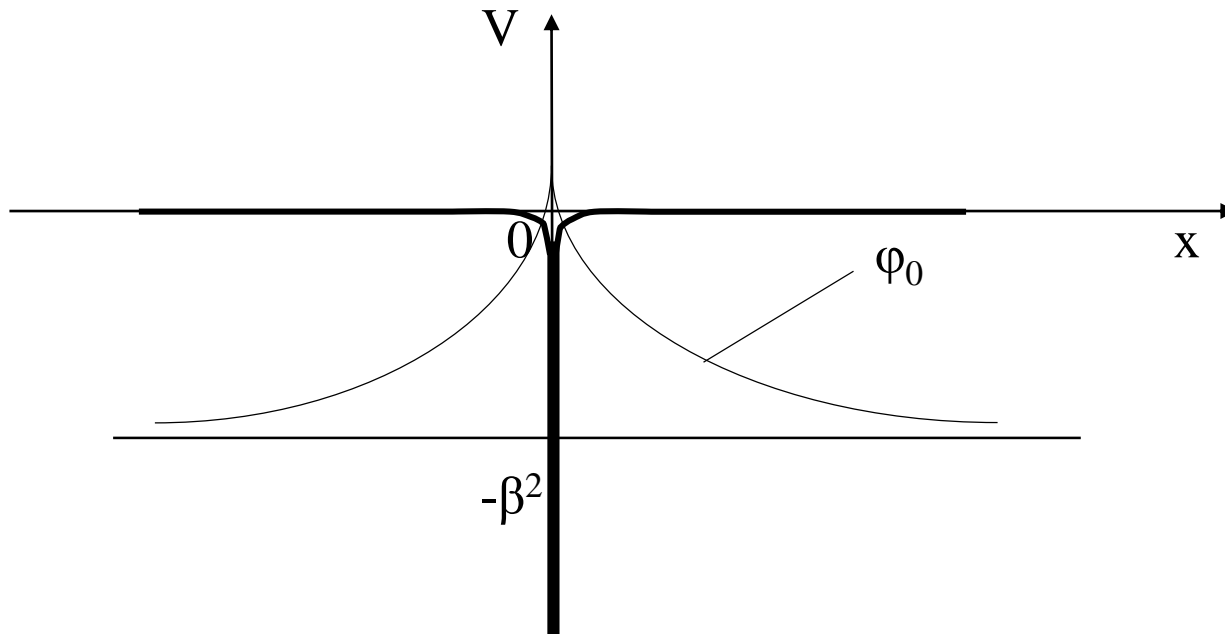
$$\psi = \begin{cases} e^{ikx} + \cos \alpha_k e^{-ikx - i\alpha_k} & x < 0 \\ i \sin \alpha_k e^{ikx - i\alpha_k} & x > 0 \end{cases} \quad \tan \alpha_k = \frac{k}{\lambda}$$

$$\varepsilon_k = k^2$$

δ -potential

The Schrödinger equation for a particle in a δ -potential reads

$$H\varphi \equiv (-\partial_x^2 - 2\beta\delta(x))\varphi = \varepsilon\varphi \quad \beta > 0$$



with natural boundary condition ($\varphi(x \rightarrow \pm\infty) = 0$) we get

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

scattering states $\varphi_k^s = \frac{1}{\sqrt{\pi}} \sin(k|x| - \alpha_k) \quad \varphi_k^{as} = \frac{1}{\sqrt{\pi}} \sin kx \quad \varepsilon_k = k^2 \quad \tan \alpha_k = k / \beta \quad k > 0$

Factorization

Decomposition

$$\mathbf{b} = \partial_x + \beta \operatorname{sign} x \quad \mathbf{b}^+ = -\partial_x + \beta \operatorname{sign} x$$

$$\begin{aligned} \mathbf{b}^+ \mathbf{b} &= -\partial_x^2 - (\beta \operatorname{sign} x)' + (\beta \operatorname{sign} x)^2 \\ &= \underbrace{-\partial_x^2 - 2\beta \delta(x)}_H + \beta^2 \end{aligned}$$

gives

$$H = \mathbf{b}^+ \mathbf{b} - \beta^2$$

From this it follows

$$\varepsilon \geq -\beta^2$$

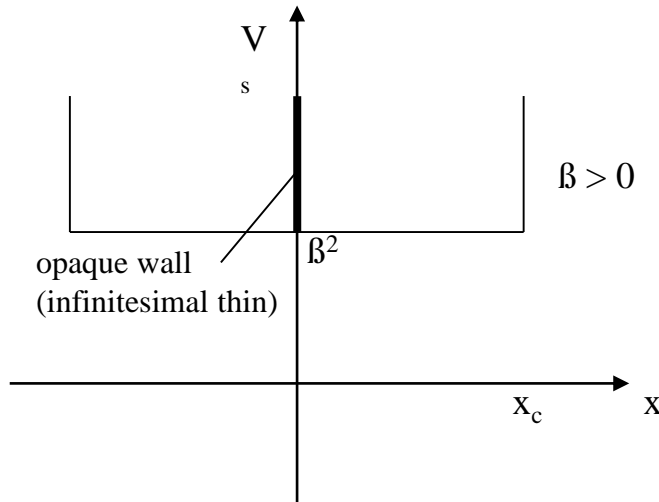
and for the ground state

$$\varepsilon_0 = -\beta^2 \quad \mathbf{b} \varphi_0 = 0 \Rightarrow \varphi_0 = N e^{-\beta|x|}$$

Schrödinger equation for infinite square well with superimposed δ -wall/hole in the middle

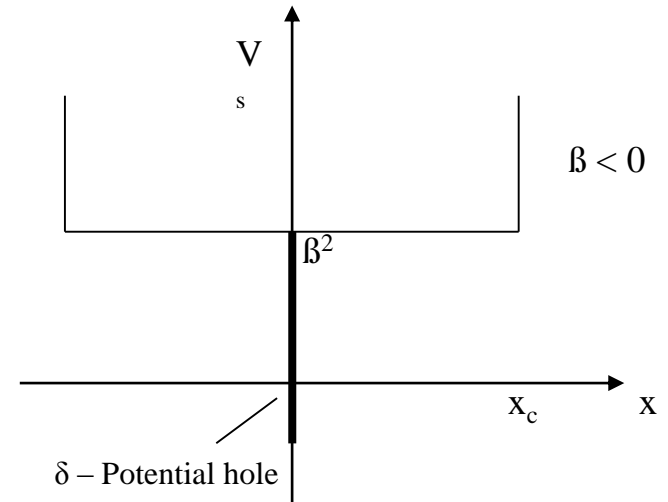
The Schrödinger equation for a infinite square well with a δ -potential in the middle reads

$$H\varphi \equiv (-\partial_x^2 + V_s) \varphi = \varepsilon \varphi \quad V_s = \begin{cases} \beta^2 + 2\beta\delta(x) & \text{for } |x| < x_c \\ \infty & \text{for } |x| \geq x_c \end{cases}$$



$$V_s = \beta^2 + 2\beta\delta(x)$$

$$\varepsilon_v = k_v^2 + \beta^2 \quad v = 0, 1, 2, \dots$$



$$V_s = \beta^2 - 2|\beta|\delta(x)$$

$$\varepsilon_v = \begin{cases} -\kappa_0^2 + \beta^2 & v = 0 & \beta x_c < -1 \\ k_v^2 + \beta^2 & v = 0, 1, 2, 3, \dots & \beta x_c > -1 \end{cases}$$

Eigenfunctions and Eigenvalues

The eigenfunctions, which automatically fulfill the infinite wall boundary conditions, are

ground state

$$\varphi_0 = \begin{cases} N_0 \sin k_0^s (|x| - x_c) & \beta x_c > -1 \\ N_0 \sinh \kappa_0^s (|x| - x_c) & \beta x_c < -1 \end{cases} \quad \varepsilon_0 = \begin{cases} k_0^{s2} + \beta^2 & \beta x_c > -1 \\ -\kappa_0^{s2} + \beta^2 & \beta x_c < -1 \end{cases}$$

excited states

$$\varphi_\nu^s = N_\nu \sin k_\nu^s (|x| - x_c) \quad \varepsilon_\nu = \beta^2 + k_\nu^{s2} \quad \nu = 1, 2, 3, \dots$$

$$\varphi_\nu^{as} = N_\nu \sin k_\nu^{as} x \quad \varepsilon_\nu = \beta^2 + k_\nu^{as2} \quad k_\nu^{as} = \frac{\nu\pi}{x_c} \quad \nu = 1, 2, 3, \dots$$

The remaining boundary condition is the jump condition $-\varphi'(0+) + \varphi'(0-) + 2\beta\varphi(0) = 0$ which has with $\varphi'^{as,s}(0+) = \pm\varphi'^{as,s}(0-)$ the simple form $\varphi'(0+) - \beta\varphi(0) = 0$ and acts only on the symmetric states

ground state

$$\tan k_0^s x_c = -\frac{k_0^s}{\beta} \quad \beta x_c > -1$$

$$\tanh \kappa_0^s x_c = -\frac{\kappa_0^s}{\beta} \quad \beta x_c < -1$$

excited states

$$\tan k_\nu^s x_c = -\frac{k_\nu^s}{\beta} \quad \nu = 1, 2, 3, \dots$$

using the principal value

$$k_\nu^s x_c = \left(\nu + \frac{1}{2}\right)\pi + \arctan(\beta/k_\nu^s)$$

Eigenfunction expansion in the limiting case $x_c \rightarrow \infty$, $\beta < 0$

The limiting case $x_c \rightarrow \infty$, $\beta < 0$ gives for the ground state

$$\varphi_0 = N_0 \sinh \kappa_0 (|x| - x_c) \rightarrow \frac{N_0}{2} e^{-\kappa_0 (|x| - x_c)} = \tilde{N}_0 e^{-|\beta||x|} \quad \varepsilon_0 = -\kappa_0^2 + \beta^2 \rightarrow 0$$

and for the symmetric scattering states

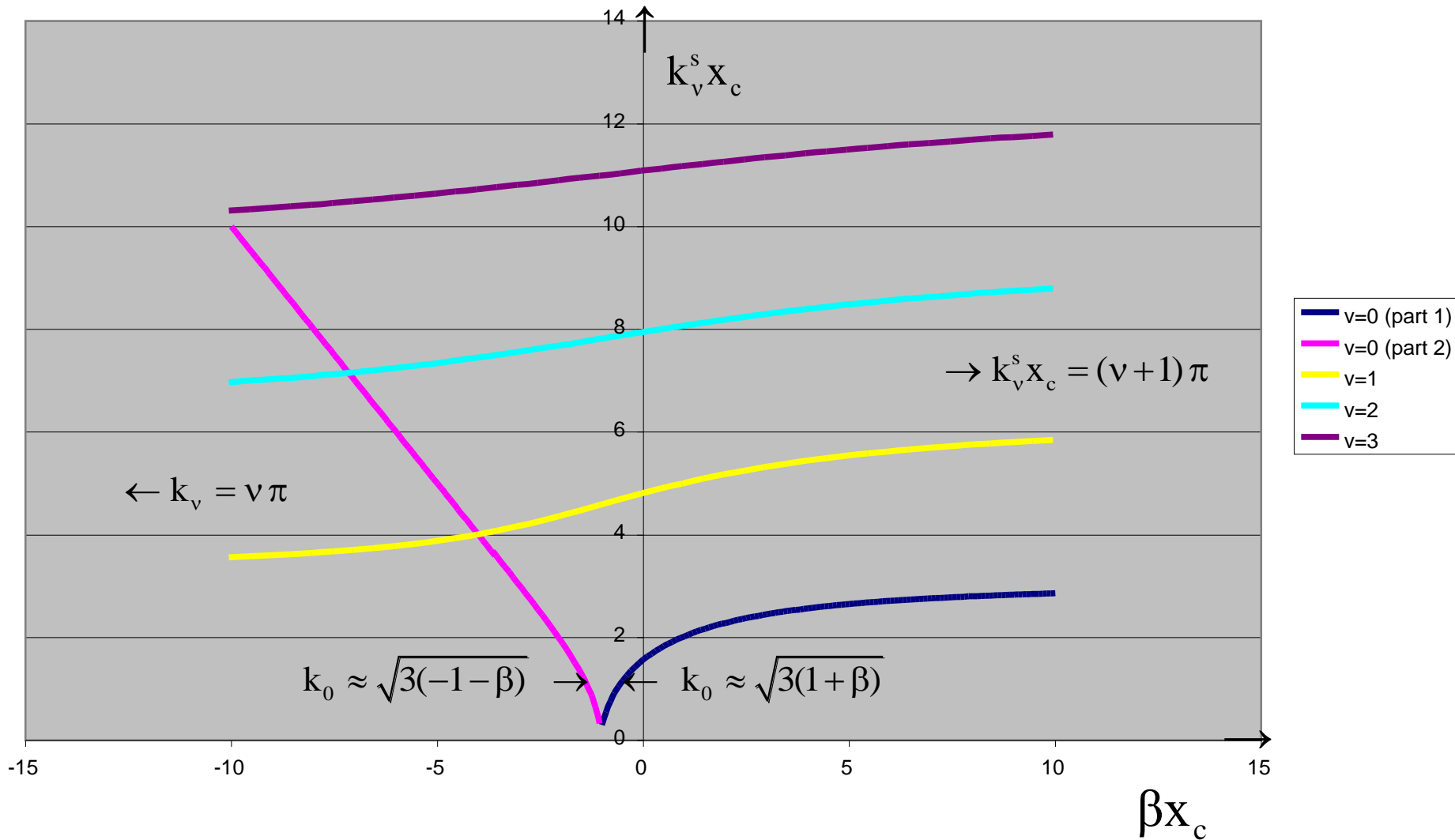
$$\varphi_\nu^s = N_\nu \sin k_\nu^s (|x| - x_c) \quad k_\nu^s x_c = \left(\nu + \frac{1}{2}\right)\pi + \arctan(\beta/k_\nu^s) \rightarrow \nu\pi \quad \nu = 1, 2, 3, \dots$$

$$\varphi_\nu^s \rightarrow N_\nu \cos k_\nu^s x \quad k_\nu^s \rightarrow \frac{\nu\pi}{2x_c} \quad \varepsilon_\nu = \beta^2 + k_\nu^{s2} \quad \nu = 1, 3, 5, \dots$$

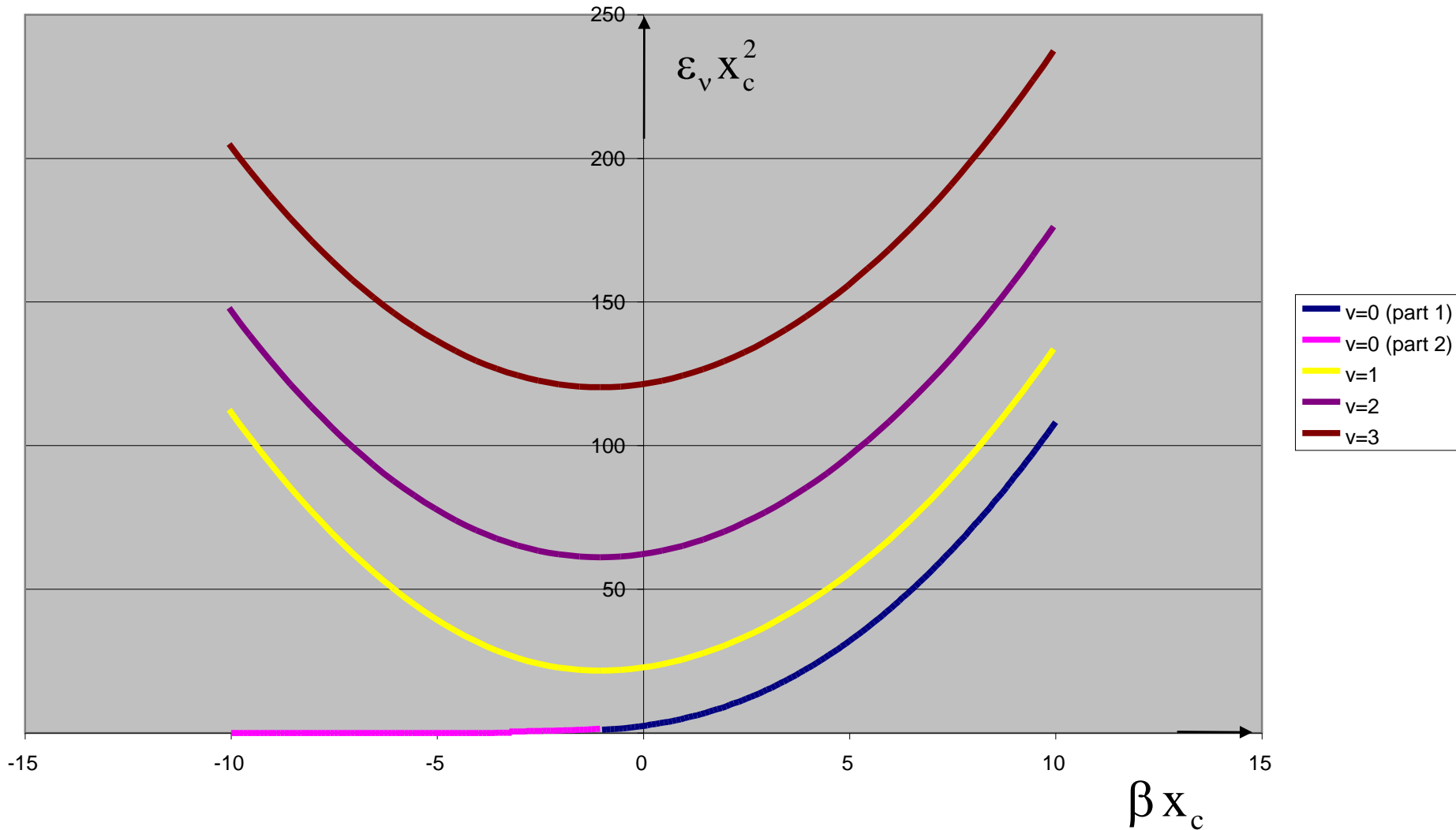
as well as for the antisymmetric scattering states

$$\varphi_\nu^{\text{as}} = N_\nu \sin k_\nu^{\text{as}} x \quad k_\nu^{\text{as}} = \frac{\nu\pi}{2x_c} \quad \varepsilon_\nu = \beta^2 + k_\nu^{\text{as}2} \quad \nu = 2, 4, 6, \dots$$

Wave numbers k_v^s of the symmetric eigenfunctions φ_v^s fulfilling the boundary conditions



eigenvalues of the Schrödinger equation



Factorization of the Schrödinger equation with the infinite square well potential and a superimposed δ -wall/hole in the middle

$$H = -\partial_x^2 + \beta^2 + 2\beta\delta(x) \quad \text{for } |x| < x_c \quad \text{with} \quad \begin{cases} \varphi_v(\pm x_c) = 0 \\ (\partial_x - \beta)\varphi_v(x)|_{x=0+} = 0 \end{cases}$$

$\beta x_c > -1$ gives

$$\varepsilon_0 = k_0^2 + \beta^2 \quad H - \varepsilon_0 = -\partial_x^2 - k_0^2 + 2\beta\delta(x) \equiv b_{k_0}^+ b_{k_0}$$

$$b_{k_0} = \partial_x - k_0 \cot k_0 (|x| - x_c) \text{sign } x$$

similar expansion of $b_{k_0}^+ b_{k_0}$ gives

$$b_{k_0}^+ b_{k_0} = -\partial_x^2 + \left(k_0 \cot k_0 (|x| - x_c) \text{sign } x\right)' + \left(k_0 \cot k_0 (|x| - x_c) \text{sign } x\right)^2$$

The expansion of $b_{k_0}^+ b_{k_0}$ finally gives

$$\begin{aligned} b_{k_0}^+ b_{k_0} &= -\partial_x^2 + k_0^2 \left(-1 - \cot^2 k_0 (|\mathbf{x}| - x_c) \right) \\ &\quad + 2k_0 \cot k_0 (|\mathbf{x}| - x_c) \delta(\mathbf{x}) + k_0^2 \cot^2 k_0 (|\mathbf{x}| - x_c) \\ &= -\partial_x^2 - k_0^2 - 2k_0 \cot k_0 x_c \delta(\mathbf{x}) \end{aligned}$$

comparison with the original gives the conditional equation for the wave number k_0

$$\cot k_0 x_c = -\frac{\beta}{k_0} \quad \text{resp.} \quad \tan k_0 x_c = -\frac{k_0}{\beta}$$

$\beta x_c < -1$ gives

$$\varepsilon_0 = -\kappa_0^2 + \beta^2 \quad \mathbf{H} - \varepsilon_0 = -\partial_x^2 + \kappa_0^2 + 2\beta \delta(x) \equiv \mathbf{b}_{\kappa_0}^+ \mathbf{b}_{\kappa_0}$$

$$\mathbf{b}_{\kappa_0} = \partial_x - \kappa_0 \coth \kappa_0 (|x| - x_c) \operatorname{sign} x$$

Expansion of $\mathbf{b}_{\kappa_0}^+ \mathbf{b}_{\kappa_0}$ gives

$$\begin{aligned} \mathbf{b}_{\kappa_0}^+ \mathbf{b}_{\kappa_0} &= -\partial_x^2 + \left(\kappa_0 \coth \kappa_0 (|x| - x_c) \operatorname{sign} x \right)' + \left(\kappa_0 \coth \kappa_0 (x - x_c) \operatorname{sign} x \right)^2 \\ &= -\partial_x^2 + \kappa_0^2 \left(1 - \coth^2 \kappa_0 (|x| - x_c) \right) \\ &\quad + 2\kappa_0 \coth \kappa_0 (|x| - x_c) \delta(x) + \kappa_0^2 \coth^2 \kappa_0 (|x| - x_c) \\ &= -\partial_x^2 + \kappa_0^2 - 2\kappa_0 \coth \kappa_0 x_c \delta(x) \end{aligned}$$

this is in accordance with the original for

$$\coth \kappa_0 x_c = -\frac{\beta}{\kappa_0}$$

which again is the condition for the wave number κ_0 to fulfill the boundary conditions

Summary of the Factorization procedure for the Schrödinger equation

The factorization procedure of the elementary Schrödinger equation application examples can be summarized as follows

We start with the decomposition

$$(\mathbf{H} - \varepsilon_v) \varphi_v \equiv (-\partial_x^2 + V_S - \varepsilon_v) \varphi_v = (\Omega^+ \Omega - (\varepsilon_v - \varepsilon_0)) \varphi_v = 0 \quad \Omega = \partial_x + W$$

The selfadjoint form gives the inequality

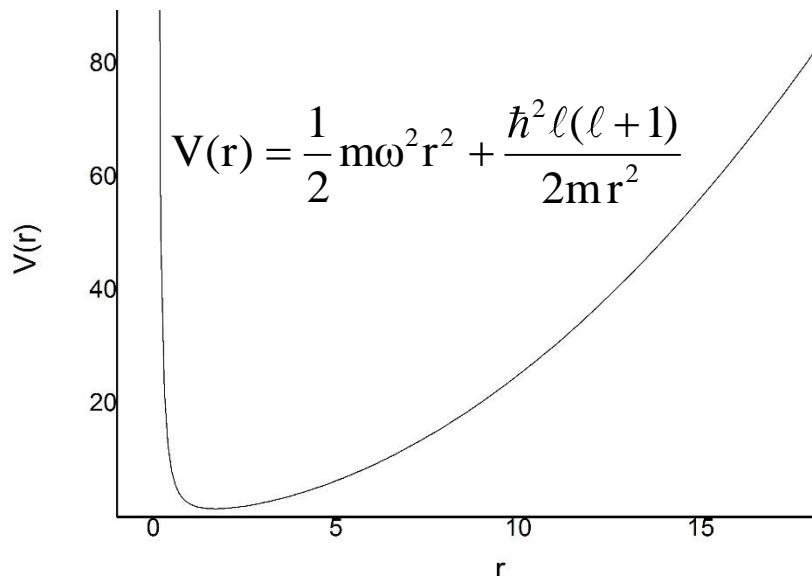
$$\varepsilon_v > \varepsilon_0 \quad \text{with} \quad \Omega \varphi_0 = 0 \Rightarrow W = -\frac{\varphi_0'}{\varphi_0} \quad \text{or} \quad -W' + W^2 = V_S - \varepsilon_0$$

where φ_0 is the ground state and ε_0 is the corresponding ground state energy.

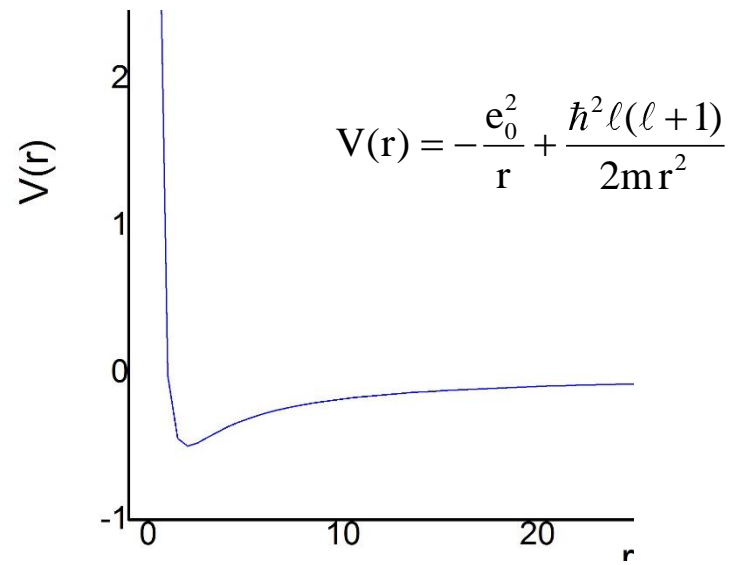
The results of the factorization for the elementary examples are put together in the adjacent table.

elementary example	ground state	factorization	eigenvalues bound states
<p>square well potential</p> $V = \begin{cases} 0 & x < 1 \\ +\infty & \text{else} \end{cases}$	$\psi_0 = \begin{cases} N_0 \cos k_0 x & x \leq 1 \\ 0 & \text{else} \end{cases}$	$H = b^+ b$ $b = \partial_x + \frac{\pi}{2} \tan \frac{\pi}{2} x$	$\epsilon_v = (1 + v)^2 \left(\frac{\pi}{2}\right)^2$
<p>rectangular potential hole</p> $V = \begin{cases} -C^2 & x < 1 \\ 0 & x > 1 \end{cases}$	$\varphi_0 = N_0 \begin{cases} \cos k_0 x \\ \cos k_0 e^{-\kappa_0(x -1)} \end{cases}$ $\kappa_0 = \sqrt{C^2 - k_0^2}$	$H = b_{k_0}^+ b_{k_0} + \epsilon_0$ $b_{k_0} = \partial_x + \begin{cases} \sqrt{C^2 - k_0^2} & x > 1 \\ k_0 \tan k_0 x & x < 1 \end{cases}$ $k_0 \tan k_0 = \sqrt{C^2 - k_0^2}$	$\epsilon_v = k_v^2 - C^2$ $k_v = v \frac{\pi}{2}$ $+ \text{Arctan} \frac{\sqrt{C^2 - k_v^2}}{k_v}$

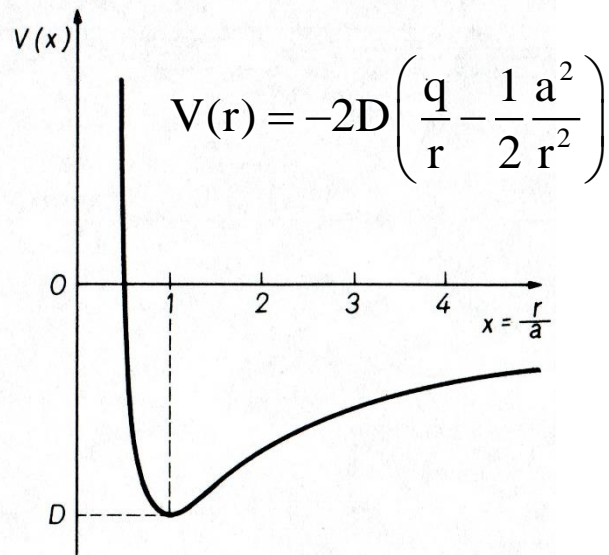
elementary example	ground state	factorization	eigenvalues bound states
δ -potential $V = -2\beta\delta(x)$	$\varphi_0 = Ne^{-\beta x }$	$H = b^+ b + \varepsilon_0$ $b = \partial_x + \beta \text{sign } x$	$\varepsilon_0 = -\beta^2$
square well with δ -wall/hole $V = \begin{cases} \beta^2 + 2\beta\delta(x) & x < 1 \\ +\infty & x > 1 \end{cases}$	$\beta x_c > -1$ $\varphi_0 = N_0 \sin k_0^s (x - x_c)$ $\beta x_c < -1$ $\varphi_0 = N_0 \sinh \kappa_0^s (x - x_c)$	$H \equiv b_{k_0}^+ b_{k_0} + \varepsilon_0$ $b_{k_0} = \partial_x - k_0 \cot k_0 (x - 1) \text{sign } x$	$\varepsilon_0 = \begin{cases} -\kappa_0^2 + \beta^2 & \beta x_c > -1 \\ k_0^2 + \beta^2 & \beta x_c < -1 \end{cases}$ $\varepsilon_\nu = k_\nu^2 + \beta^2$ $k_\nu = (\nu + \frac{1}{2})\pi + \text{Arctan} \frac{\beta}{k_\nu} \quad \nu = 1, 2, \dots$



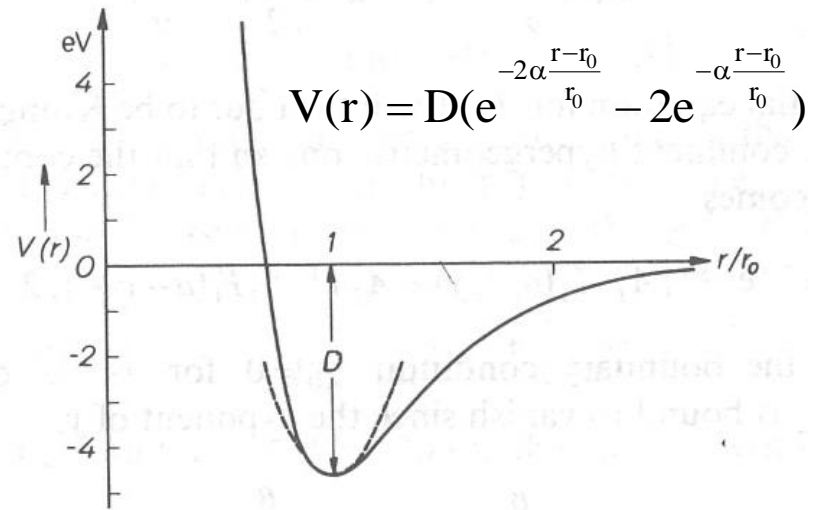
3D harm. oscillator



Coulomb potential



Kratzer potential



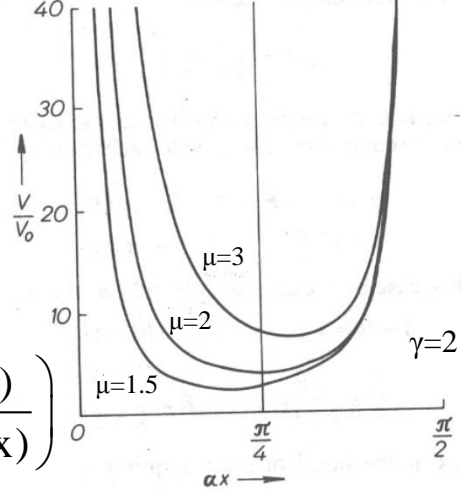
Morse potential

Summary of further exactly solvable potentials (I)

name	formula	factorization	eigenvalues
3D harm. oscillator	$V(r) = \frac{1}{4}r^2 + \frac{\ell(\ell+1)}{r^2}$	$H(\ell) = b^+(\ell)b(\ell) + \ell + \frac{3}{2}$ $b(\ell) = \partial_r + \frac{1}{2}r - \frac{\ell+1}{r}$	$\varepsilon_n(\ell) = 2n + \ell + \frac{3}{2}$
Coulomb potential	$V(r) = -\frac{2}{r} + \frac{\ell(\ell+1)}{r^2}$	$H(\ell) = b^+(\ell)b(\ell) - \frac{1}{(\ell+1)^2}$ $b(\ell) = \partial_r - \frac{\ell+1}{r} + \frac{1}{\ell+1}$	$\varepsilon_n(\ell) = -\frac{1}{(n+\ell+1)^2}$
Kratzer potential	$V(x) = \frac{-2\gamma}{x} + \frac{\lambda(\lambda-1)}{x^2}$	$H(\lambda) = b^+(\lambda)b(\lambda) - \frac{\gamma^2}{\lambda^2}$ $b(\lambda) = \partial_x - \frac{\lambda}{x} + \frac{\gamma}{\lambda}$	$\varepsilon_v(\lambda) = -\frac{\gamma^2}{(v+\lambda)^2}$
Morse potential	$V(x) = e^{-2x} - 2\gamma e^{-x}$	$H(\gamma) = b^+(\gamma)b(\gamma) - (\gamma - \frac{1}{2})^2$ $b(\gamma) = \partial_x - e^{-x} + \gamma - \frac{1}{2}$	$\varepsilon_v(\gamma) = -(\gamma - \frac{1}{2} - v)^2$

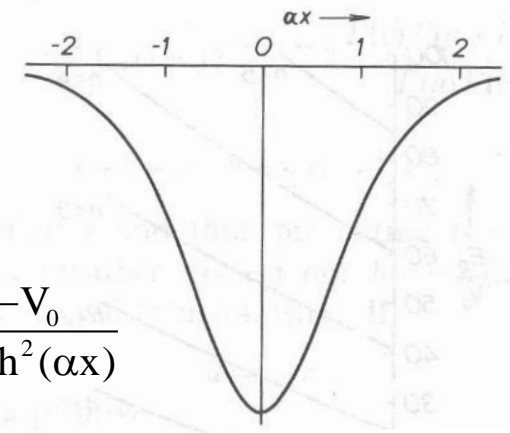
$$V(x) =$$

$$\frac{V_0}{2} \left(\frac{\mu(\mu-1)}{\sin^2(\alpha x)} + \frac{\gamma(\gamma-1)}{\cos^2(\alpha x)} \right)$$



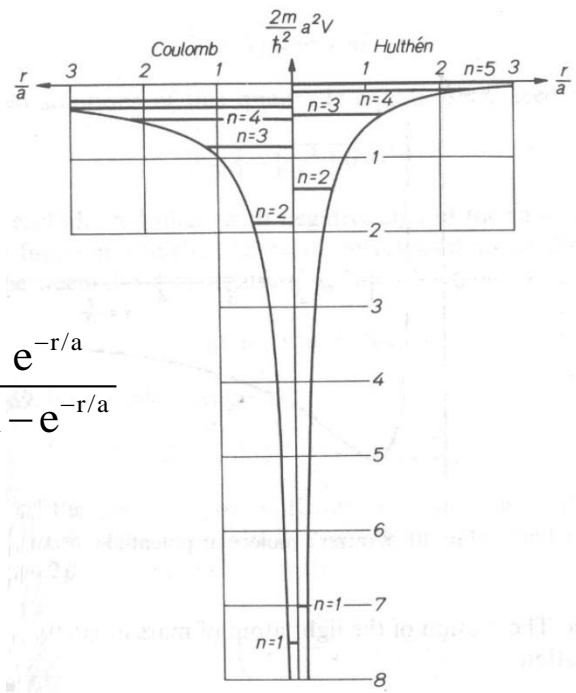
trigon. Pöschl Teller potential

$$V(x) = \frac{-V_0}{\cosh^2(\alpha x)}$$

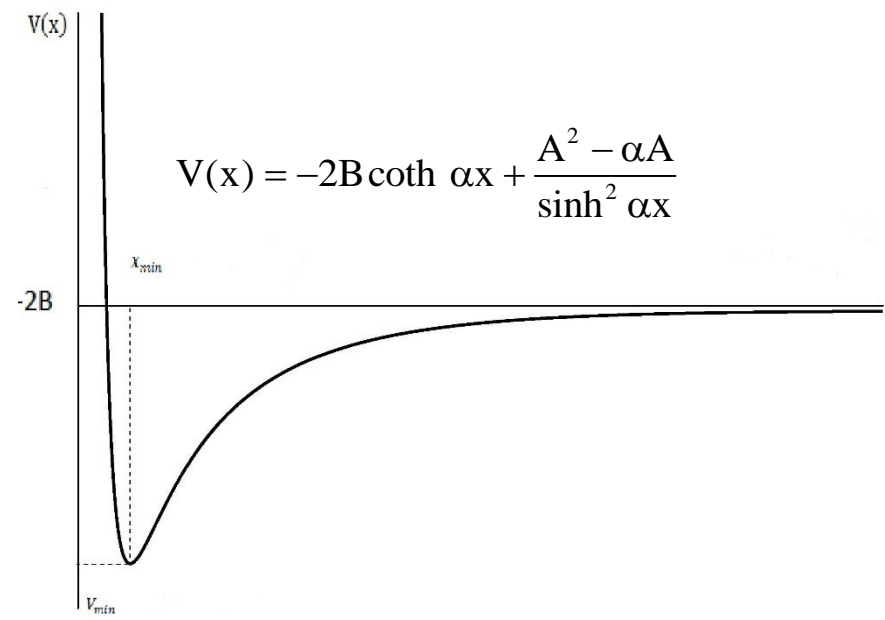


hyperbolic (modified) Pöschl Teller potential

$$V(r) = -V_0 \frac{e^{-r/a}}{1 - e^{-r/a}}$$



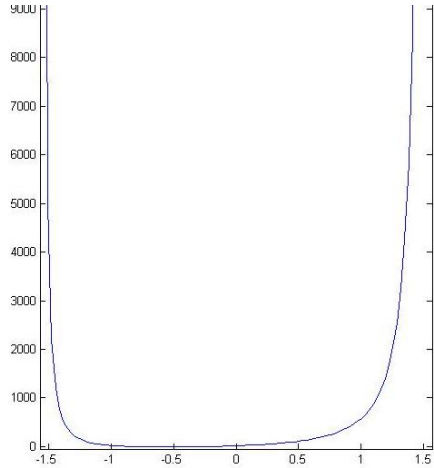
Hulthén potential



Eckart potential

Summary of further exactly solvable potentials (II)

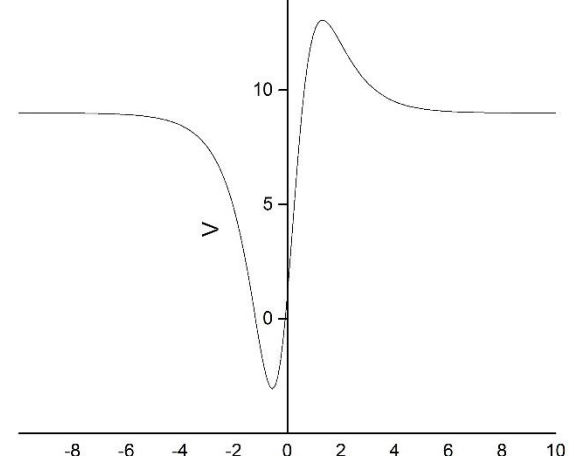
name	formula	factorization	eigenvalues
trig. Pöschl-Teller potential	$V(x) = \frac{\mu(\mu-1)}{\sin^2 x} + \frac{\gamma(\gamma-1)}{\cos^2 x}$	$H(\mu, \gamma) = B_{\mu, \gamma}^+ B_{\mu, \gamma} + (\mu + \gamma)^2$ $B_{\mu, \gamma} = \partial_x - \mu \cot x + \gamma \tan x$	$\varepsilon_\nu(\mu, \gamma) = (\mu + \gamma + 2\nu)^2$
hyperb. Pöschl-Teller potential	$V(x) = -\frac{\lambda(\lambda+1)}{\cosh^2 x}$	$H(\lambda) = \tilde{\Omega}^+(\lambda) \tilde{\Omega}(\lambda) - (\lambda-1)^2$ $\tilde{\Omega}(\lambda) = \partial_x + (\lambda-1) \operatorname{th} x$	$\varepsilon_n = -(\lambda - 1 - n)^2$
Hulthén potential	$V(x) = -\beta^2 \frac{1}{e^x - 1}$	$H = b^+ b - \left(\frac{\beta^2 - 1}{2}\right)^2$ $b = \partial_x - \frac{1}{2} \operatorname{coth} \frac{x}{2} + \frac{\beta^2}{2}$	$\varepsilon_n = -\left(\frac{\beta^2}{2(n+1)} - \frac{n+1}{2}\right)^2$
Eckart potential	$V(x) = -2B \operatorname{coth} x + \frac{A(A-1)}{\sinh^2 x}$	$H(A) = \Omega_A^+ \Omega_A - A^2 - \frac{B^2}{A^2}$ $\Omega_A = \partial_x - A \operatorname{coth} x + \frac{B}{A}$	$\varepsilon_n = -(A+n)^2 - \frac{B^2}{(A+n)^2}$



$V(x) =$

$$-A^2 + \frac{B^2 + A^2 - \alpha A}{\cos^2 \alpha x} + B(2A - \alpha) \frac{\tan \alpha x}{\cos \alpha x}$$

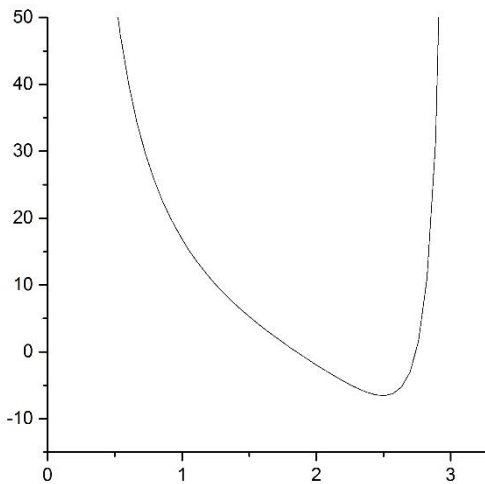
Scarf I potential



$V(x) =$

$$A^2 + \frac{B^2 - A^2 - \alpha A}{\cosh^2 \alpha x} + B(2A + \alpha) \frac{\tanh \alpha x}{\cosh \alpha x}$$

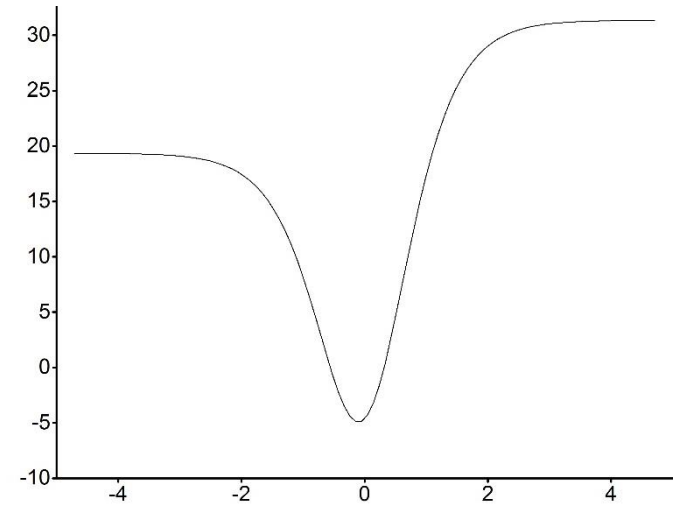
Scarf II potential



$V(x) =$

$$-A^2 + \frac{B^2}{A^2} + \frac{A(A-1)}{\sin^2 \alpha x} + 2B \cot \alpha x$$

trig. Rosen-Morse potential



$V(x) =$

$$A^2 + \frac{B^2}{A^2} - \frac{A(A+1)}{\cosh^2 \alpha x} + 2B \tanh \alpha x$$

hyperbolic Rosen-Morse potential

Summary of further exactly solvable potentials (III)

name	formula	factorization	eigenvalues
trig. Scarf potential	$V = -A^2 + \frac{B^2 + A^2 - A}{\cos^2 x} + B(2A - 1) \frac{\tan x}{\cos x}$	$H(A) = b_A^+ b_A$ $b_A = \partial_x + A \tan x + \frac{B}{\cos x}$	$\varepsilon_v(A) = (A + v)^2 - A^2$
hyp. Scarf potential	$V = A^2 + \frac{B^2 - A^2 - A}{\cosh^2 x} + B(2A + 1) \frac{\tanh x}{\cosh x}$	$H(A) = \tilde{b}_A^+ \tilde{b}_A$ $\tilde{b}_A = \partial_x + A \tanh x + \frac{B}{\cosh x}$	$\varepsilon_v(A) = -(A - v)^2 + A^2$
trig. Rosen- Morse potential	$V = -A^2 + \frac{B^2}{A^2} + \frac{A^2 - A}{\sin^2 x} + 2B \cot x$	$H(A) = b_A^+ b_A$ $b_A = \partial_x - A \cot x - \frac{B}{A}$	$\varepsilon_v(A) = (A + v)^2 - A^2 - B^2 \left(\frac{1}{(A + v)^2} - \frac{1}{A^2} \right)$
hyp. Rosen- Morse potential	$V = A^2 + \frac{B^2}{A^2} - \frac{A^2 + A}{\cosh^2 x} + 2B \tanh x$	$H = \tilde{b}_A^+ \tilde{b}_A$ $\tilde{b}_A = \partial_x + A \tanh x + \frac{B}{A}$	$\varepsilon_v(A) = A^2 - (A - v)^2 + B^2 \left(\frac{1}{A^2} - \frac{1}{(A - v)^2} \right)$

Generalization for the group of all shape invariant potentials

Generally all Schrödinger equations with shape invariant potentials can be solved algebraically and are characterized by the property

$$V_-(x, a_2) = V_+(x, a_1) + \Theta$$

where a_1 and a_2 are 2 parameters, Θ is a constant eventually depending on a_1 and/or a_2 , and V_{\pm} are amenable to the Riccati equation

$$V_{\pm}(x, a) = W^2(x, a) \pm \frac{\partial W(x, a)}{\partial x}$$

The Hamiltonian of the considered Schrödinger equation reads

$$H(a) = -\partial_x^2 + V_-(x, a)$$

$$= (-\partial_x + W(x, a))(\partial_x + W(x, a)) = B^+(a)B(a)$$

The substitution $a_1 \rightarrow a_2$ in the original Hamiltonian gives

$$\begin{aligned} H(a_2) &= -\partial_x^2 + V_-(x, a_2) = B^+(a_2)B(a_2) \\ &= -\partial_x^2 + W^2(x, a_2) - \frac{\partial W(x, a_2)}{\partial x} \end{aligned}$$

Inserting the property of shape invariant potentials yields

$$\begin{aligned} H(a_2) &= -\partial_x^2 + W^2(x, a_1) + \frac{\partial W(x, a_1)}{\partial x} + \Theta \\ &= B(a_1)B^+(a_1) + \Theta \end{aligned}$$

Multiplying the starting Schrödinger equation $H(a_2)\psi = \varepsilon_v(a_2)\psi$ from left with $B^+(a_1)$ gives

$$\begin{aligned} &B^+(a_1)H(a_2)\psi_v(a_2) \\ &= B^+(a_1)\underbrace{B^+(a_2)B(a_2)}_{B(a_1)B^+(a_1)+\Theta}\psi_v(a_2) = B^+(a_1)\varepsilon_v(a_2)\psi_v(a_2) \end{aligned}$$

Thus inserting of the property of the shape invariant potentials yields

$$\begin{aligned}
 & \mathbf{B}^+(\mathbf{a}_1)\mathbf{H}(\mathbf{a}_2)\psi_v(\mathbf{a}_2) \\
 &= \left(\mathbf{B}^+(\mathbf{a}_1)\mathbf{B}(\mathbf{a}_1) + \Theta \right) \underbrace{\mathbf{B}^+(\mathbf{a}_1)\psi_v(\mathbf{a}_2)}_{\sim \psi_{v+1}(\mathbf{a}_1)} = \varepsilon_v(\mathbf{a}_2) \underbrace{\mathbf{B}^+(\mathbf{a}_1)\psi_v(\mathbf{a}_2)}_{\sim \psi_{v+1}(\mathbf{a}_1)}
 \end{aligned}$$

which can be summarized as

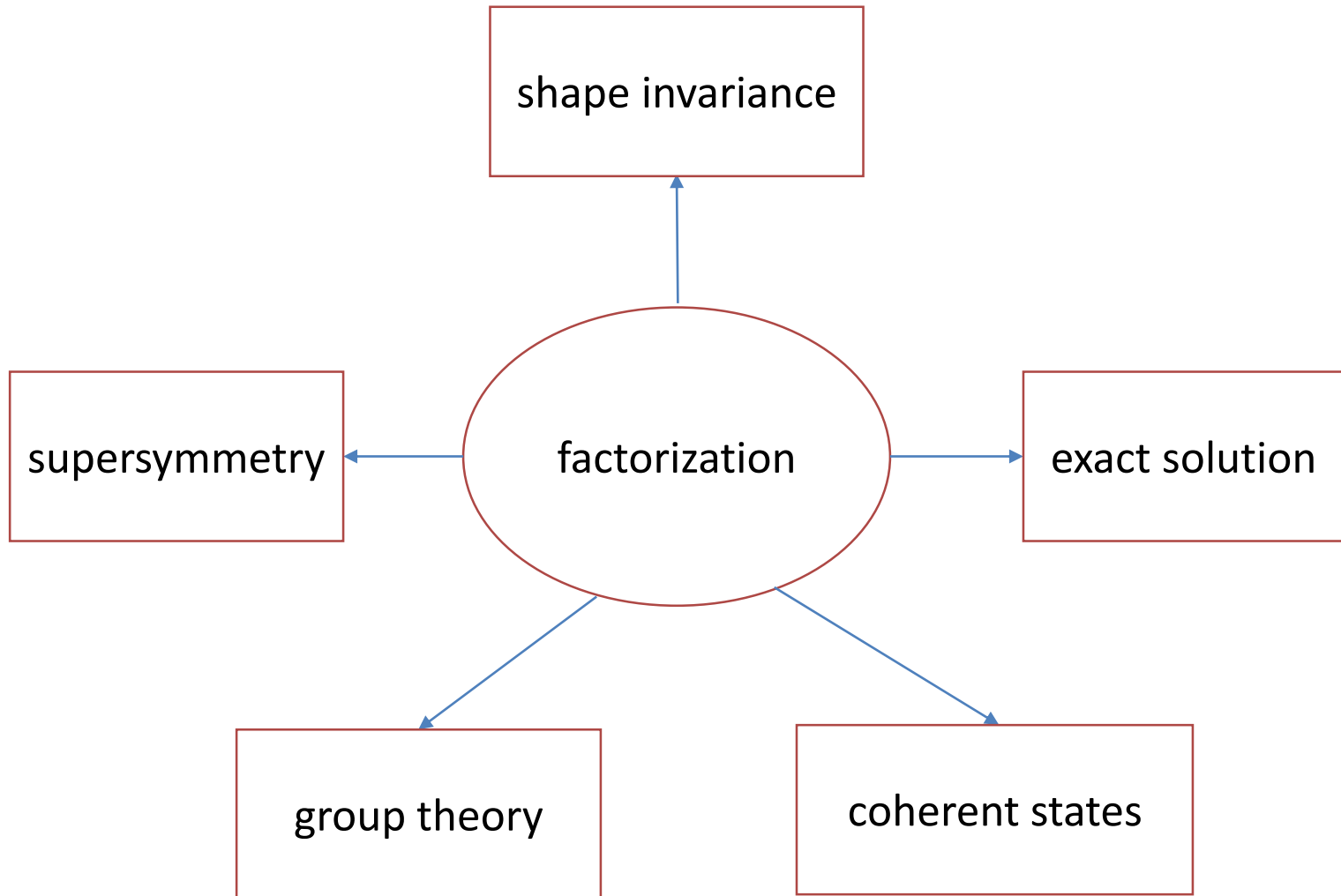
$$\varepsilon_{v+1}(\mathbf{a}_1) + \Theta = \varepsilon_v(\mathbf{a}_2) \quad \psi_{v+1}(\mathbf{a}_1) \sim \mathbf{B}^+(\mathbf{a}_1)\psi_v(\mathbf{a}_2)$$

allowing the inaugurated ladder array in case of discrete eigenstates

Relations among shape invariant potentials

- algebraic approach
- mapping by canonical transformation
- Lie algebraic methods

Factorization of the Schrödinger equation as central module for exact solutions, supersymmetry, shape invariance, group theory, and coherent states in quantum mechanics



The relation to generate the energy eigenvalues of the Schrödinger equation for supersymmetric, shape invariant potentials can be summarized as a Lie algebra approach

The Lie algebra uses a calculus, which starts with the commutation relation

$$[L_i, L_j] = \varepsilon_{ijk} L_k \quad \varepsilon_{ijk} = \text{Levi - symbol} = \begin{cases} i, j, k \in 1, 2, 3 \\ +1 \text{ for } i, j, k \text{ even permutation of } 1, 2, 3 \\ -1 \text{ for } i, j, k \text{ odd permutation of } 1, 2, 3 \\ 0 \text{ for any 2 of } i, j \text{ or } k \text{ are equal} \end{cases}$$

A Lie algebra is a vector space \mathfrak{g} over a field K together with an inner operation $[\cdot, \cdot]: \mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$, $(x, y) \mapsto [x, y]$. The inner operation is called *Lie-bracket* and is subject to the following conditions:

- The inner operation is bilinear, that means it is linear in both arguments.
 $[ax+by, z] = a[x, z] + b[y, z]$ and $[z, ax+by] = a[z, x] + b[z, y]$ valid for all $a, b \in K$ and all $x, y, z \in \mathfrak{g}$.
- The inner operation fulfills the Jacobi identity. The Jacobi identity reads:
 $[x, [y, z]] + [y, [z, x]] + [z, [x, y]] = 0$ valid for all $x, y, z \in \mathfrak{g}$.
- $[x, x] = 0$ is valid for all $x \in \mathfrak{g}$.

The Schrödinger equation with the hyperbolic Scarf potential (generalized Huthén potential) as an example for algebraic approach defining creation and annihilation operators*)

$$V = A^2 + \frac{B^2 - A^2 - A}{\cosh^2 x} + B(2A+1) \frac{\tanh x}{\cosh x} \quad H(A) = \tilde{b}_A^+ \tilde{b}_A \quad \tilde{b}_A = \partial_x + A \tanh x + \frac{B}{\cosh x}$$

$$H(A)\psi_{n+1}(A) = \varepsilon_{n+1}(A)\psi_{n+1}(A) \quad \varepsilon_n(A+1) = \varepsilon_{n+1}(A) \quad \varepsilon_n = A^2 - (A-n)^2$$

$$\psi_{n+1}(A) \sim \tilde{b}_A^+ \psi_n(A-1) = \tilde{b}_A^+ e^{-\partial_A} \psi_n(A) \equiv \hat{L}_+ \psi_n(A) \quad \text{resp.} \quad \hat{L}_- = e^{\partial_A} \tilde{b}_A = \tilde{b}_{A+1} e^{\partial_A}$$

The definition of L_- and L_+ leads to the commutation relation

$$[\hat{L}_-, \hat{L}_+] = \hat{L}_- \hat{L}_+ - \hat{L}_+ \hat{L}_- = e^{\partial_A} \tilde{b}_A \tilde{b}_A^+ e^{-\partial_A} - \tilde{b}_A^+ e^{-\partial_A} e^{\partial_A} \tilde{b}_A = \tilde{b}_{A+1} \tilde{b}_{A+1}^+ - \tilde{b}_A^+ \tilde{b}_A$$

whereas $\tilde{b}_{A+1} \tilde{b}_{A+1}^+ = \tilde{b}_A^+ \tilde{b}_A + (2A+1)$ gives $[\hat{L}_-, \hat{L}_+] = 2A + 1 \equiv 2\hat{L}_0$

*) Balantekin, A. B., Algebraic approach to shape invariance, Phys. Rev. A57 (1998) pp.4981 91

The further commutation relations read

$$\begin{aligned}
\left[\hat{L}_0, \hat{L}_+ \right] &= \hat{L}_0 \hat{L}_+ - \hat{L}_+ \hat{L}_0 = \left(A + \frac{1}{2} \right) \tilde{b}_A^+ e^{-\partial_A} - \tilde{b}_A^+ e^{-\partial_A} \left(A + \frac{1}{2} \right) \\
&= \left(A + \frac{1}{2} \right) \tilde{b}_A^+ e^{-\partial_A} - \tilde{b}_A^+ \left(A - \frac{1}{2} \right) e^{-\partial_A} = \left(A + \frac{1}{2} \right) \tilde{b}_A^+ e^{-\partial_A} - \left(A - \frac{1}{2} \right) \tilde{b}_A^+ e^{-\partial_A} = \tilde{b}_A^+ e^{-\partial_A} = \hat{L}_+ \\
\left[\hat{L}_0, \hat{L}_- \right] &= \hat{L}_0 \hat{L}_- - \hat{L}_- \hat{L}_0 = \left(A + \frac{1}{2} \right) e^{\partial_A} \tilde{b}_A - e^{\partial_A} \tilde{b}_A \left(A + \frac{1}{2} \right) \\
&= \left(A + \frac{1}{2} \right) e^{\partial_A} \tilde{b}_A - e^{\partial_A} \left(A + \frac{1}{2} \right) \tilde{b}_A = \left(A + \frac{1}{2} \right) e^{\partial_A} \tilde{b}_A - \left(A + \frac{3}{2} \right) e^{\partial_A} \tilde{b}_A = - e^{\partial_A} \tilde{b}_A = -\hat{L}_-
\end{aligned}$$

and can be summarized as the Lie brackets

$$\left[\hat{L}_-, \hat{L}_+ \right] = 2\hat{L}_0 \quad , \quad \left[\hat{L}_0, \hat{L}_+ \right] = \hat{L}_+ \quad , \quad \left[\hat{L}_0, \hat{L}_- \right] = -\hat{L}_-$$

which are connected to the ladder operators

$$\hat{L}_+ \psi_n(\mathbf{y}) = \ell_+ \psi_{n+1}(\mathbf{y}) \quad \hat{L}_- \psi_n(\mathbf{y}) = \ell_- \psi_{n-1}(\mathbf{y}) \quad \hat{L}_0 = A + \frac{1}{2}$$

Application Examples

A Disaster description

- Brownian motion and Schrödinger equation
- Stochastic description of waterlevel undulations
- First passage time distribution

B Traffic breakdown propagation

- Korteweg-de Vries equation, Lax pairs and Schrödinger equation
- Conservation law in traffic modeling
- Korteweg-de Vries equation for wide moving jams

Brownian motion and Schrödinger equation

Langevin equation as starting point

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

with δ – correlated fluctuations

$$\langle \Gamma \rangle = 0 \quad \langle \Gamma(t)\Gamma(t') \rangle = 2D\delta(t - t')$$

and

$$F = -\partial_x \Phi \quad (\text{force derived from potential})$$

summary

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

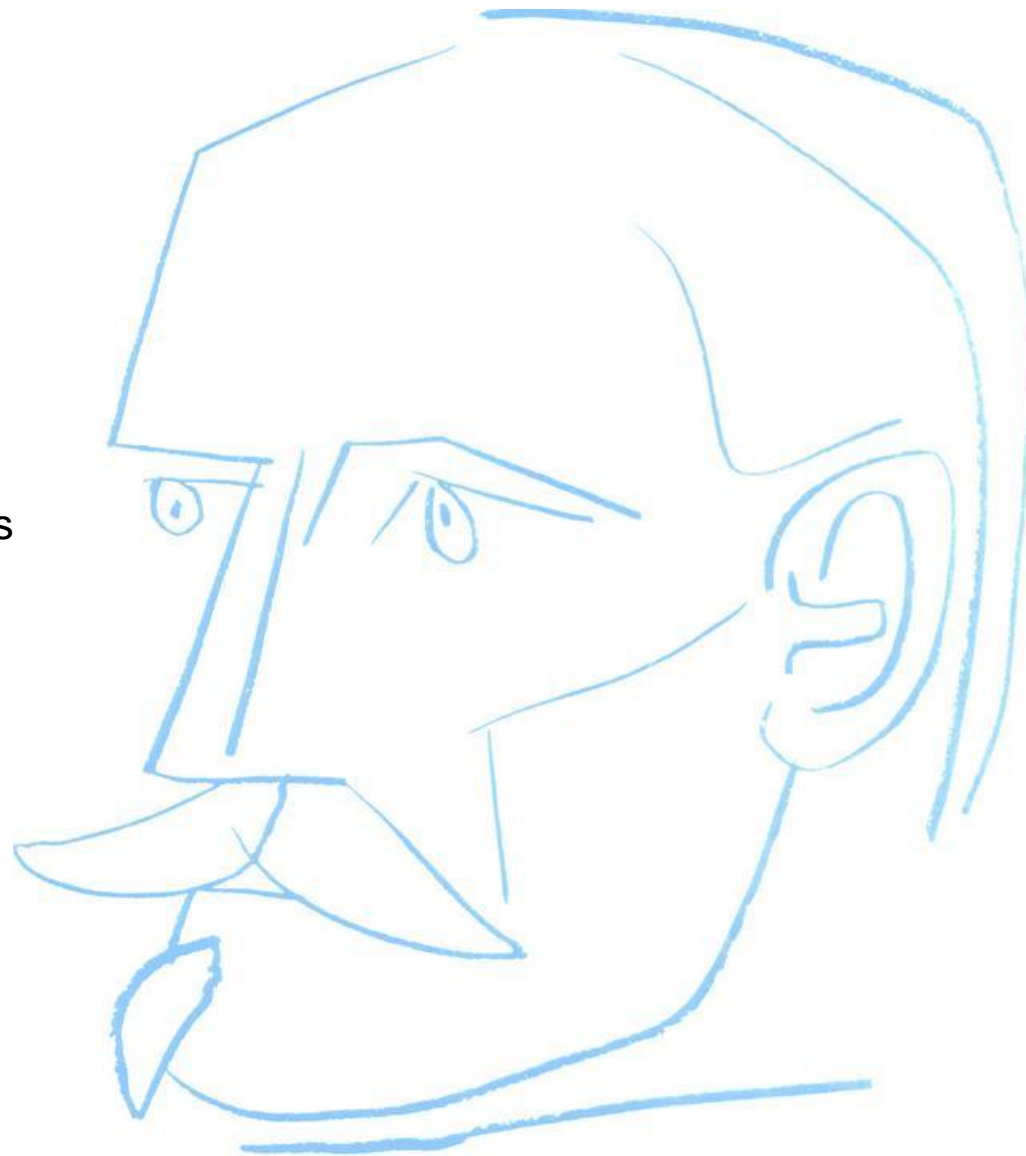
$$\dot{x} = -\partial_x \Phi + \Gamma \quad (\text{Langevin equation})$$

Paul Langevin

* January 23.1872

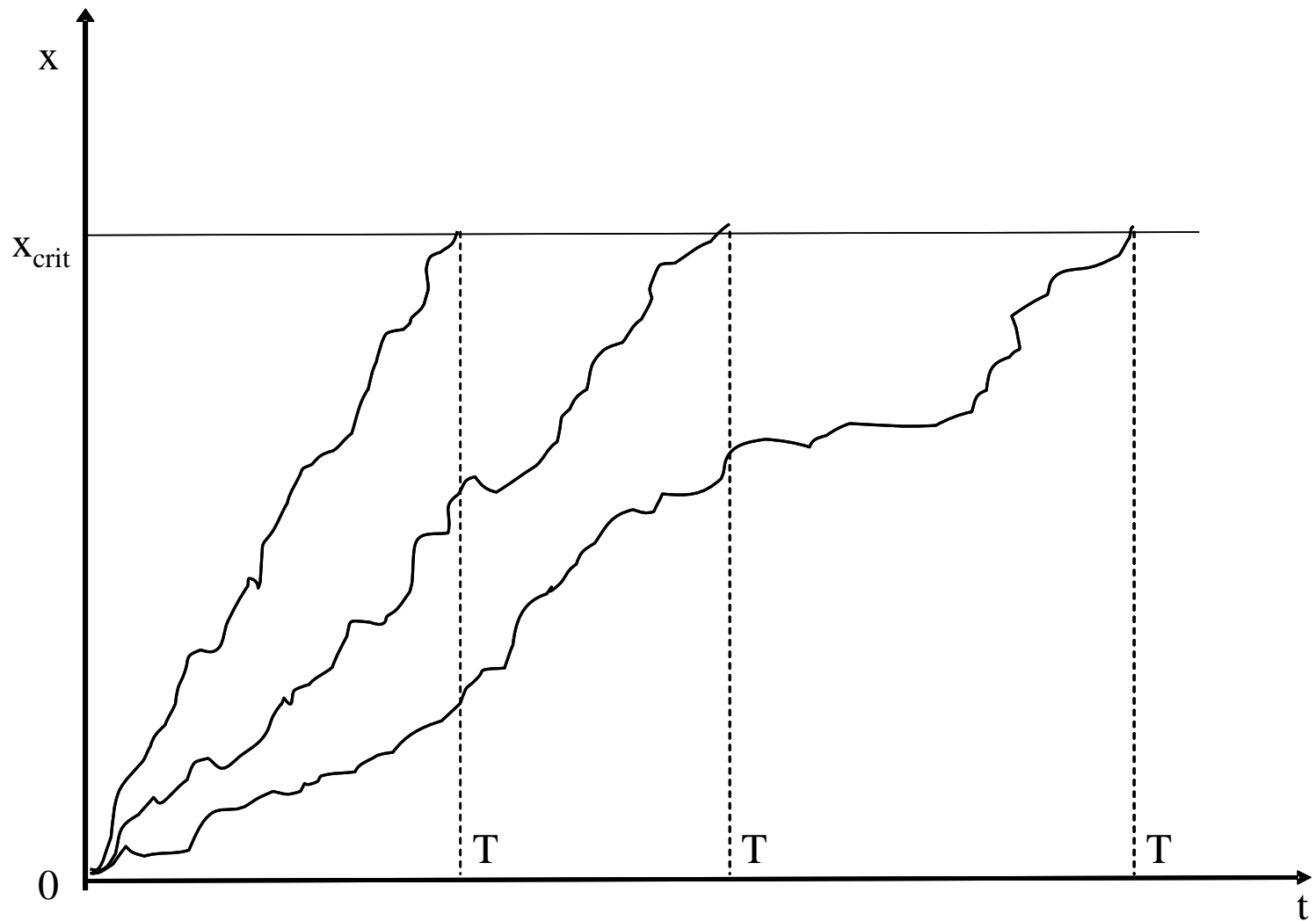
† December 19.1946

- french physicist
- studied at the Ecole Supérieure 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

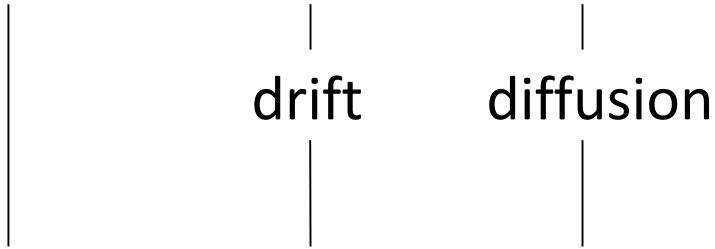


Trajectories of the system status with common start at $x=0$

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

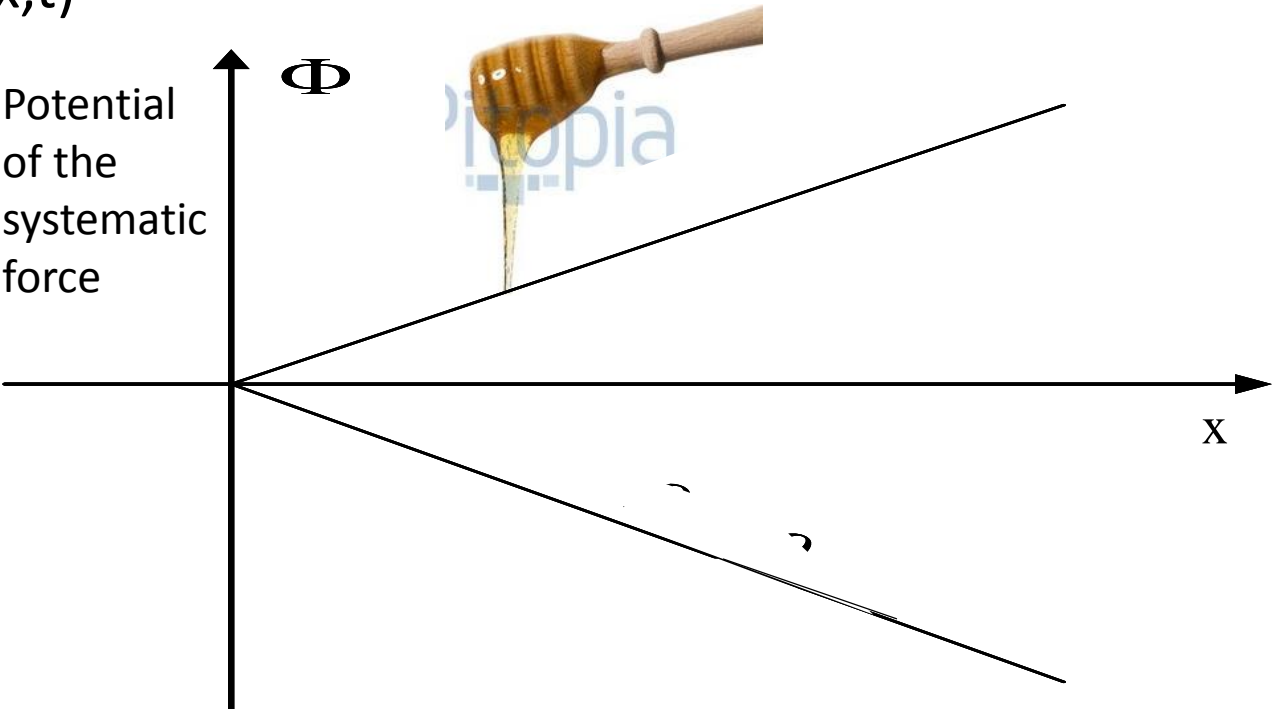
Langevin equation

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



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

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



Special cases to interpret the Fokker-Planck equation

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

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

Solution by method of characteristics

$$P(\mathbf{x},t) \equiv P(\mathbf{x}(t))$$

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

= sharp movement along the trajectory $\mathbf{x}=\mathbf{x}(t)$

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

$$P(\mathbf{x},t) = \frac{1}{\sqrt{2\pi Dt}} e^{-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{4Dt}}$$

= dissolving Gaussian distribution

General Solution for $P(x,t)$ by Separation

Starting equation (Fokker-Planck equation)

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

$\partial_t = 0$ gives stationary solution

$$0 = \partial_x \left(\Phi'(x) + \partial_x \right) P^{\text{st}}(x) \quad \Rightarrow \quad P^{\text{st}}(x) = N e^{-\Phi(x)}$$

separation ansatz for complete solution

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

gives

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

or

$$\begin{aligned} \lambda \varphi &= \left(-\partial_x + \frac{1}{2}\Phi' \right) \left(\partial_x + \frac{1}{2}\Phi' \right) \varphi \\ &= \left(-\partial_x^2 + \frac{1}{4}\Phi'^2 - \frac{1}{2}\Phi'' \right) \varphi \end{aligned}$$

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

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

and the correspondence

energy eigenvalue $E \Leftrightarrow$ time constant λ

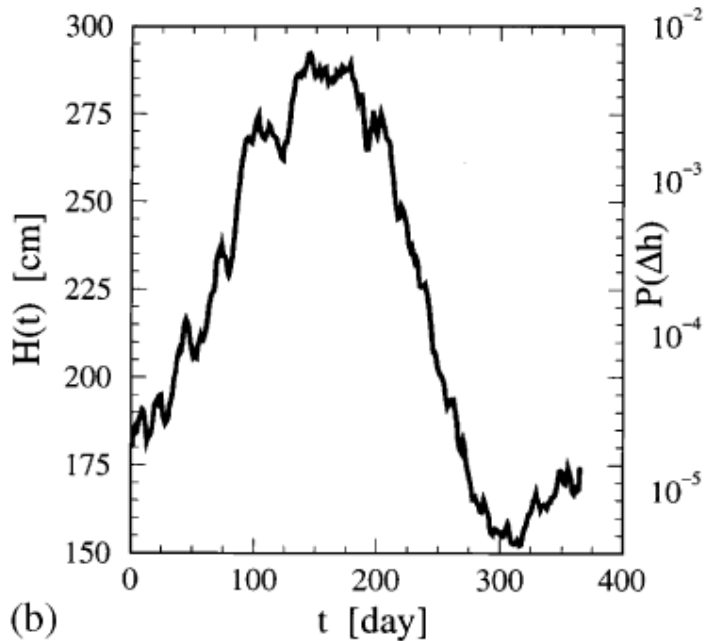
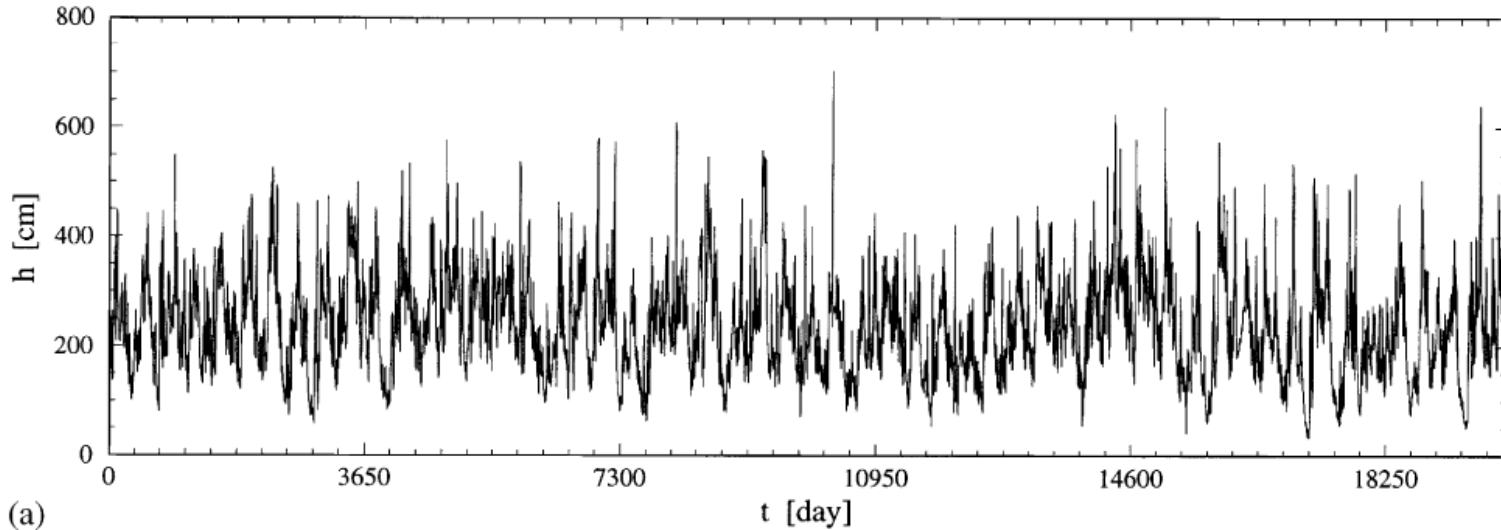
particle density $\psi^*\psi \Leftrightarrow$ probability density P

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

A short ethymology

- dis – aster (latin origin):
non/wrong constellation (dis) of stars (aster)-
our ancestors believed in the influence of stars on
natural disasters (floods, earthquakes,...)
- catastrophe (greek origin: *καταστροφή*):
revolution of planets around a central star, again-
the influence of stars on our live

Danube water level time series



Stochastic description of water level undulations

h_t = daily water level of a specific day for year t

simple approach with constant flow rate γ and fluctuations

$$h_{t+1} = h_t + \begin{cases} -2\gamma h_t & \text{if } h_t > \bar{h} \\ +2\gamma h_t & \text{if } h_t < \bar{h} \end{cases} + \Gamma(t)$$

no
change

in / out flow

fluctuations

$$\underbrace{\frac{h_{t+1} - h_t}{1}}_{\dot{h}(t)} = \underbrace{\begin{cases} -2\gamma h_t \\ +2\gamma h_t \end{cases}}_{\begin{cases} -2\gamma h(t) \\ +2\gamma h(t) \end{cases}} + \Gamma$$

Langevin
equation

$$(x = \ln(h(t) / \bar{h}))$$

$$\dot{x} = -2\gamma \text{sign } x + \tilde{\Gamma} \quad \langle \tilde{\Gamma}(t) \tilde{\Gamma}(t') \rangle = 2D \delta(t - t')$$

$$= \underbrace{-\Phi'(x)}_{\text{drift}} + \underbrace{\tilde{\Gamma}}_{\text{diffusion}}$$

Fokker-Planck equation
for probability $P(x,t)$

$$\dot{P} = \partial_x \Phi' P + \partial_x^2 P$$

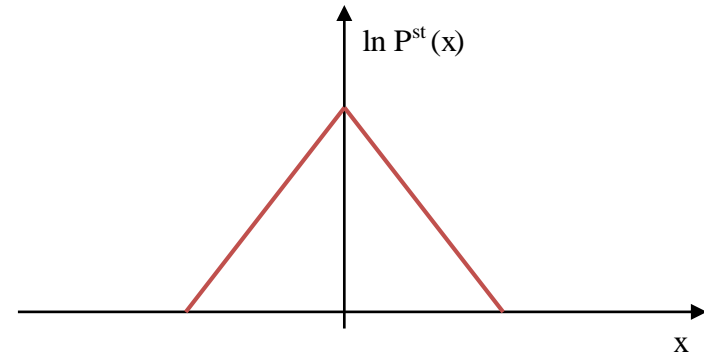
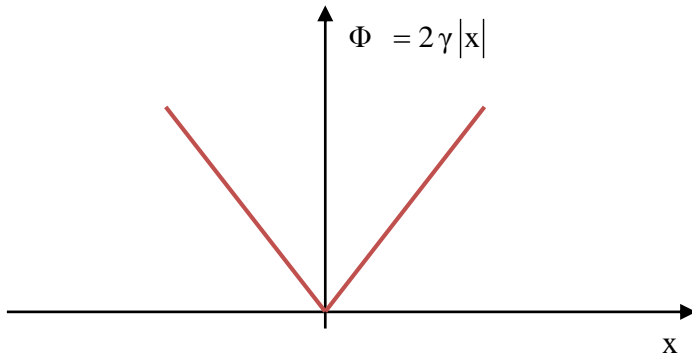
$$\Phi' = 2\gamma \text{sign } x$$

$$\Phi = 2\gamma |x|$$

Stationary solution

$$\dot{P}^{\text{st}} = 0 \quad \text{gives} \quad (\Phi' + \partial_x) P^{\text{st}}(x) = 0$$

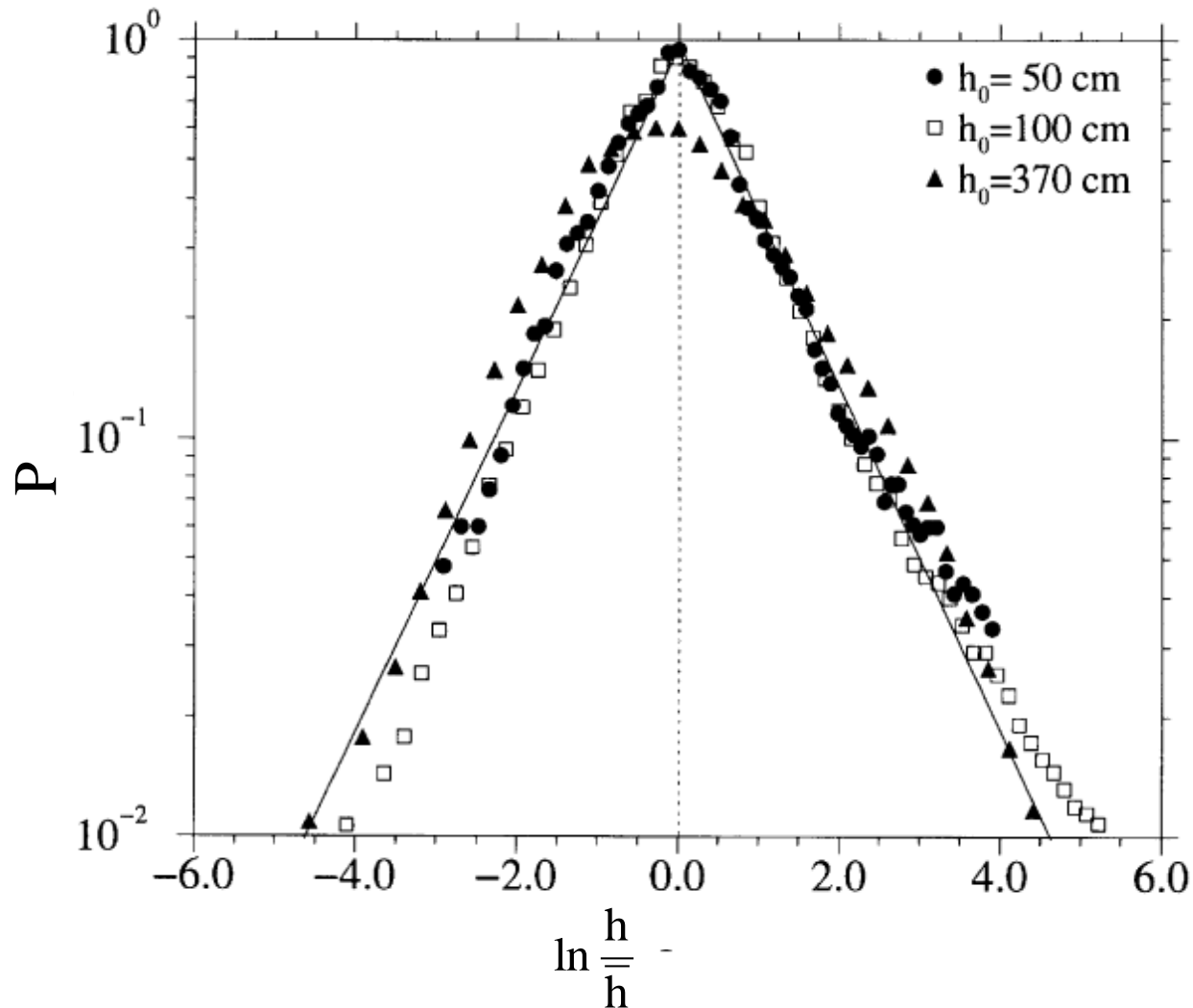
$$\text{from this follows} \quad P^{\text{st}}(x) = \gamma e^{-2\gamma|x|} \quad \ln P^{\text{st}}(x) = -2\gamma|x| + \ln \gamma$$



transformation to
original variable

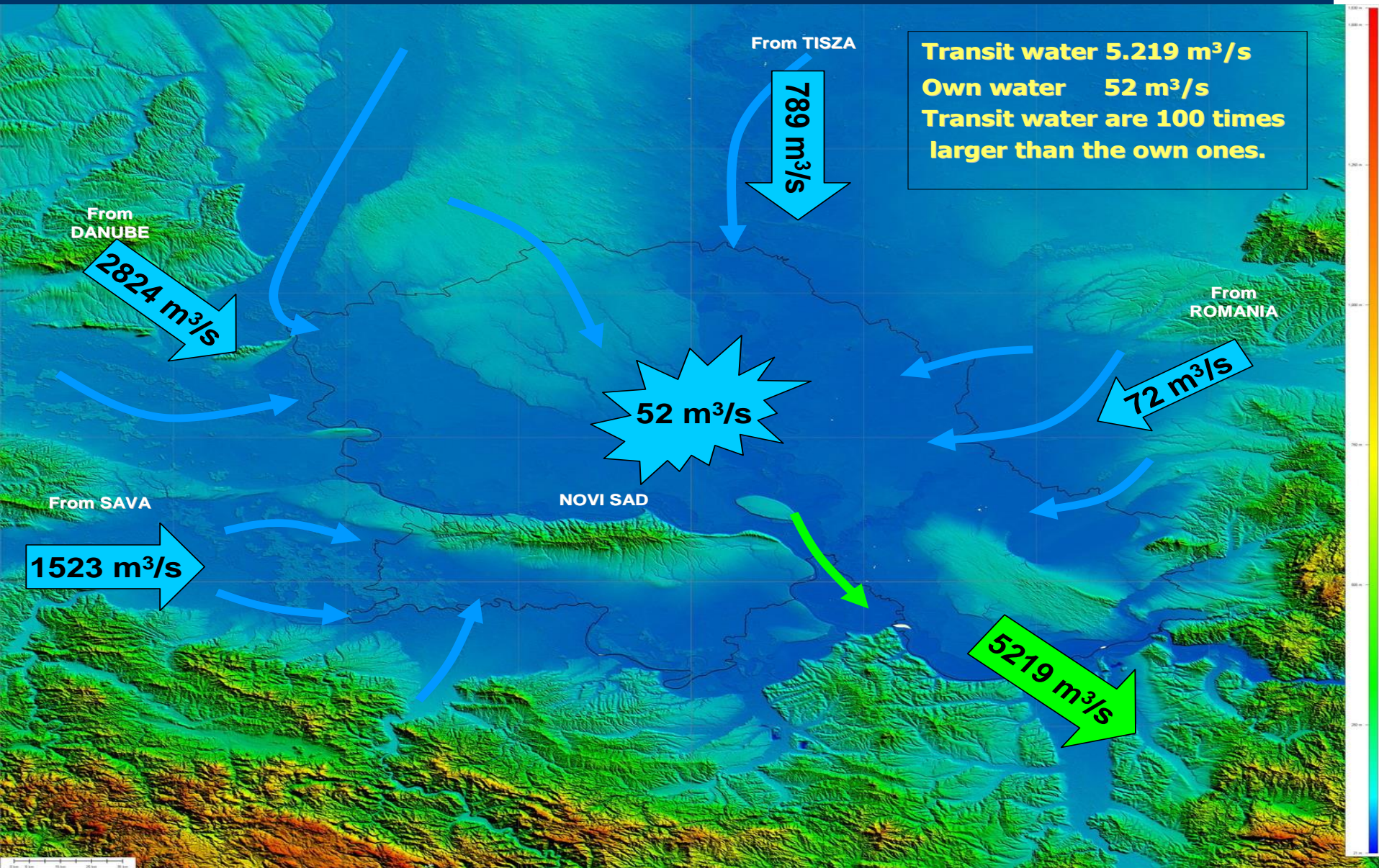
$$\tilde{P}^{\text{st}}(h) = P^{\text{st}}(x) \left| \frac{dx}{dh} \right|_{x=\ln \frac{h}{\bar{h}}} = \frac{\gamma}{\bar{h}} \cdot \begin{cases} \left(\frac{h}{\bar{h}}\right)^{-2\gamma-1} & h > \bar{h} \\ \left(\frac{h}{\bar{h}}\right)^{2\gamma-1} & h < \bar{h} \end{cases}$$

Danube water level



probability density distribution as a function of the logarithmic rate of change. The data approximately collapse upon the universal (thin solid line).

Water Balance in Vojvodina Region



Source: Atila Salvai, university of Novi Sad (presentation – Ulm, city hall 6. of November 2007)

Eigenfunction expansion for the V-shaped potential with natural boundaries

Separation $P = e^{-\frac{\phi(x)}{2}} \varphi(x) e^{-\lambda t}$ with $\phi(x) = 2\gamma|x|$

transforms the Fokker Planck equation

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

into a Schrödinger equation

$$\lambda\varphi = \left(-\partial_x + \frac{\Phi'}{2}\right)\left(\partial_x + \frac{\Phi'}{2}\right)\varphi \equiv \left(-\partial_x^2 + \gamma^2 - 2\gamma\delta(x)\right)\varphi$$

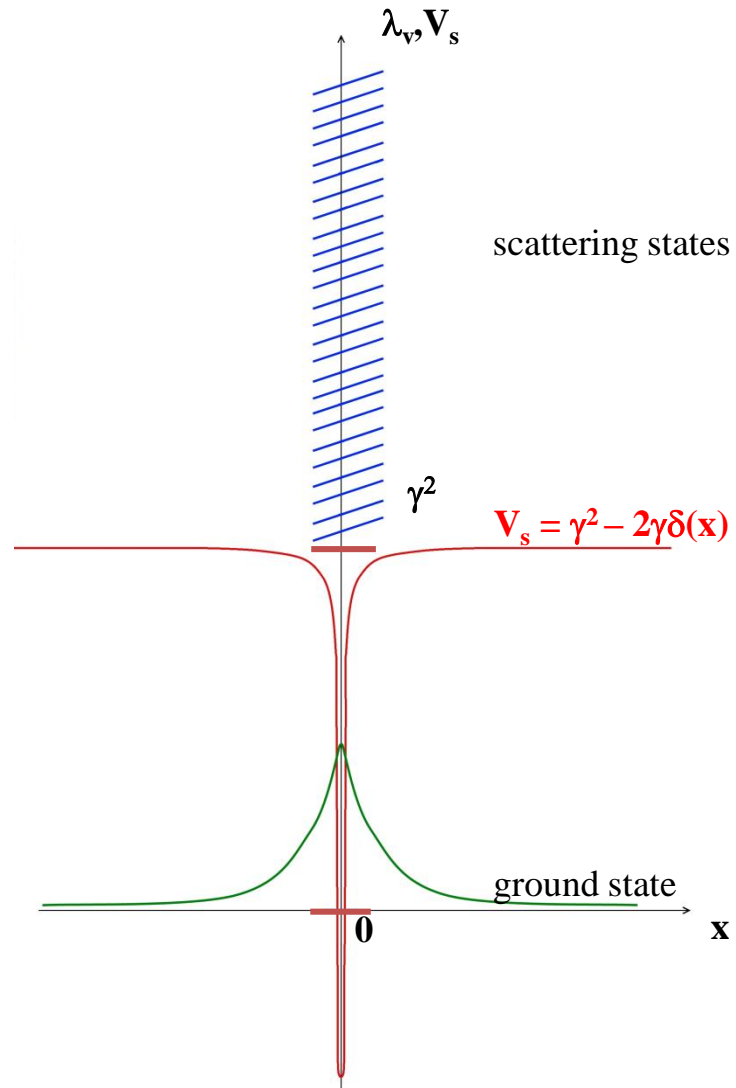
with natural boundary condition $(\varphi(x \rightarrow \pm\infty) = 0)$

ground state $\lambda_0 = 0$ $\varphi_0 = \sqrt{\gamma}e^{-\gamma|x|}$

symmetric/ antisymmetric scattering states

$$\varphi_k^s = \frac{1}{\sqrt{\pi}} \sin(k|x| - \alpha_k) \quad \tan \alpha_k = k/\gamma \quad \varphi_k^{as} = \frac{1}{\sqrt{\pi}} \sin kx \quad \lambda_k = \gamma^2 + k^2, k > 0$$

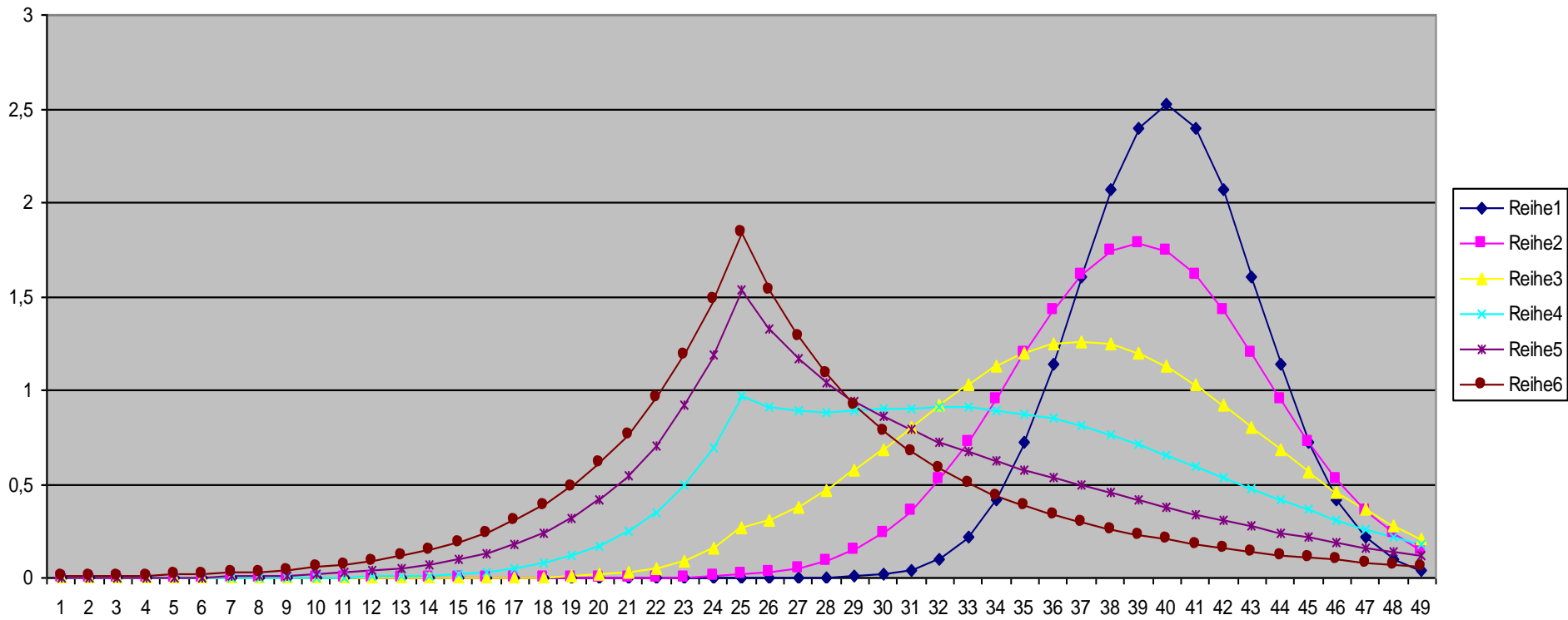
Term scheme

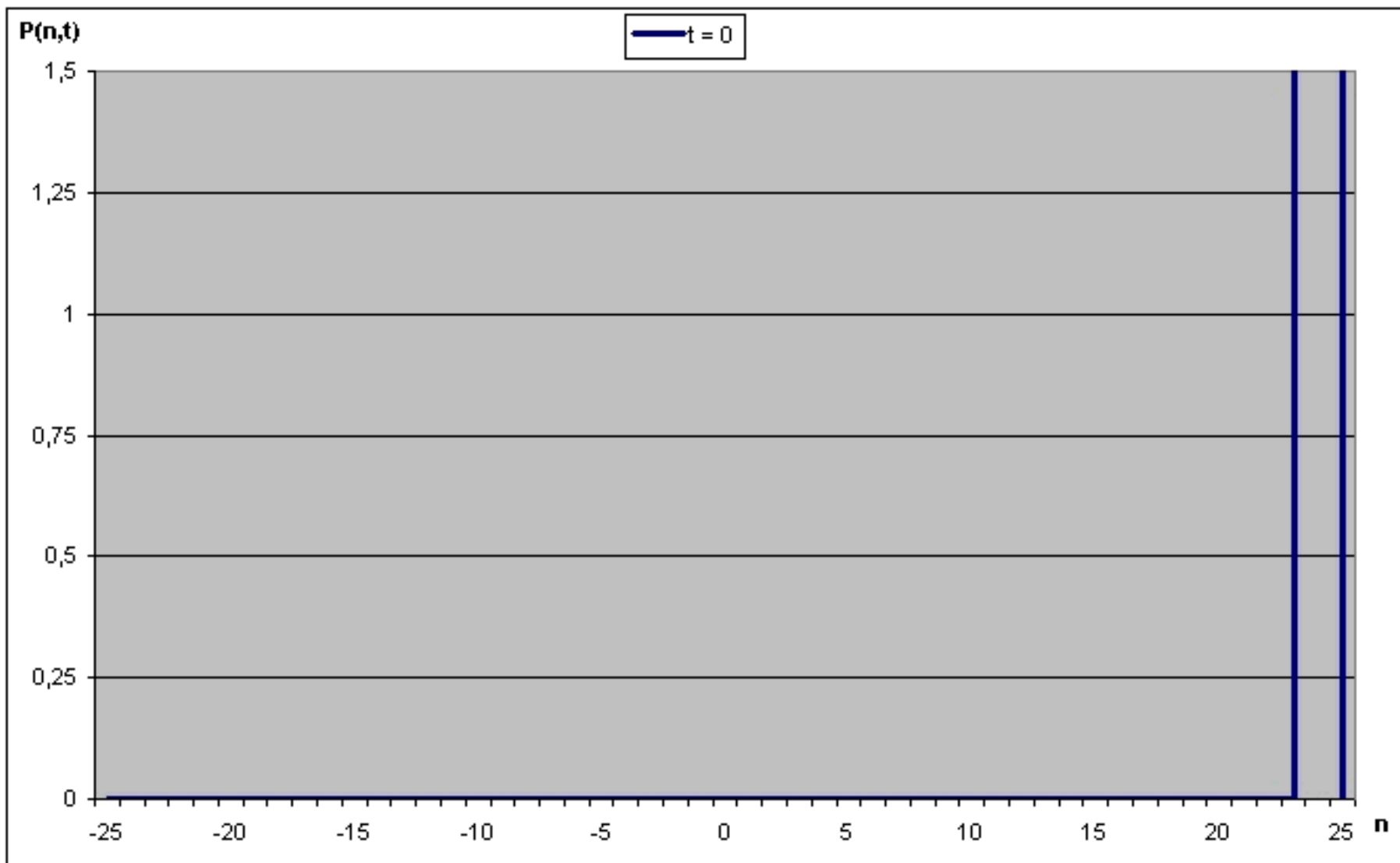


(Matthew 22:14 – For many are called, but few are chosen)

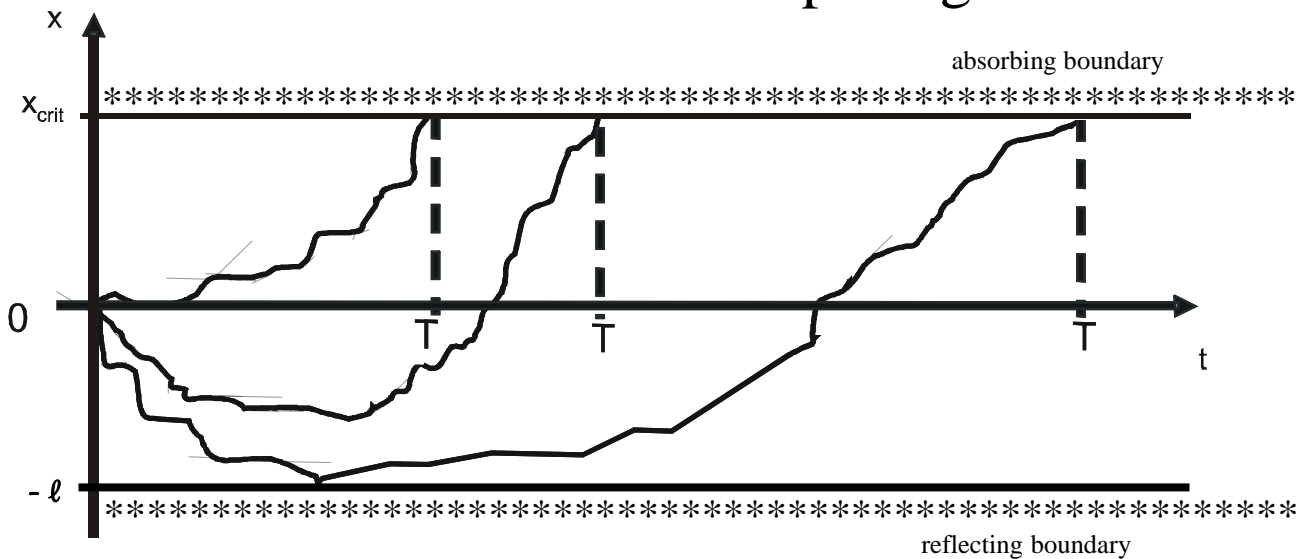
Construction of the time dependent (conditional) probability distribution using the completeness relation

$$P(x, t | x_0, 0) = e^{-\frac{1}{2}\phi(x) + \frac{1}{2}\phi(x_0)} \sum_k \varphi_k(x) \varphi_k(x_0) e^{-\lambda_k t} \rightarrow \begin{cases} \delta(x - x_0) & \text{for } t = 0 \\ \gamma e^{-2\gamma|x|} & \text{for } t \rightarrow \infty \end{cases}$$





First passage time

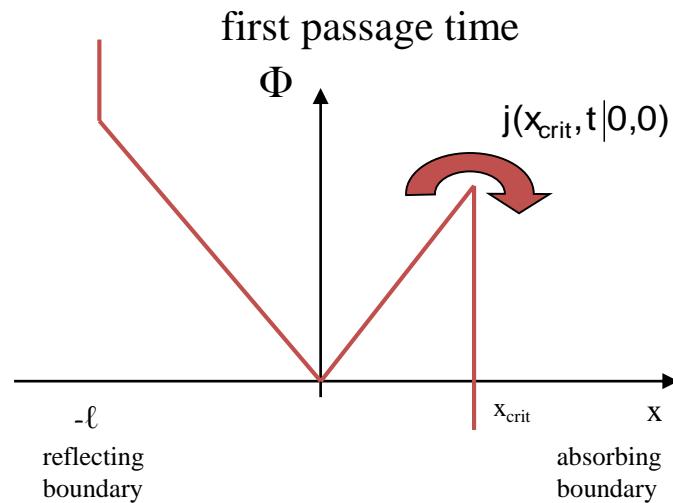


Probability and temporal drop of finding x anywhere below x_{crit}

$$W(t) = \int_{-\ell}^{x_{\text{crit}}} P(x,t|0,0) dx \quad -\frac{dW(t)}{dt} = -\int_{-\ell}^{x_{\text{crit}}} \dot{P}(x,t|0,0) dx = p(t)$$

Probability of flow over x_{crit}

$$p(t) = -\int_{-\ell}^{x_{\text{crit}}} \dot{P}(x,t|0,0) dx = j(x_{\text{crit}}, t | 0,0)$$



Eigenfunction expansion

Using the completeness relation

$$\int \varphi_\nu(\mathbf{x}) \varphi_\nu(0) = \delta(\mathbf{x})$$

allows the decomposition

$$P(\mathbf{x}, t | 0, 0) = e^{-\frac{1}{2}\Phi(\mathbf{x}) + \frac{1}{2}\Phi(0)} \sum \varphi_\nu(\mathbf{x}) \varphi_\nu(0) e^{-\lambda_\nu t}$$

with

$$P(\mathbf{x}, t | 0, 0) \Big|_{t=0} = \delta(\mathbf{x})$$

transforms the Fokker Planck equation into an eigenvalue equation

$$\left(-\partial_x^2 + \frac{1}{4}\Phi'^2(\mathbf{x}) - \frac{1}{2}\Phi''(\mathbf{x})\right)\varphi_\nu(\mathbf{x}) = \lambda_\nu \varphi_\nu(\mathbf{x})$$

which has to be solved under the boundary conditions

$$\left[\left(\partial_x + \frac{\Phi'(\mathbf{x})}{2} \right) \varphi_\nu(\mathbf{x}) = 0 \right]_{x = -\ell} \quad \text{reflecting boundary}$$

$$\varphi_\nu(\mathbf{x}) \Big|_{x = x_{\text{crit}}} = 0 \quad \text{absorbing boundary}$$

$\ell \rightarrow \infty$ gives

bound state

$$\varphi_0(x) = \begin{cases} N \frac{\sinh \kappa_0 (x_{\text{crit}} - x)}{\sinh \kappa_0 x_{\text{crit}}} & 0 < x < x_{\text{crit}} \\ N e^{\kappa_0 x} & x < 0 \end{cases} \quad \lambda_0 = \gamma^2 - \kappa_0^2, \quad \kappa_0 > 0$$

jump condition

$$-\varphi_0'(\varepsilon) + \varphi_0'(-\varepsilon) = 2\gamma \varphi_0(0)$$

$$1 - \frac{\kappa_0}{\gamma} = e^{-2\kappa_0 x_{\text{crit}}} \quad \text{only solutions for } \gamma x_{\text{crit}} > \frac{1}{2}$$

and normalization gives

$$N^2 = \frac{1}{\gamma} \frac{\kappa_0^2}{1 - 2\gamma x_{\text{crit}} e^{-2\kappa_0 x_{\text{crit}}}}$$

scattering states

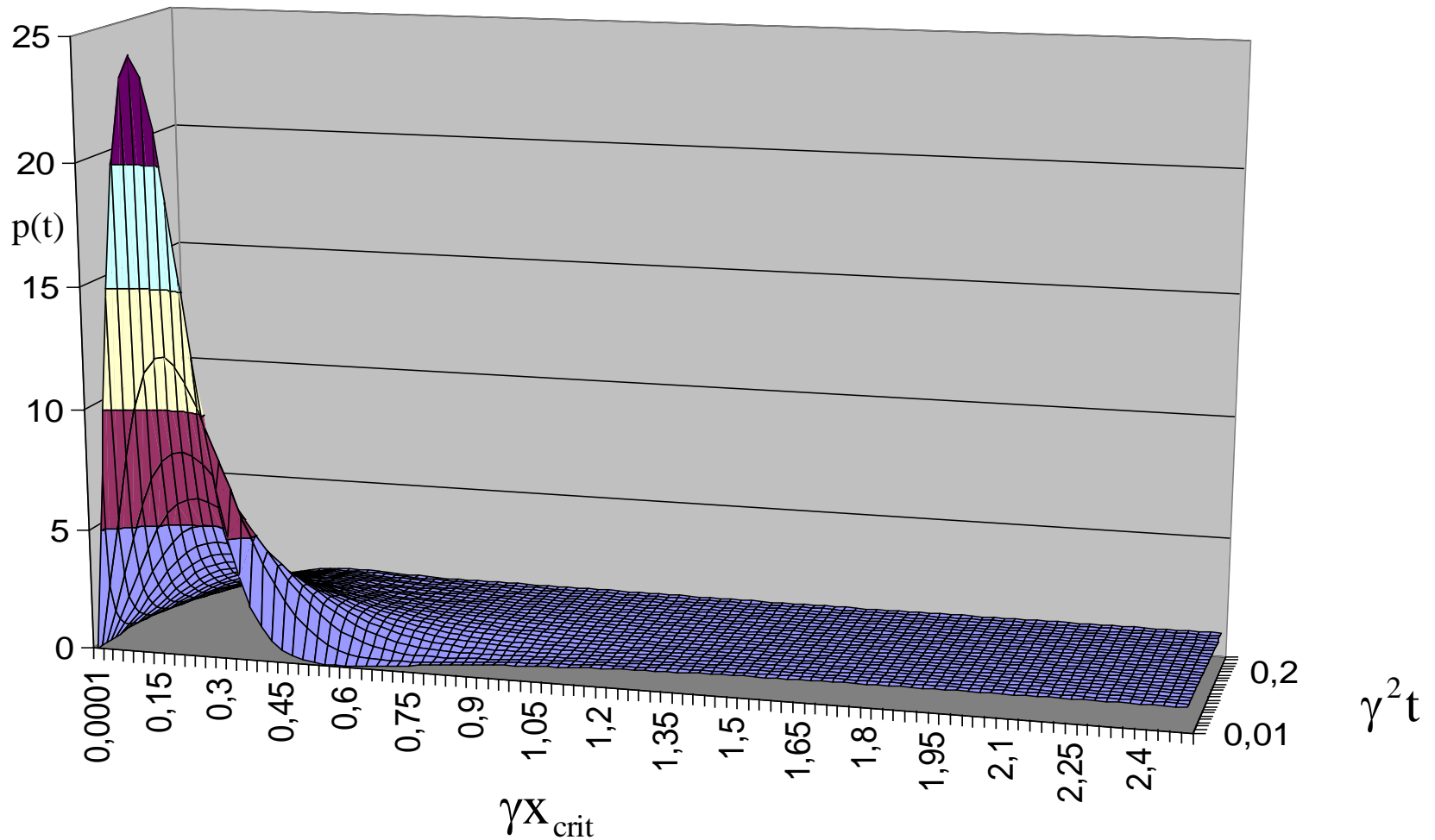
$$\varphi_k(x) = \begin{cases} \sqrt{\frac{2}{\pi}} \frac{\sin \alpha}{\sin kx_{\text{crit}}} \sin k(x_{\text{crit}} - x) & 0 \leq x \leq x_{\text{crit}} \\ \sqrt{\frac{2}{\pi}} \sin(kx + \alpha) & x \leq 0 \end{cases} \quad \lambda_k = \gamma^2 + k^2, \quad k > 0$$

with jump condition at $x = 0$

$$\cot kx_{\text{crit}} + \cot \alpha = 2 \frac{\gamma}{k}$$

First passage time probability distribution

$$p(t) = \frac{2\kappa_0^2 e^{-\gamma x_{\text{crit}} - \kappa_0 x_{\text{crit}}}}{1 - 2\gamma x_{\text{crit}} e^{-2\kappa_0 x_{\text{crit}}}} e^{-(\gamma^2 - \kappa_0^2)t} \cdot \begin{cases} 0 & \gamma x_{\text{crit}} < 1/2 \\ 1 & \gamma x_{\text{crit}} > 1/2 \end{cases} + e^{-\gamma x_{\text{crit}}} \int_0^\infty \frac{dk}{\pi/2} k \frac{\sin^2 \alpha}{\sin k x_{\text{crit}}} e^{-(\gamma^2 + k^2)t}$$



Korteweg-de Vries equation and Schrödinger equation

For the description of

(1) shallow water waves

(2) tidal bores, Tsunamis ([Amazon tidal bore.avi](#))

(3) wide moving jams

the Korteweg-de Vries equation is perfect suitable as equation of motion with competing nonlinear and dispersion terms

$$u_t + 6uu_x - u_{xxx} = 0$$

Korteweg-de Vries equation and Schrödinger equation (cont'd)

Introducing the linear operator L

$$L = -\partial_x^2 + u$$

where u is the solution of the Korteweg de-Vries equation. The spectral problem of the linear operator is represented by a Schrödinger-like equation

$$L\psi \equiv -\psi_{xx} + u\psi = E\psi$$

The eigenfunctions $\psi[x,E,t]$ and the eigenvalues E of L depend on t as a parameter and when t is fixed this equation is the well known time-independent linear Schrödinger equation of quantum mechanics for a particle in the potential $u(x,t)$

Korteweg-de Vries equation and Schrödinger equation (cont'd)

Note that if $u(x,t)$ evolves according to the Korteweg de-Vries equation

$$u_t + 6uu_x - u_{xxx} = 0$$

and, if we chose

$$A = 4i\partial_x^3 - 3i(u\partial_x + \partial_x u) = 4i\partial_x^3 - 3i(2u\partial_x + u_x)$$

the linear operator L satisfies the operator equation

$$i\frac{\partial L}{\partial t} = [A, L]$$

The operators L and A form a “Lax pair” *).

*)Lax, P.D., Integrals of nonlinear equations of evolution and solitary waves, Comm. Pure Appl. Math., **21**, pp. 467...490, 1968

Proof of the Lax pair relation

Inserting

$$A = 4i\partial_x^3 - 3i(u\partial_x + \partial_x u) = 4i\partial_x^3 - 3i(2u\partial_x + u_x)$$

gives for the commutator relation

$$\begin{aligned} [A, L] &= [4i\partial_x^3 - 3i(u\partial_x + \partial_x u), -\partial_x^2 + u] \\ &= -4i \underbrace{[\partial_x^3, \partial_x^2]}_0 + 4i \underbrace{[\partial_x^3, u]}_{u_{xxx} + 3(u_{xx} + u_x \partial_x) \partial_x} + 3i \underbrace{[\partial_x^2, (u\partial_x + \partial_x u)]}_{-u_{xxx} - 4u_{xx} \partial_x - 4u_x \partial_x^2} - 3i \underbrace{[(u\partial_x + \partial_x u), u]}_{2uu_x} \\ &= 4i(u_{xxx} + 3(u_{xx} \partial_x + u_x \partial_x^2)) - 3i(u_{xxx} + 4u_{xx} \partial_x + 4u_x \partial_x^2) - 6iuu_x \\ &= iu_{xxx} - 6iuu_x \end{aligned}$$

together with $iL_t = iu_t$ the relation $iL_t = [A, L]$ is thus exactly equivalent to the Korteweg de-Vries equation

$$u_t = u_{xxx} - 6uu_x$$

As a consequence of the decomposition of the Schrödinger operator L and the corresponding Lax pair operator A the time development of the eigenfunctions ψ satisfying the eigenvalue equation

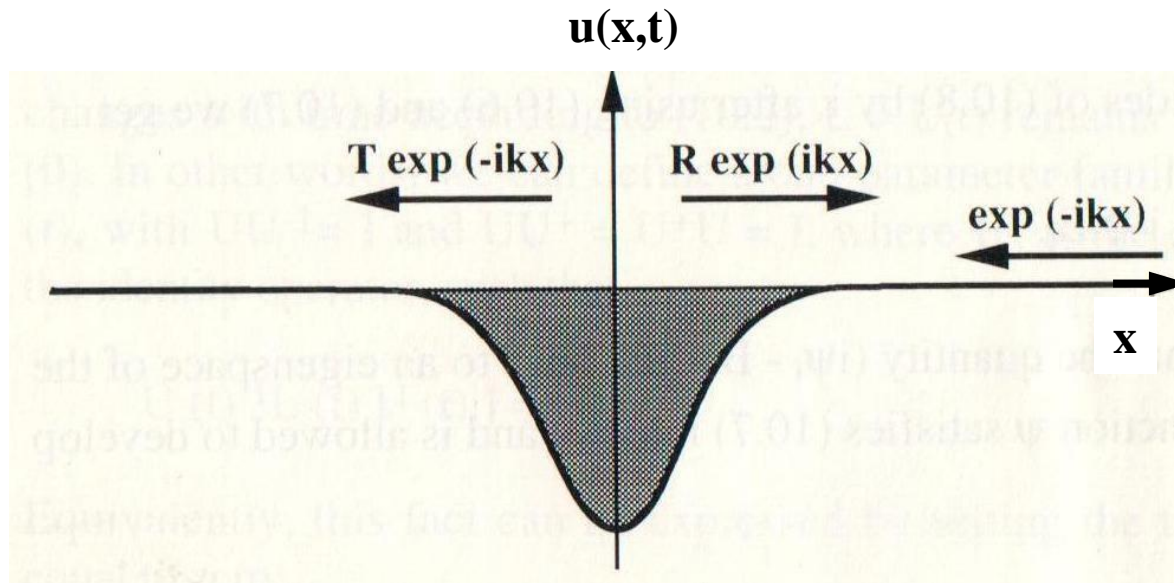
$$L\psi = E\psi$$

can be written as

$$i\frac{\partial\psi}{\partial t} = A\psi$$

So it is possible to associate the linear operator L with the Korteweg-de Vries equation and to reinforce the solution to a spectral problem of the operator A .

For solving the spectral problem of the Lax pair operators we assume that the solutions $u(x,t)$ of the Korteweg-de Vries equation are (1) continuous, (2) bounded, and (3) tend to 0 for $|x| \rightarrow \infty$



Scattering solutions corresponding to the continuous spectrum of the linear operator L

For the time evolution of the eigenfunctions of the self-adjoint linear Schrödinger-like operator L we split the eigenvalues E into bound state and continuous state values

$$E = \begin{cases} -\kappa_n^2 & \text{bound states} \\ k^2 & \text{continuous states} \end{cases}$$

and introduce the asymptotic eigenfunctions

$$\begin{aligned} \psi_n &\rightarrow \begin{cases} e^{-\kappa_n|x|} & \text{for } x \rightarrow +\infty \\ c_n(t)e^{-\kappa_n|x|} & \text{for } x \rightarrow -\infty \end{cases} && \text{bound states} \\ \psi_k &\rightarrow \begin{cases} e^{-ikx} + R(k,t)e^{ikx} & \text{for } x \rightarrow +\infty \\ T(k,t)e^{-ikx} & \text{for } x \rightarrow -\infty \end{cases} && \text{continuous states} \end{aligned}$$

For the discrete spectrum of the time development governed by the Lax pair operators

$$i \frac{\partial \psi_n}{\partial t} = A \psi_n$$

in the asymptotic limit $|x| \rightarrow \infty$ where $A \rightarrow 4i\partial_x^3$, since u vanishes, we get

$$\frac{\partial c_n}{\partial t} = 4\kappa_n^3 c_n$$

This is simply solved and gives

$$c_n(t) = c_n(0) e^{4\kappa_n^3 t}$$

where $c_n(0)$ is determined by the initial data $u(x,0)$ of the Korteweg de-Vries equation

For the continuous spectrum we get

$$\psi_k = a(k,t)e^{ikx} + b(k,t)e^{-ikx} \quad x \rightarrow +\infty$$

inserting this in the time development

$$i \frac{\partial \psi_k}{\partial t} = A \psi_k$$

gives with the asymptotic expression

$$A \rightarrow 4i\partial_x^3$$

$$i\partial_t \left(a(k,t)e^{ikx} + b(k,t)e^{-ikx} \right) = 4i\partial_x^3 \left(a(k,t)e^{ikx} + b(k,t)e^{-ikx} \right)$$

or because of the linear independence of the exponential

functions

$$\partial_t a(k,t) = -4ik^3 a(k,t), \quad \partial_t b(k,t) = 4ik^3 b(k,t)$$

Integration leads to

$$a(k,t) = a(k,0)e^{-4ik^3 t}, \quad b(k,t) = b(k,0)e^{4ik^3 t}$$

and for the reflection coefficient to

$$R(k,t) = a(k,t)/b(k,t) = R(k,0)e^{-8ik^3 t}$$

Exactly solvable potentials with the asymptotic $u(|x| \rightarrow \infty) = 0$

name	formula	factorization	eigenvalues
δ -potential	$u = -2\gamma\delta(x)$	$H = b^+ b - \gamma^2$ $b = \partial_x + \gamma \text{sign } x$	$\varepsilon_0 = -\gamma^2$
Pöschl-Teller potential	$u = -\frac{\lambda(\lambda-1)}{\cosh^2 x}$	$H = b^+(\lambda) b(\lambda) - (\lambda-1)^2$ $b(\lambda) = \partial_x + (\lambda-1) \text{th } x$	$\varepsilon_\nu = -(\lambda-1+\nu)^2$
rectangular potential hole	$u = \begin{cases} -C^2 & x < 1 \\ 0 & x > 1 \end{cases}$	$H = b^+ b + \varepsilon_0$ $b = \partial_x + \begin{cases} \kappa_0 & x > 1 \\ k_0 \tan k_0 x & x < 1 \end{cases}$ with $k_0 \tan k_0 = \kappa_0$	$\varepsilon_0 = -\kappa_0^2$ κ_0 from $k_0 \tan k_0 = \kappa_0$ with $k_0 = \sqrt{C^2 - \kappa_0^2}$
Scarf II potential	$u = A^2 + \frac{B^2 - A^2 - A}{\cosh^2 \alpha x} + B(2A+1) \frac{\tanh \alpha x}{\cosh \alpha x}$	$H(A) = \tilde{b}_A^+ \tilde{b}_A$ $\tilde{b}_A = \partial_x + A \tanh x + \frac{B}{\cosh x}$	$\varepsilon_\nu(A) = -(A-\nu)^2 + A^2$

Inverse scattering theory

Given the energy levels of the Schrödinger equation

$$\left(-\partial_x^2 + u\right)\psi = \lambda\psi$$

find the potential u

1) Asymptotic behavior for $|x| \rightarrow \infty$

Assumption $u(|x| \rightarrow \infty) = 0$

scattering states

$$\lambda = k^2 > 0 \quad \psi_k = \begin{cases} e^{ikx} + \underbrace{R e^{-ikx}}_{\text{reflected wave}} & x \rightarrow +\infty \\ \text{incident wave} & \\ T e^{ikx} & x \rightarrow -\infty \\ \text{transmitted wave} & \end{cases}$$

bound states

$$\lambda = -\kappa_n^2 \quad \psi_n(x) = \begin{cases} e^{-\kappa_n x} & \text{for } x \rightarrow \infty \\ c_n e^{\kappa_n x} & \text{for } x \rightarrow -\infty \end{cases}$$

2) Complete solution

With the Green's function of the asymptotic of the Schrödinger equation

$$\left(-\partial_x^2 - k^2\right)G(x,x') = \delta(x - x') \Rightarrow G(x,x') = \frac{i}{2k} e^{ik|x-x'|}$$

the solution of the complete Schrödinger equation

$$\left(-\partial_x^2 + u(x)\right)\psi_k(x) = k^2 \psi_k(x) \text{ or } \left(-\partial_x^2 - k^2\right)\psi_k(x) = \underbrace{-u(x)\psi_k(x)}_{I(x)}$$

reads

$$\psi_k(x) = \psi_k^{\text{hom}}(x) + \int_{-\infty}^{\infty} dx' G(x,x') I(x') = e^{ikx} - \frac{i}{2k} \int_{-\infty}^{\infty} dx' e^{ik|x-x'|} u(x') \psi_k(x')$$

The complete solution is a linear integral equation representing the sum of an incident plane wave and an outgoing wave

$$\lim_{x \rightarrow \infty} \psi_k(x) = e^{ikx} + R(k)e^{-ikx} \quad k > 0$$

Together with the bound states the integral equation can be put in the general form

$$g(x,y) + F(x+y) + \int_x^\infty dz F(y+z)g(x,z) = 0$$

$$F(\xi) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} R(k)e^{ik\xi} dk + \sum c_n^2 e^{-\kappa_n \xi} \quad u(x,t) = -2 \frac{d}{dx} g(x, y=x)$$

as shown by Gelfand and Levitan*). The function $F(x+y)$ is related to the scattering data $R(k), c_n,$ and κ_n .

*)Gelfand, I.M., Levitan, B. M., On the determination of a differential equation from its spectral function
Am. Math. Soc. Trans. **1**, 253...304, 1951

Inserting the spectral data for the evolution of the Korteweg-de Vries equation

Inserting the time developments of the coefficients in the eigenfunctions found for the Korteweg-de Vries equation

$$c_n(t) = c_n(0) e^{4\kappa_n^3 t}, \quad R(k,t) = R(k,0) e^{-8ikt}$$

into the Gelfand-Levitan integral equation, we obtain

$$F(x+y,t) = \sum_1^N c_n^2(0) e^{-\kappa_n(x+y) + 8\kappa_n^3 t} + \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk R(k,0) e^{ik(x+y) - 8ik^3 t}$$

Discrete spectrum only: one soliton solution

If the potential $u(x,t)$ has only a discrete spectrum and is reflectionless (i.e. $R(k,0)=0$) and if we first consider $N=1$ (i.e. $E=-\kappa^2$ is the only eigenvalue), then the solution of the Gelfand-Levitan integral equation

$$g(x, y, t) + F(x + y, t) + \int_x^{\infty} dz F(x + y, t) g(x, y, t) = 0$$

can be put in the form

$$g(x, y, t) = -c^2(0) e^{-\kappa(x+y)+8\kappa^3 t} - c^2(0) e^{8\kappa^3 t} \int_x^{\infty} dz e^{-\kappa(z+y)} g(x, z, t)$$

from which

$$u(x,t) = -2 \frac{d}{dx} g(x, y=x, t) = -2 \frac{\kappa^2}{\cosh^2(\kappa(x - x^0) + 4\kappa^3 t)}$$

follows

Discrete spectrum only: N soliton solution

If we next consider a discrete spectrum with N bound states $E_n = -\kappa_n^2$ and again a reflectionless potential, we get for the Gelfand-Levitan integral equation

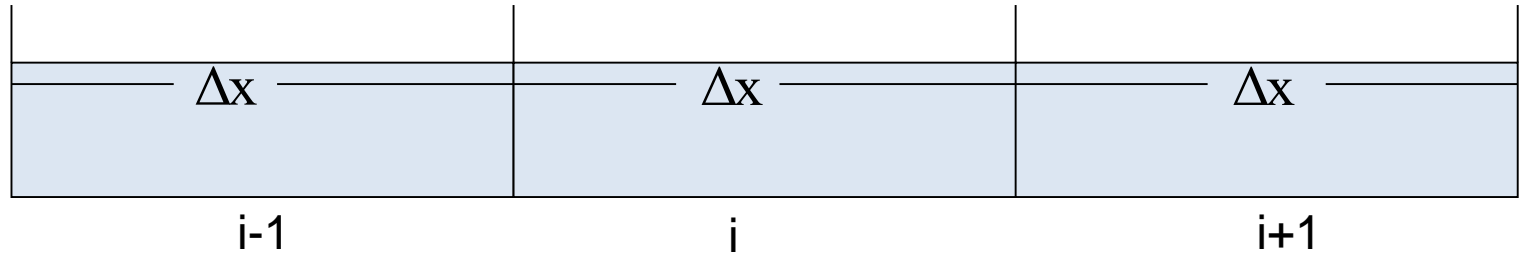
$$g(x, y, t) = -\sum_1^N c_n^2(0) e^{8\kappa_n^3 t} \left(e^{-\kappa_n x} + \int_x^\infty dz e^{-\kappa_n z} g(x, z, t) \right) e^{-\kappa_n y}$$

with the N soliton solution

$$u(x, t) = -2 \sum_1^N \frac{\kappa_n^2}{\cosh^2(\kappa_n (x - x_n^0) + 4\kappa_n^3 t)}$$

Each soliton has a velocity $-4\kappa_n^2$, and the bigger solitons travel faster.

Conservation law



$$N(i, t) = k(i, t) \cdot \Delta x$$

$$\frac{dN(i, t)}{dt} = k_t(i, t) \Delta x = -q_{\text{out}} + q_{\text{in}}$$

Traffic flow as forward difference*)
gives

$$q(i \rightarrow i + 1, t) = k(i, t)v(i + 1, t)$$

The approach reflects the forward orientation of the drivers and the asymmetric interaction in contrast to molecules in a gas or atoms in a solid state

The forward difference approach is summarized

$$q_{\text{out}} = k(i, t)v(i + 1, t) \quad q_{\text{in}} = k(i - 1, t)v(i, t)$$

*) Hilleges, M., Ein phänomenologisches Modell des dynamischen Verkehrsflusses in Schnellstraßennetzen, Diss., Uni Stuttgart, 1994 .

Conservation law (cont'd)

A continuum approximation allows the Taylor expansion

$$q_{\text{out}} = q(i \rightarrow i + 1, t) = k(x, t) \left(v(x, t) + \Delta x v_x(x, t) + \frac{(\Delta x)^2}{2} v_{xx}(x, t) + \frac{(\Delta x)^3}{6} v_{xxx}(x, t) + \dots \right)$$

$$q_{\text{in}} = q(i - 1 \rightarrow i, t) = \left(k(x, t) - \Delta x k_x(x, t) + \frac{(\Delta x)^2}{2} k_{xx}(x, t) - \frac{(\Delta x)^3}{6} k_{xxx}(x, t) + \dots \right) v(x, t)$$

Inserted into $\frac{dN(i, t)}{dt} = k_t(i, t)\Delta x = -q_{\text{out}} + q_{\text{in}}$

gives the conservation law

$$k_t = -(kv_x + k_x v) + \frac{\Delta x}{2} (-kv_{xx} + k_{xx} v) - \frac{(\Delta x)^2}{6} (kv_{xxx} + k_{xxx} v) + \dots$$

This can be transformed into a new conservation law

$$k_t + q_x = 0, \quad q = kv + \frac{\Delta x}{2} (kv_x - k_x v) + \frac{(\Delta x)^2}{6} (kv_{xx} + k_{xx} v - k_x v_x) + \dots (1)$$

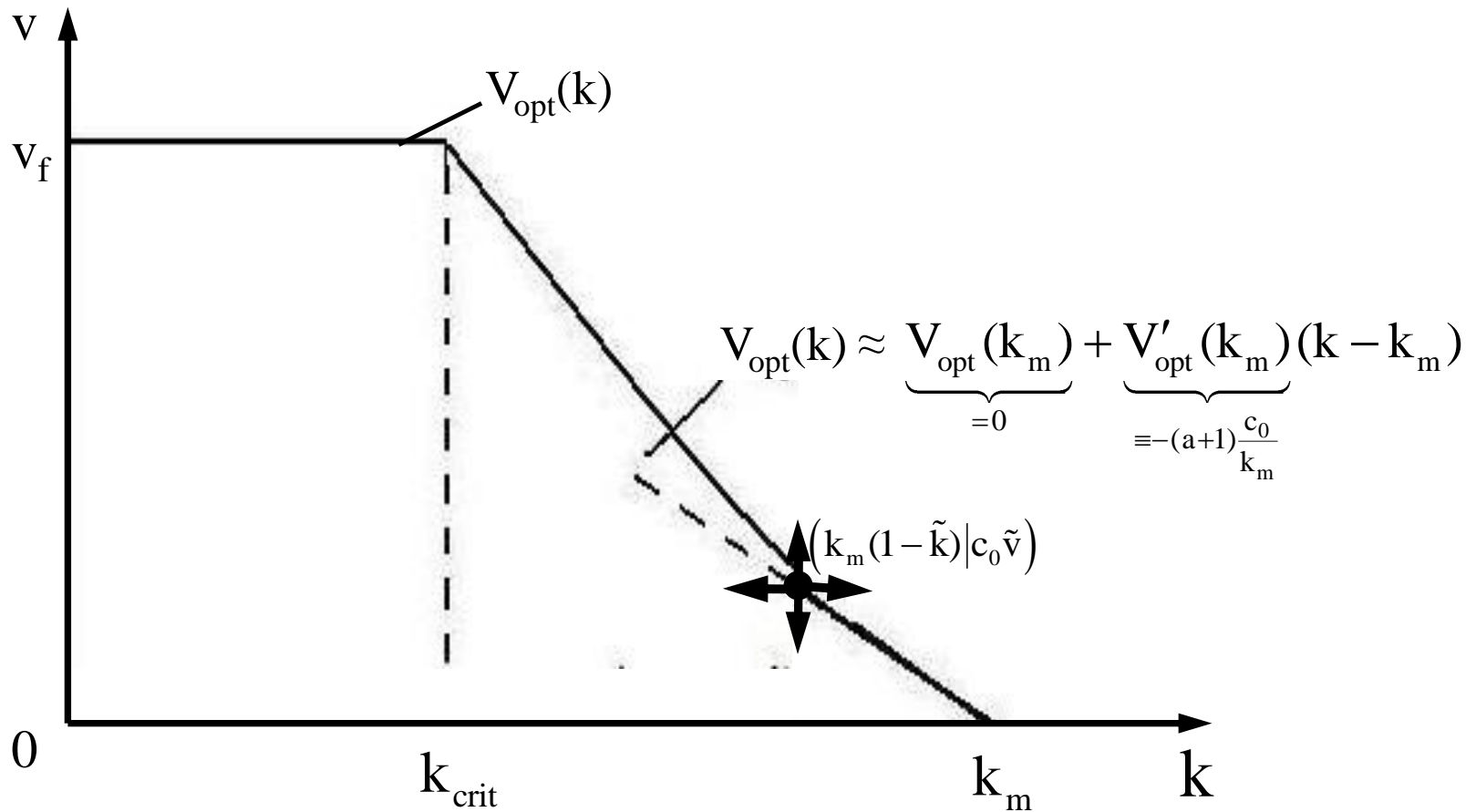
For the speed variation we assume, that the density k follows instantaneously an optimum velocity function:

$$v = V_{\text{opt}}(k) \quad (2)$$

$V_{\text{opt}}(k)$ is the equilibrium speed-density relation from the fundamental diagram. (1) and (2) is a modification (i.e. infinitesimal relaxation time) of the macro-scopic traffic flow model firstly introduced by Bando et al.*).

*)Bando, M., et al.: Phys. Rev. E Vol.5, pp. 1035(1995)

Selecting an operating point in very dense traffic



Decomposition for very dense traffic

$$\mathbf{k} = \mathbf{k}_m (1 - \tilde{\mathbf{k}}) \quad \mathbf{v} = \mathbf{c}_0 \tilde{\mathbf{v}} \quad \text{with} \quad \mathbf{c}_0 = \frac{\Delta \mathbf{x}}{2\tau} \quad \mathbf{V}_{\text{opt}}(\mathbf{k}_m) = 0$$

gives

$$-\frac{1}{\mathbf{c}_0} \tilde{\mathbf{k}}_t + \tilde{\mathbf{v}}_x - (\tilde{\mathbf{k}}\tilde{\mathbf{v}})_x = \frac{\Delta \mathbf{x}}{2} \left(-\tilde{\mathbf{v}}_{xx} + \tilde{\mathbf{k}}\tilde{\mathbf{v}}_{xx} - \tilde{\mathbf{k}}_{xx} \tilde{\mathbf{v}} \right) - \frac{(\Delta \mathbf{x})^2}{6} \left(\tilde{\mathbf{v}}_{xxx} - \tilde{\mathbf{k}}\tilde{\mathbf{v}}_{xxx} - \tilde{\mathbf{k}}_{xxx} \tilde{\mathbf{v}} \right) + \dots \quad (1)$$

$$\tilde{\mathbf{v}} = \underbrace{-\frac{\mathbf{k}_m}{\mathbf{c}_0} \mathbf{V}'_{\text{opt}}(\mathbf{k}_m)}_{a+1} \tilde{\mathbf{k}} \quad (2)$$

Inserting the second relation

$$-(a+1)\tilde{k} + \tilde{v} = 0$$

and sorting the terms yields to

$$\left(\tilde{v}_x + \frac{\Delta x}{2} \tilde{v}_{xx} + \frac{(\Delta x)^2}{6} \tilde{v}_{xxx} + \dots \right)$$

$$-\frac{1}{a+1} \left(\frac{1}{c_0} \tilde{v}_t + (\tilde{v}^2)_x + \frac{(\Delta x)^2}{3} \tilde{v} \tilde{v}_{xxx} + \dots \right) = 0$$

Proper scaling $\tilde{v} = \lambda \tilde{v}'$ $\partial_t = \lambda \partial_{t'}$ ('suppressed)
separates the equation of motion in terms of $O(\lambda)$ and $O(\lambda^2)$.

Synchronized traffic description

$O(\lambda)$ contains only linear terms and no temporal changes

$$\tilde{v}_x^{(0)} + \frac{\Delta x}{2} \tilde{v}_{xx}^{(0)} + \frac{(\Delta x)^2}{6} \tilde{v}_{xxx}^{(0)} + \dots = 0 \Rightarrow \tilde{v}^{(0)} = \text{const.} \doteq \tilde{v}_{\text{syn}}$$

The constant solution $\tilde{v}^{(0)}$ is “synchronized traffic”: in very dense traffic creeping shows undulations only on a coarse scale, and the behavior in adjacent lanes shows no big differences (traffic in adjacent lanes seems to be synchronized*).

*)Palmer, J., et al. Quality of Congested Traffic Int'l J. Adv. Systems 4 pp.168-182 (2011)

Korteweg-de Vries equation for speed drop propagation (wide moving jam)

In $O(\lambda^2)$ the time derivative and the nonlinear terms prevail

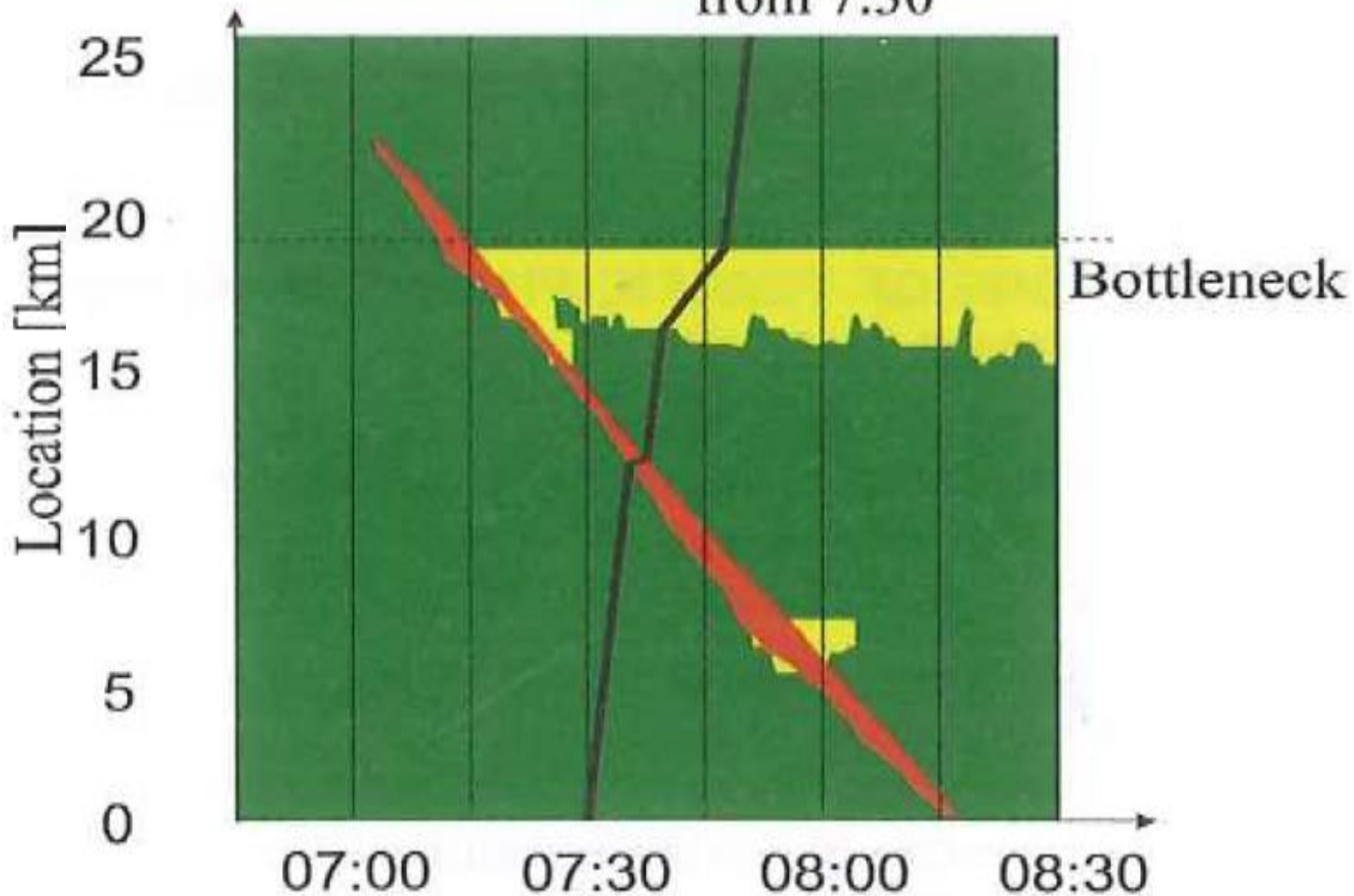
$$\frac{1}{c_0} \tilde{v}_t^{(1)} + ((\tilde{v}^{(1)})^2)_x + \frac{(\Delta x)^2}{3} \tilde{v}^{(1)} \tilde{v}_{xxx}^{(1)} + \dots = 0 \quad \Rightarrow \quad \tilde{v}^{(1)} = \text{solution of non-linear equation}$$

$\tilde{v}^{(1)}$ follows a nonlinear equation for the spatio-temporal speed variations of the Korteweg-de Vries type: in very dense traffic other traffic patterns than the synchronized traffic can occur under certain parameter configurations.

Wide moving jam

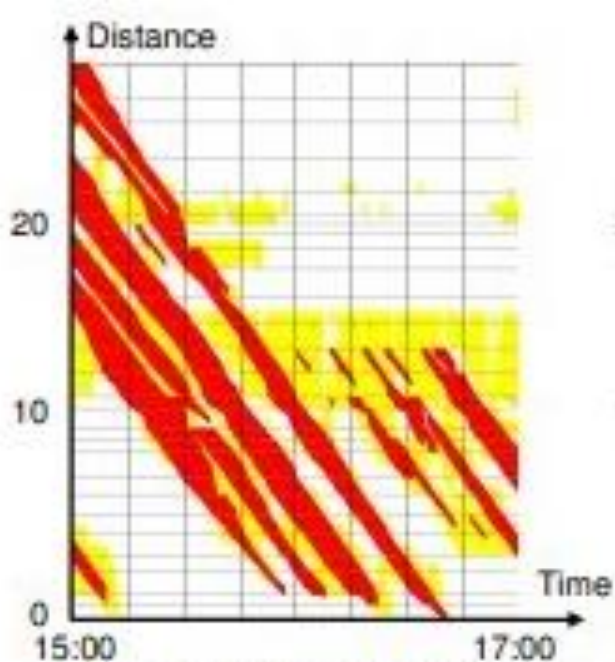
Trajectory of a vehicle
from 7:30

example *)
of a back-
wards
running
jam, stable
over more
than 20 km

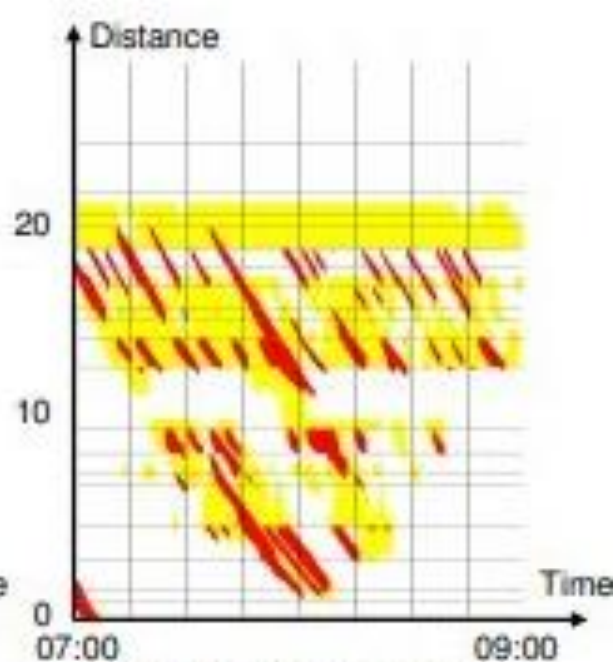


Free Flow Synchronised flow Wide moving jam

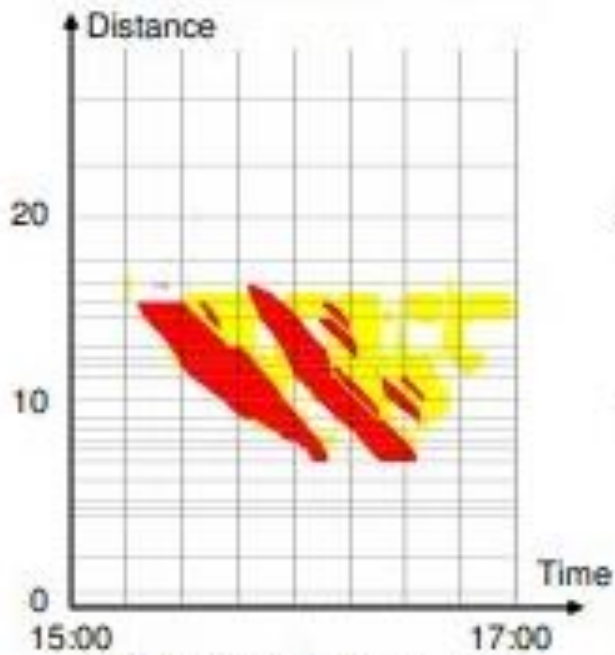
*) R.-P. Schäfer et al., "A study about probe vehicle data to verify the three-phase traffic theory". Traffic Engineering and Control, Vol 52, No 5, Pages 225-231, 2011



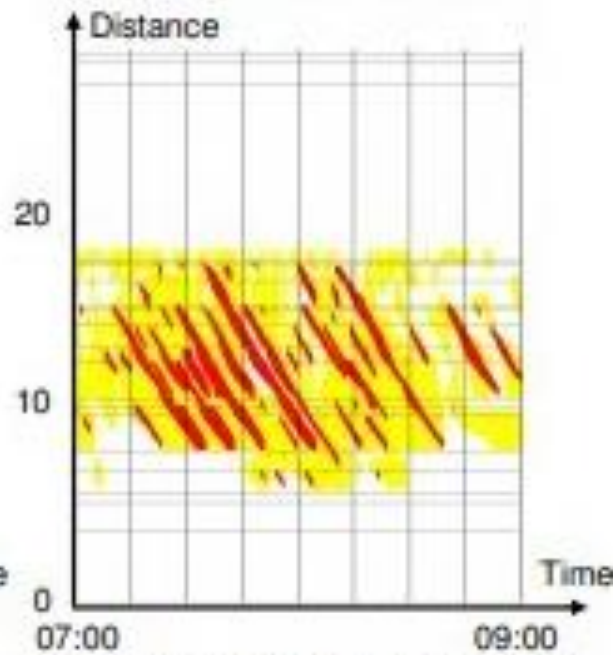
A5, Hessen, Germany



M42, United Kingdom



A3, Bavaria, Germany



I405, Orange County, USA

Distance time diagrams from traffic patterns in very dense traffic showing stable backwards running shockwaves remaining stable over long distances *)
 (red=low speed, yellow=high speed)

*)Palmer, J., Rehborn, H., Congested Traffic Patterns, ITS World Congress, Stockholm,2009

Using a mean field approximation for the third order derivative term as indicated

$$\frac{(\Delta x)^2}{3} \tilde{v}^{(1)} \tilde{v}_{xxx}^{(1)} \approx \frac{(\Delta x)^2}{3} \bar{\tilde{v}}^{(1)} \tilde{v}_{xxx}^{(1)} = -\frac{(\Delta x)^2}{3} \left| \bar{\tilde{v}}^{(1)} \right| \tilde{v}_{xxx}^{(1)}$$

with the mean value $\bar{\tilde{v}}^{(1)}$ as profile average

$$\bar{\tilde{v}}^{(1)} = \frac{1}{2\Lambda} \int_{-\Lambda}^{+\Lambda} dx \tilde{v}^{(1)}(x, t)$$

determined by a self consistency condition
later on

and a change in the variables (``suppressed)

$$t'' = \left| \tilde{v}^{(1)} \right| \frac{c_0}{3\Delta x} t' \quad x'' = \frac{x}{\Delta x} \quad u = \frac{1}{\left| \tilde{v}^{(1)} \right|} \tilde{v}^{(1)}$$

gives for the temporal and spatial behavior of the (normalized) speed u

$$u_t + 6u u_x - u_{xxx} = 0$$

(nonlinear wave equation also called Korteweg-de Vries equation)

This is exactly the Korteweg-de Vries equation, describing waves with long wavelengths running stable like a Tsunami*).

The Korteweg-de Vries equation as a nonlinear equation for the spatio-temporal speed variations describes the impressive wide moving jams in very dense traffic, i.e. the backward running shockwaves, which are so stable, that even traffic from interchanges do not destroy their structure (compare distance-time diagrams shown above).

*) Remoissenet, M., Waves Called Solitons, Springer publ., 1999

The solution can be found either by the Cole-Hopf transformation*)

$$u = -2(\ln F)_{zz}$$

which converts the Korteweg-de Vries equation into a homogeneous quadratic differential equation or by a direct ansatz, which is shown in the following section and leads to the solution

$$u(x, t) = -\frac{N}{\cosh^2 \left(\kappa(x - x^0) + \omega t \right)}$$

*) Whitham, G.B., Linear and Nonlinear Waves, Wiley, 1974

Soliton solution of the general Korteweg-de Vries equation

The general Korteweg-de Vries equation reads

$$u_t + \alpha u u_x - \beta u_{xxx} = 0$$

Introducing the collective coordinate

$$z = \kappa(x - x^0) + \omega t \quad \text{or} \quad \partial_t = \omega \partial_z \quad \partial_x = \kappa \partial_z$$

gives

$$\frac{\omega}{\kappa} u_z + \alpha u u_z - \beta \kappa^2 u_{zzz} = 0 \quad \text{resp.} \quad \frac{\omega}{\kappa} u + \frac{\alpha}{2} u^2 - \beta \kappa^2 u_{zz} = C$$

The boundary condition $u=0$ for $x \rightarrow \pm\infty$

leads to

$$\frac{\omega}{\kappa} u + \frac{\alpha}{2} u^2 - \beta \kappa^2 u_{zz} = 0$$

The ansatz fulfills the Korteweg- de Vries equation for

$$\frac{\omega}{\kappa} = 4\beta \kappa^2 \quad , \quad \frac{\alpha}{2} = \beta \kappa^2 \frac{6}{N}$$

As simple case the following parameter set is chosen

$$\alpha = 6 \quad \beta = 1 \quad N = 2\kappa^2 \quad \omega = 4\kappa^3$$

With this the self consistency condition

$$1 = \frac{1}{2\Lambda} \int_{-\Lambda}^{+\Lambda} dx \frac{2\kappa^2}{\cosh^2(\kappa(x - x^0) + 4\kappa^3 t)}$$

is for $\kappa = \Lambda/2$ automatically fulfilled.

As final result, if we restrict to second order and take \tilde{v}_{syn} as the asymptotic speed, we get for the speed profile in very dense traffic

$$\tilde{v} = \tilde{v}_{\text{syn}} \left(1 - \frac{2\kappa^2}{\cosh^2(\kappa(x - x^0) + 4\kappa^3 t)} \right) \Big|_{\kappa = \Lambda/2}$$

which describes a temporal and spatial variation, with a low speed at the very tails and a stable backward running breakdown.

The ansatz $u = N \frac{1}{\cosh^2 z}$, $u_z = -2N \frac{\text{th } z}{\cosh^2 z}$

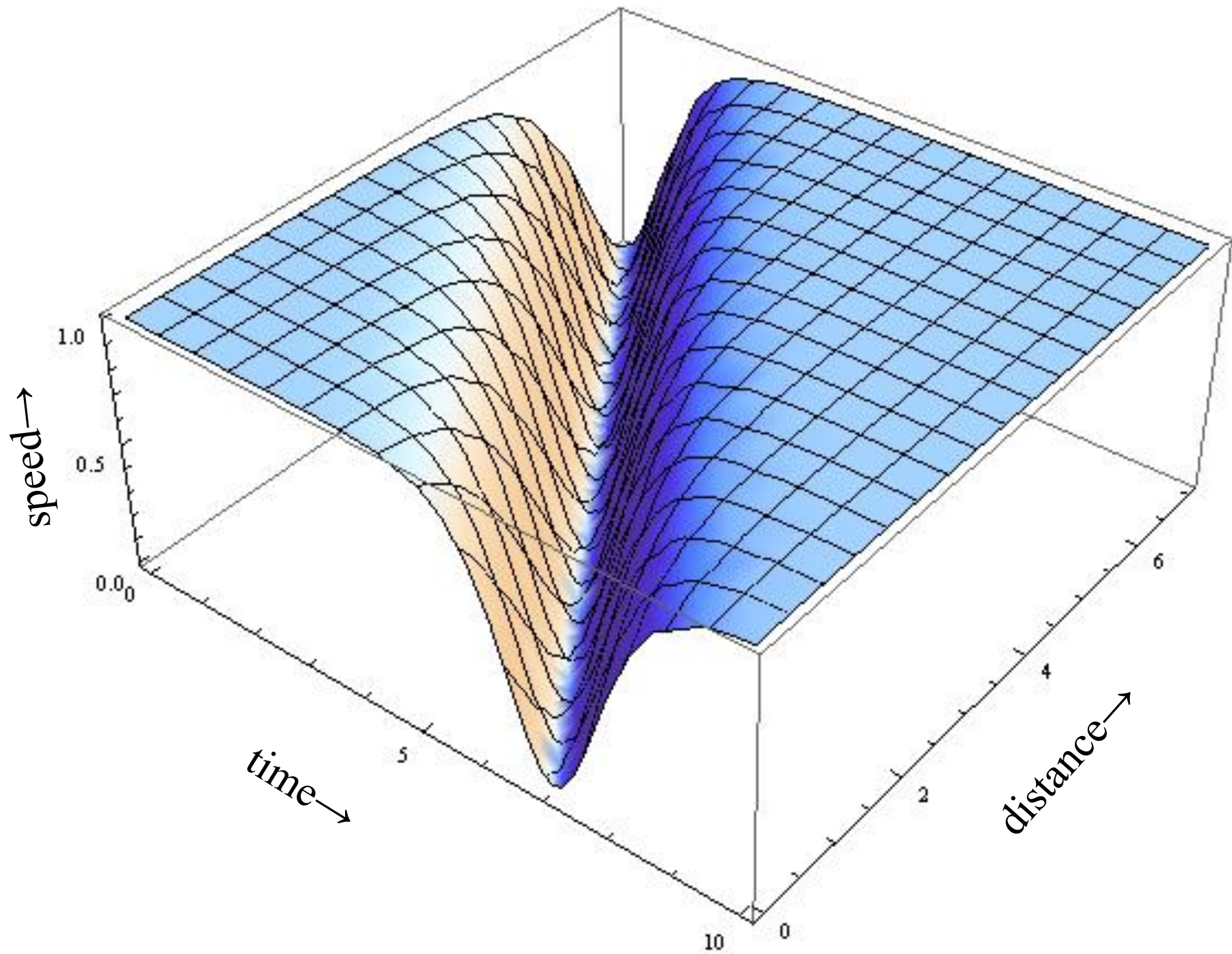
gives

$$u_{zz} = -2N \frac{1 - 2 \cosh^2 z \text{ th}^2 z}{\cosh^4 z} = -\frac{6}{N} u^2 + 4u$$

and leads to $\frac{\omega}{\kappa} = 4\beta \kappa^2$, $\frac{\alpha}{2} = \beta \kappa^2 \frac{6}{N}$

As simple case the following parameter set is

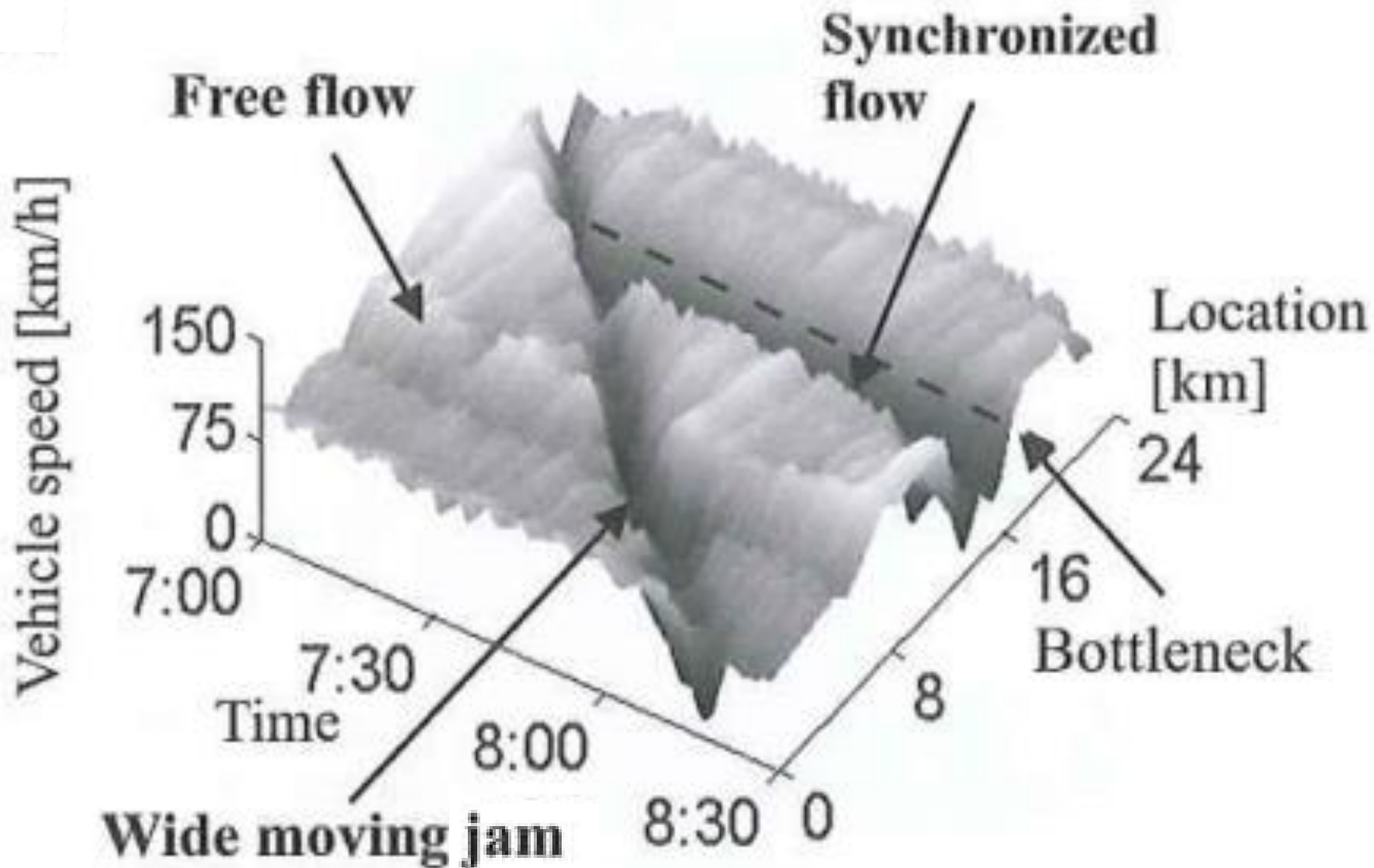
chosen $\alpha = 6$ $\beta = 1$ $N = 2\kappa^2$ $\omega = 4\kappa^3$



This result fits excellently with the empirically observed data from vehicle probes or inductive loops in very dense traffic situations.

These data of the spatio-temporal patterns allow the determination of the parameters like backwards speed and breakdown amplitude and make the perturbation approach very reasonable.

Traffic patterns from free flow to very dense*)



*) Kerner, B., et al. Methods for tracing and forecasting congested traffic patterns, Traffic Engineering & Control 42, pp282-287, 2001

The multi-soliton solution of the original Korteweg-de Vries equation

$$u_t + 6uu_x - u_{xxx} = 0$$

can be obtained under proper initial conditions and under the boundary conditions $u=0$ for $x \rightarrow \pm\infty$ as shown in the above inverse scattering theory section, or when we set

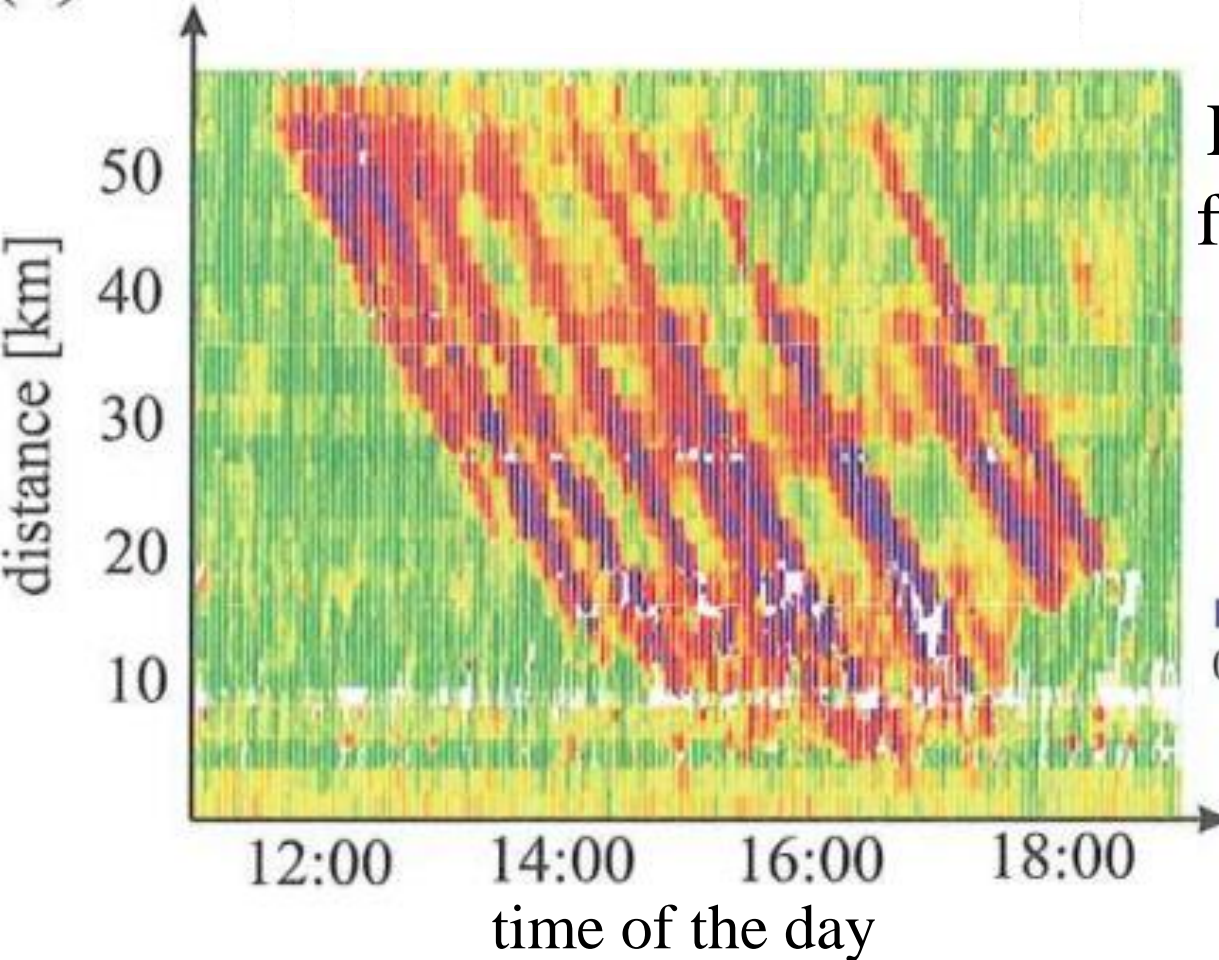
$$u = -2 \left(\ln f(x, t) \right)_{xx}$$

$$f(x, t) = \det(M)$$

$$M_{i,j}(x, t) = \delta_{i,j} + \frac{2\sqrt{\kappa_i \kappa_j}}{\kappa_i + \kappa_j} e^{\frac{1}{2}(z_i + z_j)}$$

$$z_i = \kappa_i (x - x_i^0) + \kappa_i^3 t$$

with the collective coordinates $z_i = \kappa_i (x - x_i^0) + \omega_i t = \kappa_i (x - x_i^0) + \kappa_i^3 t$ as the only independent variables.

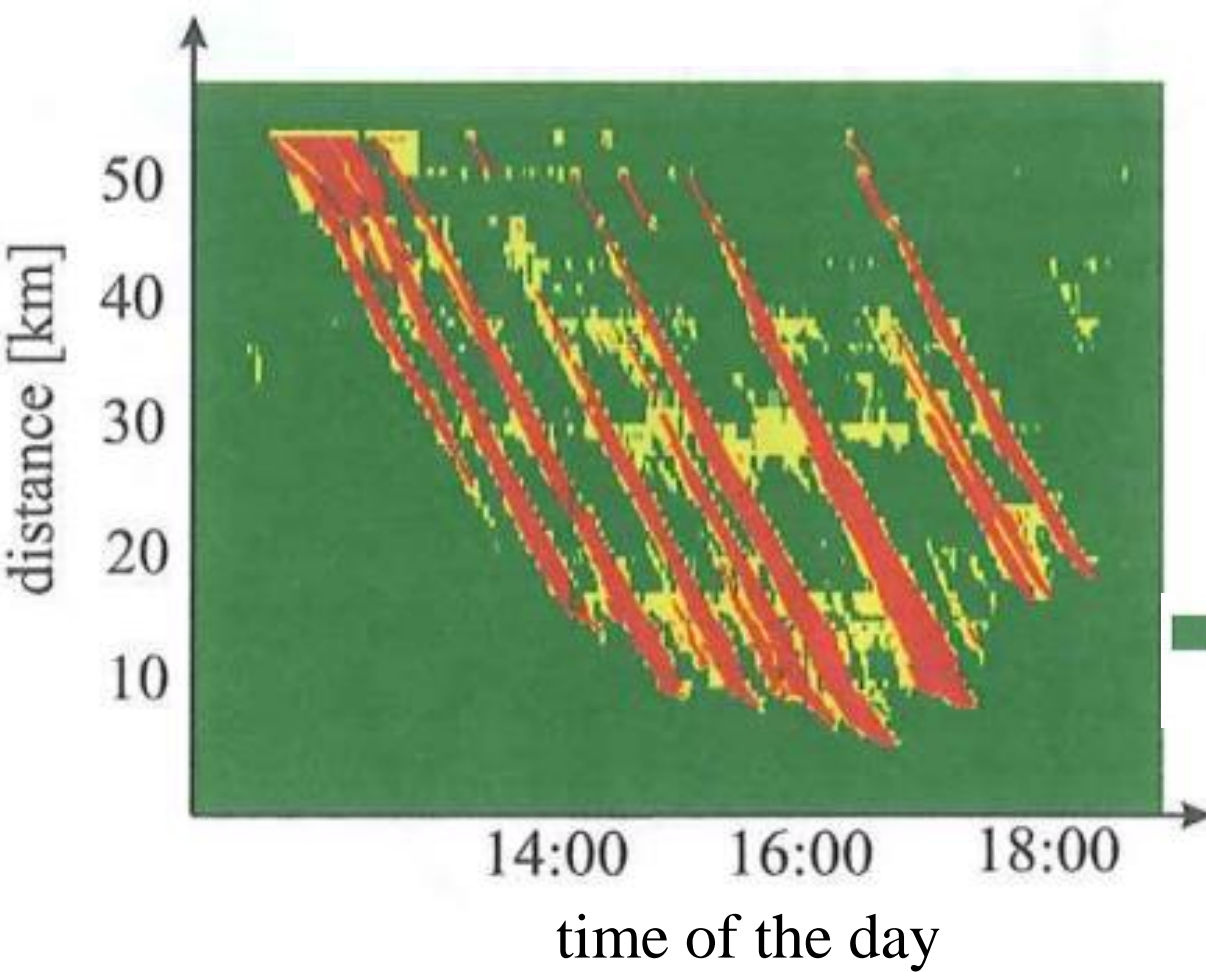


Distance-time patterns
from probe vehicle data
autobahn A5 North
May 12, 2010

Multi-soliton solutions as explanation for distance
time pattern with several wide moving jams

R.-P. Schäfer et al., "A study about probe vehicle data to verify the three-
phase traffic theory".

Traffic Engineering and Control, Vol 52, No 5, Pages 225-231, 2011



Distance-time patterns
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Free Flow Synchronised flow
Wide moving jam

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