A Simple application of orthogonal polynomials to Physics

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Review QM

WAVE FUNCTIONS (STATES): $\varphi_n(x)$ (or ket $|n\rangle$)
OPERATORS: Hamiltonian, transition operators.

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x).$$

(Independent of time) Schroedinger eq.:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\varphi_n(x) = E_n\varphi_n(x)$$

plus the corresponding boundary conditions PROVIDE $\varphi_n(x)$:

- finite
- single valued
- continuous

Normalization:

$$\int_{\text{all space}} dx\ \varphi_n^*(x)\varphi_m(x) = \delta_{n,m}$$

Algebraic approach to QM

If the potential is independent on time, the Schroedinger equation to be solved is the eigenvalue equation

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x)$$

$\hat{H}$ is the system Hamiltonian which contains the kinetic energy and the potential energy

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x).$$

For a general potential, one has to solve the corresponding differential equation.
An alternative to this method is the algebraic approach. This is based on the following simple idea. Suposse an operator $\hat{A}$ defined in a given vectorial space of dimension 2 and we have to solve the eigenvalue problem

$$\hat{A}\ \vec{u}_n = \lambda_n\ \vec{u}_n,$$

Algebraic approach...continue

One can consider a basis $\{\vec{e}_1, \vec{e}_2\}$ of the vector space. The action of $\hat{A}$ on the basis vectors will be:

$$\begin{aligned} \hat{A}\ \vec{e}_1 &= a\ \vec{e}_1 + b\ \vec{e}_2, \\ \hat{A}\ \vec{e}_2 &= c\ \vec{e}_1 + d\ \vec{e}_2. \end{aligned}$$

The eigenstates $\vec{u}$ will be linear combinations of the basis vectors

$$\vec{u} = u_1\ \vec{e}_1 + u_2\ \vec{e}_2.$$

Thus, finding the $\hat{A}$ eigenvectors, $\vec{u}$, is equivalent to getting the coefficients u_1 y u_2 in the given basis.
All the above can be written in matrix form

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}.$$

Algebraic approach...continue

Consequently, solving the eigenvalue problem $\hat{A}\vec{u} = \lambda\vec{u}$ is equivalent to diagonalize the matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \vec{e}_1 \cdot \hat{A}\vec{e}_1 & \vec{e}_2 \cdot \hat{A}\vec{e}_1 \\ \vec{e}_1 \cdot \hat{A}\vec{e}_2 & \vec{e}_2 \cdot \hat{A}\vec{e}_2 \end{pmatrix} \equiv \begin{pmatrix} \hat{A}_{1,1} & \hat{A}_{1,2} \\ \hat{A}_{2,1} & \hat{A}_{2,2} \end{pmatrix}$$

Lets go now to our problem of solving the time independent Schroedinger equation: $\hat{A} = \hat{H}$.

$$\hat{H}\varphi_k = E_k\varphi_k \ .$$

Following what we have discussed above, what we need is a basis of the Hilbert space of the problem: $\{\phi_n\}$, with $n = 1, 2, \ldots$. The $\hat{H}$ eigenstates, φ_k, can be written as a linear combination of basis states $\{\phi_n\}$:

$$\varphi_k = \sum_{n=1}^{\infty} c_n^{(k)} \phi_n.$$

Algebraic approach...continue

Putting this last expanssion into the Schrödinger equation:

$$H\sum_{n=1}^{\infty} c_n^{(k)}\phi_n = E_k \sum_{n=1}^{\infty} c_n^{(k)}\phi_n,$$

bring us to the conclusion that getting the eigenstates $\{\varphi_k\}$ is equivalent to determining the expanssion coefficients in the selected basis, $\{c_n^{(k)}\}$.
Left multiplication of the last equation by an arbitrary element of the basis ϕ_m^* and integration to the whole space give (Dirac notation: $\phi_n \longrightarrow |n\rangle$)

$$\sum_{n=1}^{\infty} c_n^{(k)}\langle m|H|n\rangle = E_k \sum_{n=1}^{\infty} c_n^{(k)}\langle m|n\rangle = E_k c_m^{(k)},$$

$$\int dV\ \phi_m^*\phi_n \quad \longrightarrow \quad \langle m|n\rangle,$$

$$\int dV\ \phi_m^* H\phi_n \quad \longrightarrow \quad \langle m|H|n\rangle.$$

The preceding equation can be written in matrix notation as ($H_{nm} \equiv \langle n|H|m\rangle$)

$$\begin{pmatrix} H_{1,1} & H_{1,2} & H_{1,3} & \dots \\ H_{2,1} & H_{2,2} & H_{2,3} & \dots \\ H_{3,1} & H_{3,2} & H_{3,3} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1^{(k)} \\ c_2^{(k)} \\ c_3^{(k)} \\ \vdots \end{pmatrix} = E_k \begin{pmatrix} c_1^{(k)} \\ c_2^{(k)} \\ c_3^{(k)} \\ \vdots \end{pmatrix}$$

CONCLUSION: Solving the time independent Schrödinger equation is equivalent to diagonalize the Hamiltonian matrix in a basis of the Hilbert space of the problem

$$\begin{pmatrix} H_{1,1} & H_{1,2} & H_{1,3} & \dots \\ H_{2,1} & H_{2,2} & H_{2,3} & \dots \\ H_{3,1} & H_{3,2} & H_{3,3} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

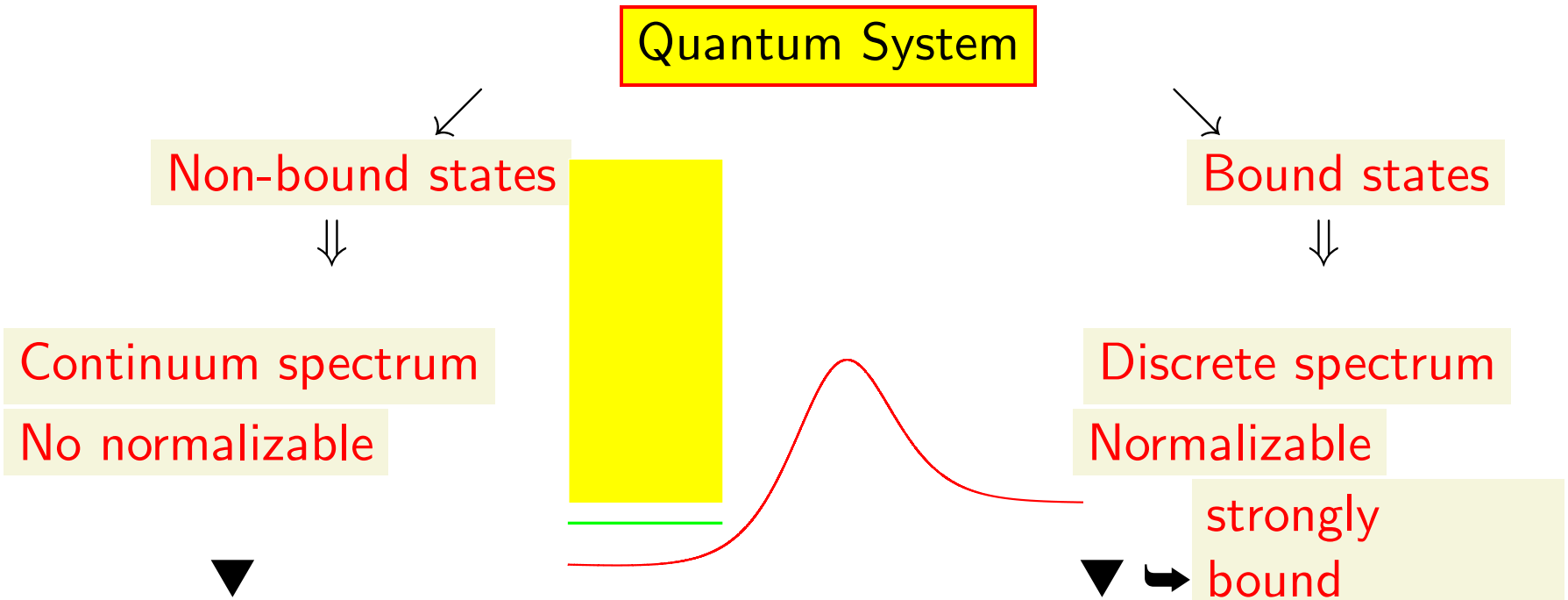
One can choose any appropriate basis !!!.

Weakly bound systems

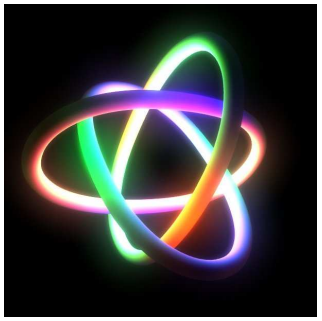
For any realistic composite quantum mechanical system (atoms, molecules, nuclei, ...) the treatment of the continuous part of the spectrum is a difficult task.
Weakly-bound systems: both bound and unbound states have to be treated on equal footing

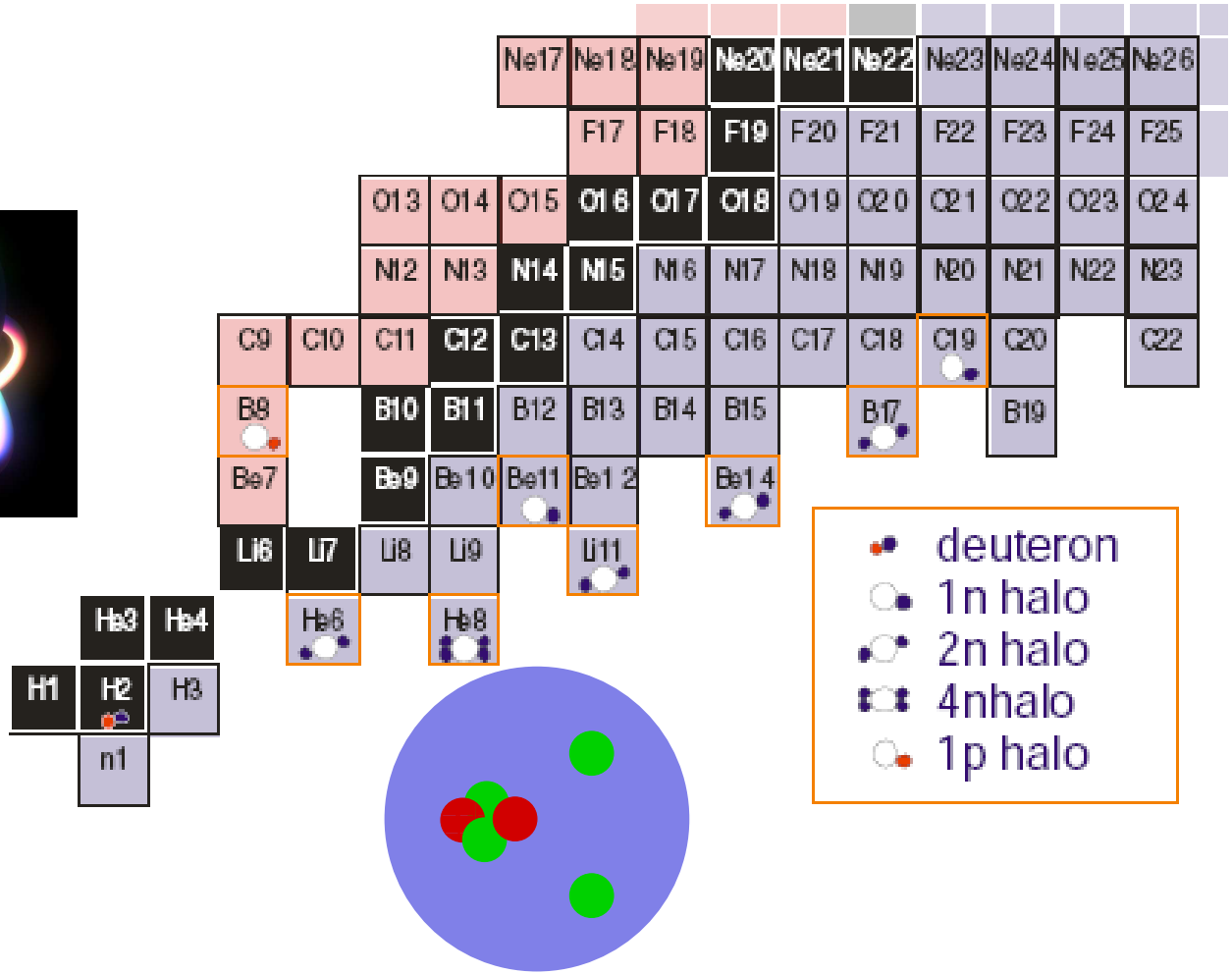
- The continuum wave functions depend on a continuously varying parameter (the energy or the wave number) and are not normalizable, which make them awkward for actual applications.
- Explicit inclusion of the continuum states in structure or reaction calculations requires a discretization of the continuum $\Rightarrow$ the continuum is substituted by a discrete set of normalizable states which becomes a complete set as the number of states considered tends to infinity.

Scheme


Quantum System
Non-bound states
Bound states
Continuum spectrum
No normalizable
Discrete spectrum
Normalizable
strongly bound system
weakly bound system
Discretization method ◆ OP

Motivation




Ne17 Ne18 Ne19 Ne20 Ne21 Ne22 Ne23 Ne24 Ne25 Ne26
F17 F18 F19 F20 F21 F22 F23 F24 F25
O13 O14 O15 O16 O17 O18 O19 O20 O21 O22 O23 O24
N12 N13 N14 N15 N16 N17 N18 N19 N20 N21 N22 N23
C9 C10 C11 C12 C13 C14 C15 C16 C17 C18 C19 C20 C22
B8 B10 B11 B12 B13 B14 B15 B17 B19
Be7 Be9 Be10 Be11 Be12 Be14
Li6 Li7 Li8 Li9 Li11
He3 He4 He6 He8
H1 H2 H3
n1
deuteron
1n halo
2n halo
4nhalo
1p halo

The Schroedinger equation

If the potential is independent on time, the Schroedinger equation to be solved is the eigenvalue equation

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x)$$

$\hat{H}$ is the system Hamiltonian which contains the kinetic energy and the potential energy

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x).$$

For a general potential, one has to solve the corresponding differential equation. General potentials $V(x)$ have both types of solutions: i) discrete and normalizable, and ii) continuous and non-normalizable.

- When treating deeply bound states the approximation of considering just the discrete states is reasonably good
- However, for loosely bound states the continuous part has to be necesarily included.

The solution of the Schroedinger equation (including the appropriate boundary conditions)

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x)$$

provide the eigenvalues, *energies*, and eigenfunctions, $\{\varphi_n(x)\}$. these are orthogonal in the sense

$$\int_{\text{all space}} dx\varphi_n^*(x)\varphi_m(x) = \delta_{n,m}$$

$\{\varphi_n(x)\}$ is a basis for the Hilbert space of the problem (include all eigenstates, discrete and continuous).

Sometimes the solution of the differential equation is difficult $\Rightarrow$ ALTERNATIVE!

Classical orthogonal polynomials

A system of polyomials $P_n(x)$ (degree n) is called orthogonal in an interval $a \leq x \leq b$, with respect to a weight function $\omega(x)$, if

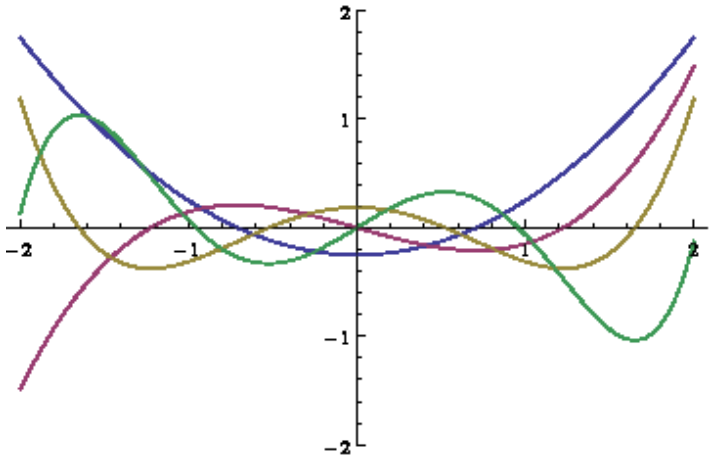
$$\int_a^b dx\ \omega(x) P_n(x) P_m(x) = 0 \qquad n \neq m \qquad n, m = 0, 1, 2, \cdots$$

$\omega(x)$ determines the polynomials up to a constant factor for each polynomial in the family. The specification of these coefficients is known as standarization.

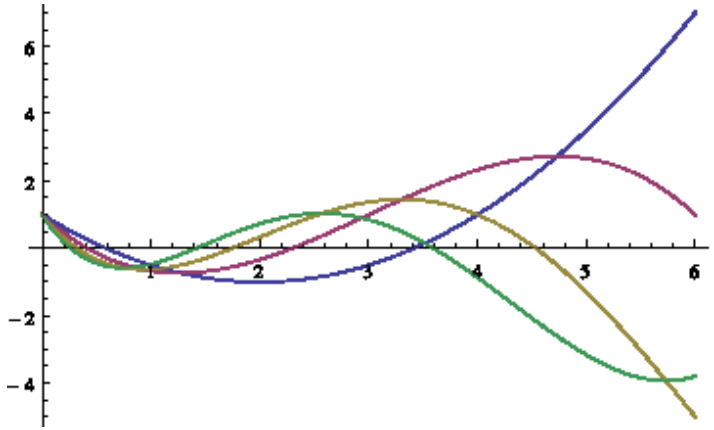
Examples:

name	$\omega(x)$	(a, b)
Hermite $H_n(x)$	e^{-x^2}	$(-\infty, +\infty)$
Laguerre $L_n(x)$	e^{-x}	$(0, +\infty)$
Laguerre generalized $L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$(0, +\infty)$
Gegenbauer $C_n^{(\alpha)}(x)$	$(1-x^2)^{\alpha-1/2}$	$(-1, 1)$

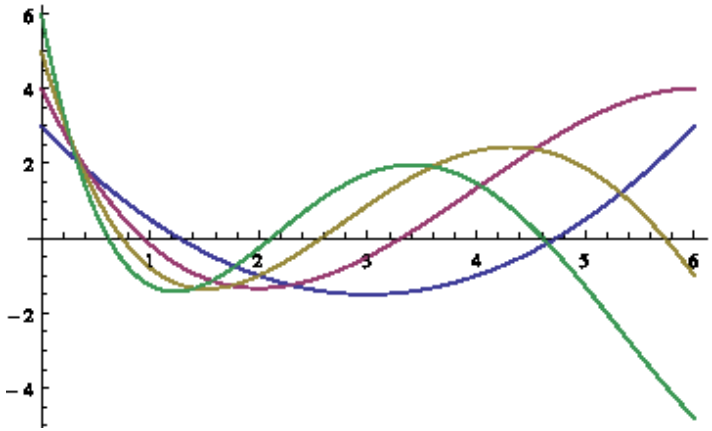
Figures



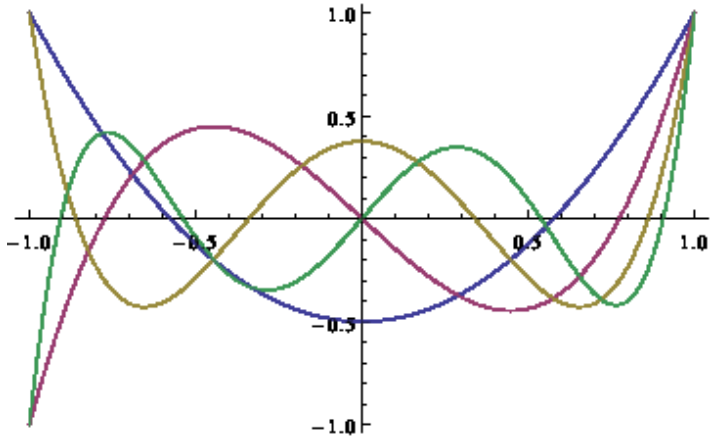
Hermite/n^3, n=2-5



Laguerre, n=2-5



Generalized Laguerre, $\alpha = 1$, n=2-5



Gegenbauer, $\alpha = 0{,}5$, n=2-5

1D case: orthogonal polynomials

A one-dimensional hamiltonian:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + v(x) \quad ,$$

The ground state wave function $\varphi_0(x)$ is known, either analytically or numerically,

$$H\varphi_0(x) = e_0\varphi_0(x) \quad .$$

Define a weight function $\omega(s)$ as

$$\omega(s) = \frac{dx}{ds}\,|\varphi_0(x)|^2 \quad ,$$

$s(x)$ is an arbitrary function continuous, single-valued, and monotonously increasing or decreasing, taking values in an interval $[a, b]$

1D case: orthogonal polynomials II

Defined interval and weight function, construct a family of orthogonal polynomials $\{P_n(s); n = 0, 1, 2, \dots\}$ that fulfill

$$\int_a^b ds\ \omega(s) P_n(s) P_m(s) = \frac{1}{\mathcal{N}_n \mathcal{N}_m} \delta_{n,m} \quad .$$

From these polynomials and the ground state wave function, it is straightforward to construct a set of orthonormal wave functions

$$\phi_m(x) = \langle x | OP, n \rangle = \mathcal{N}_m \varphi_0(x) P_m(s(x)) \quad ,$$

that fulfill

$$\int_{-\infty}^{+\infty} dx\ \phi_m^*(x) \phi_n(x) = \delta_{n,m} \quad .$$

The functions $\phi_n(x)$, excepting $\phi_0(x)$ which is actually the ground state wave function, are not eigenfunctions of the hamiltonian, but constitute a basis in which the hamiltonian can be diagonalized.

Examples: Trivial orthogonal polynomials

1. Trivial weight: $s = x$. The ground state wave function in terms of s is just $\varphi_0(x)$. The weight function is

$$\omega(x) = |\varphi_0(x)|^2.$$

Orthogonal polynomials, $P_n(x)$, in the interval $(-\infty, +\infty)$ with respect to this weight function can be found by a Gram-Schmidt procedure. From these and the ground state wave function, the basis wave functions are obtained as

$$\phi_n^{TOP}(x) = \mathcal{N}_n \varphi_0(x) P_n(x).$$

$P_n(x)$ can be written

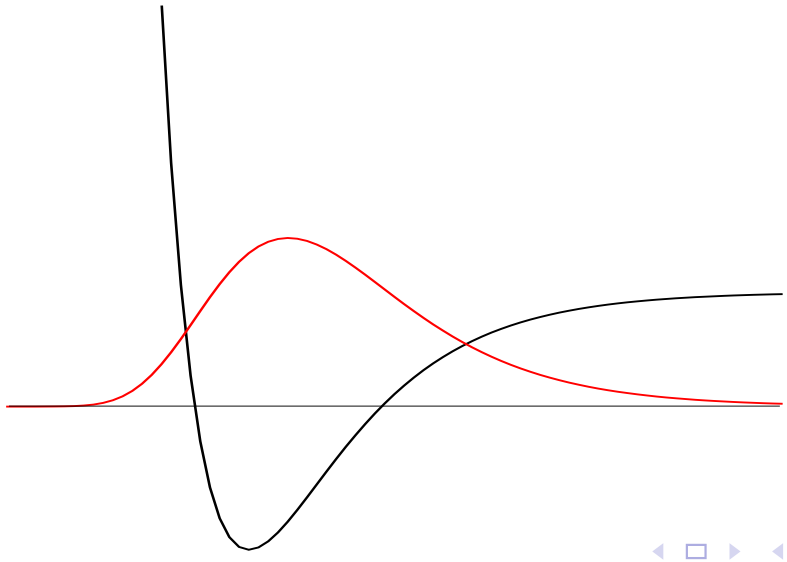
$$P_n(x) = \sum_{k=0}^{n} C_{n,k} x^k.$$

NOP: Morse

1. The Morse potential is

$$v(x) = D\left((1-\exp(-x))^2 - 1\right) \; ; D = \frac{1}{2}\left(j+\frac{1}{2}\right)^2,$$

   1. $s = (2j+1)\exp[-x]$
   2. weight: $\omega(s) = \frac{1}{\Gamma[2j]} s^{2j-1}\exp[-s]$
   3. interval: $[0,\infty)$.
   4. Laguerre polynomials $L_n^{(2j-1)}(s)$,

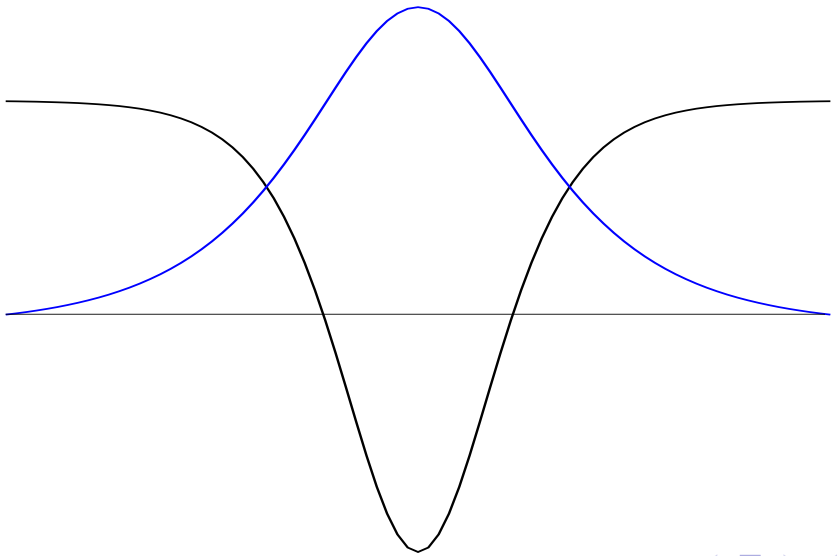


NOP: Poeschl-Teller

1. The Pöschl-Teller potential

$$v(x) = -D\,\frac{1}{\cosh^2(x)}\;;\; D=\frac{1}{2}j(j+1)$$

   1. $s=\tanh[x]$
   2. weight: $\omega(s)=\frac{(2j-1)!!}{2^j(j-1)!}\,(1-s^2)^{j-1}$
   3. interval: $(-1,1)$.
   4. Gegenbauer polynomials $C_n^{(j-1/2)}(s)$,



Continuum discretization with THO

One-dimensional weakly bound system with hamiltonian

$$h = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + v(x)$$

- x: relative coordinate of two particles.
- m: reduced mass.
- $v(x)$: interaction between both particles.

We assume only one bound state:

$$h\psi_B(x) = E_B\psi_B(x)$$

Objective

Develop a procedure to describe approximately the states in the continuum by means of a *finite number of normalizable states*.

THO method (1D)

1. THO: the local scale transformation transforms the ground state wave function in the ground state wave function of a harmonic oscillator

$$\int_{-\infty}^{x} |\varphi_0(x')|^2 dx' = \int_{-\infty}^{s} |\phi_0^{HO}(s')|^2 ds' = \frac{1+\mathrm{erf}(s)}{2} \quad .$$

Direct integration provides $s(x)$. THO basis: $\omega(s) = e^{-s^2}$, interval $(-\infty, +\infty) \Rightarrow$ relevant polynomials are Hermite).

$$\phi_n^{THO}(x) = \mathcal{N}_n \varphi_0(x) H_n(s(x)),$$

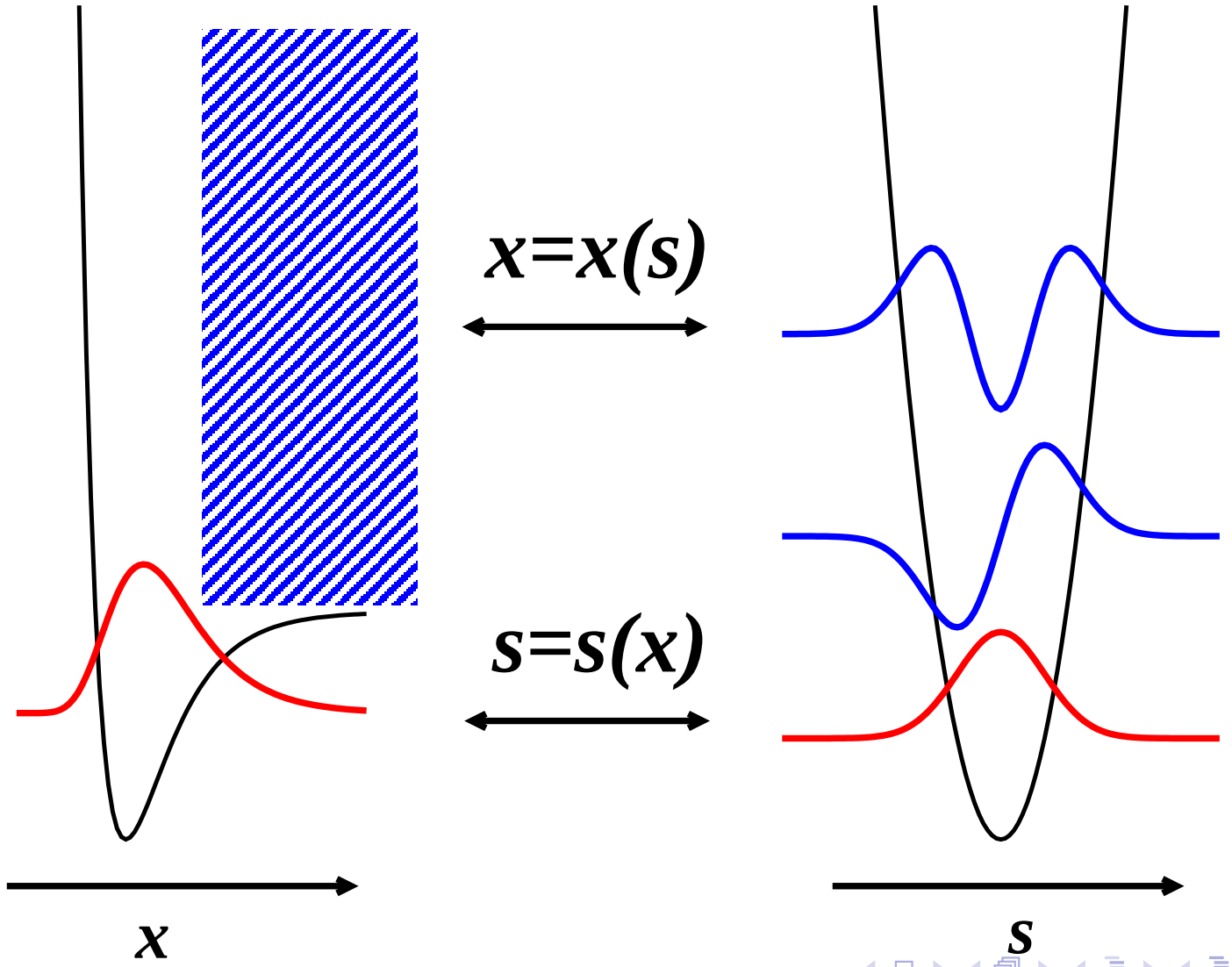
2. If x-values restricted to positive values,

$$\int_{0}^{x} |\varphi_0(x')|^2 dx' = \int_{0}^{s} |\phi_0^{HO}(s')|^2 ds'.$$

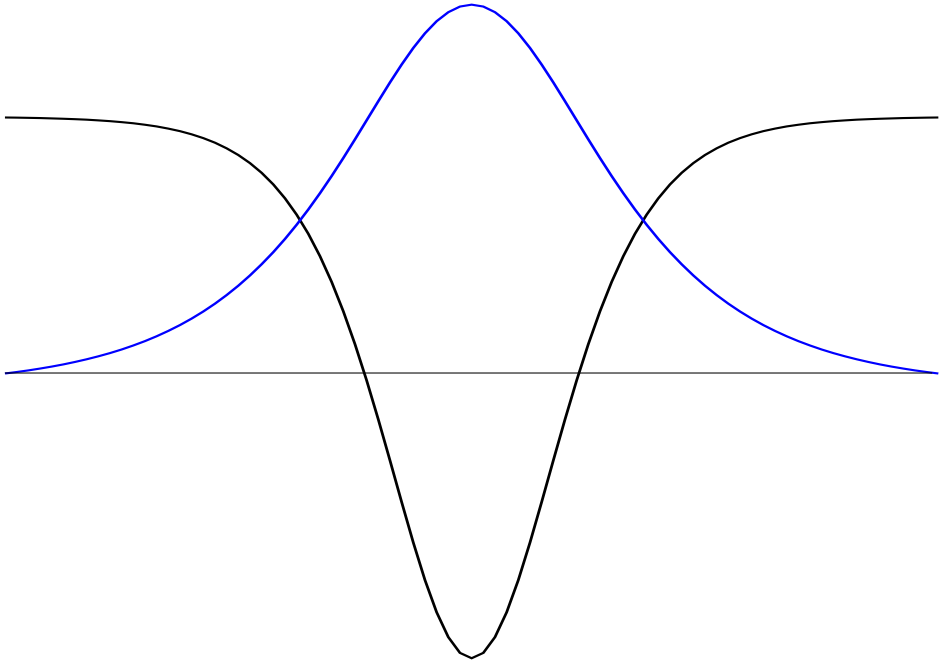
THO basis (relevant polynomials are generalized Laguerre in $s(x)^2$).

$$\phi_n^{THO'}(x) = \mathcal{N}'_n \varphi_0(x) L_n^{1/2}((s(x))^2),$$

The LST for HO $\Rightarrow$ THO method



Poeschl-Teller Potential



$$V(x) = -D \frac{1}{\cosh^2(\alpha x)}$$

THO basis for PT potential

$$\frac{\exp(-s^2)}{\sqrt{\pi}}ds = \frac{1}{2cosh^2(x)}dx$$

$$tanh(x) = erf(s)$$

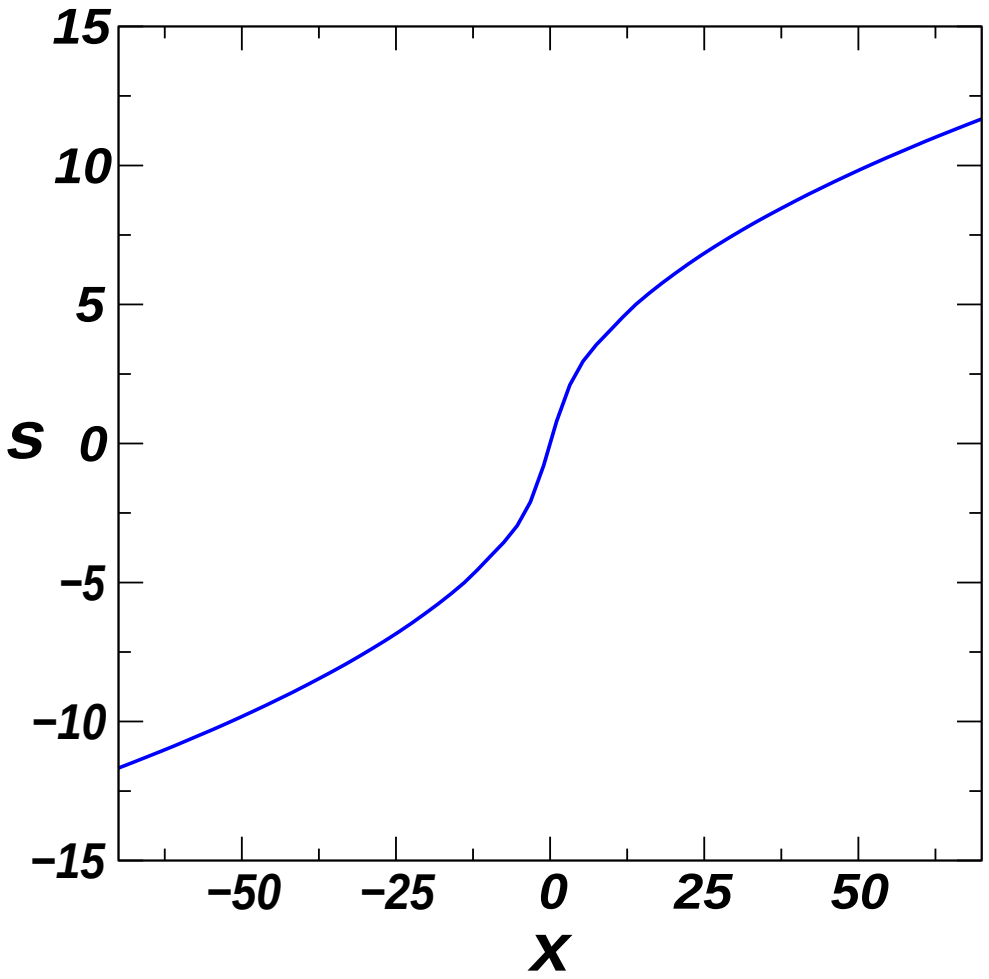
$$\frac{ds}{dx} = \frac{\sqrt{\pi}}{2}\exp(-s^2)(1 - erf^2(s))$$

$$\varphi_n^{THO}(x) = \langle x|\, THO, n\rangle = \mathcal{N}_n\varphi_0(x)H_n(s(x)) = \sqrt{\frac{ds}{dx}}\phi_n^{HO}(s(x))$$

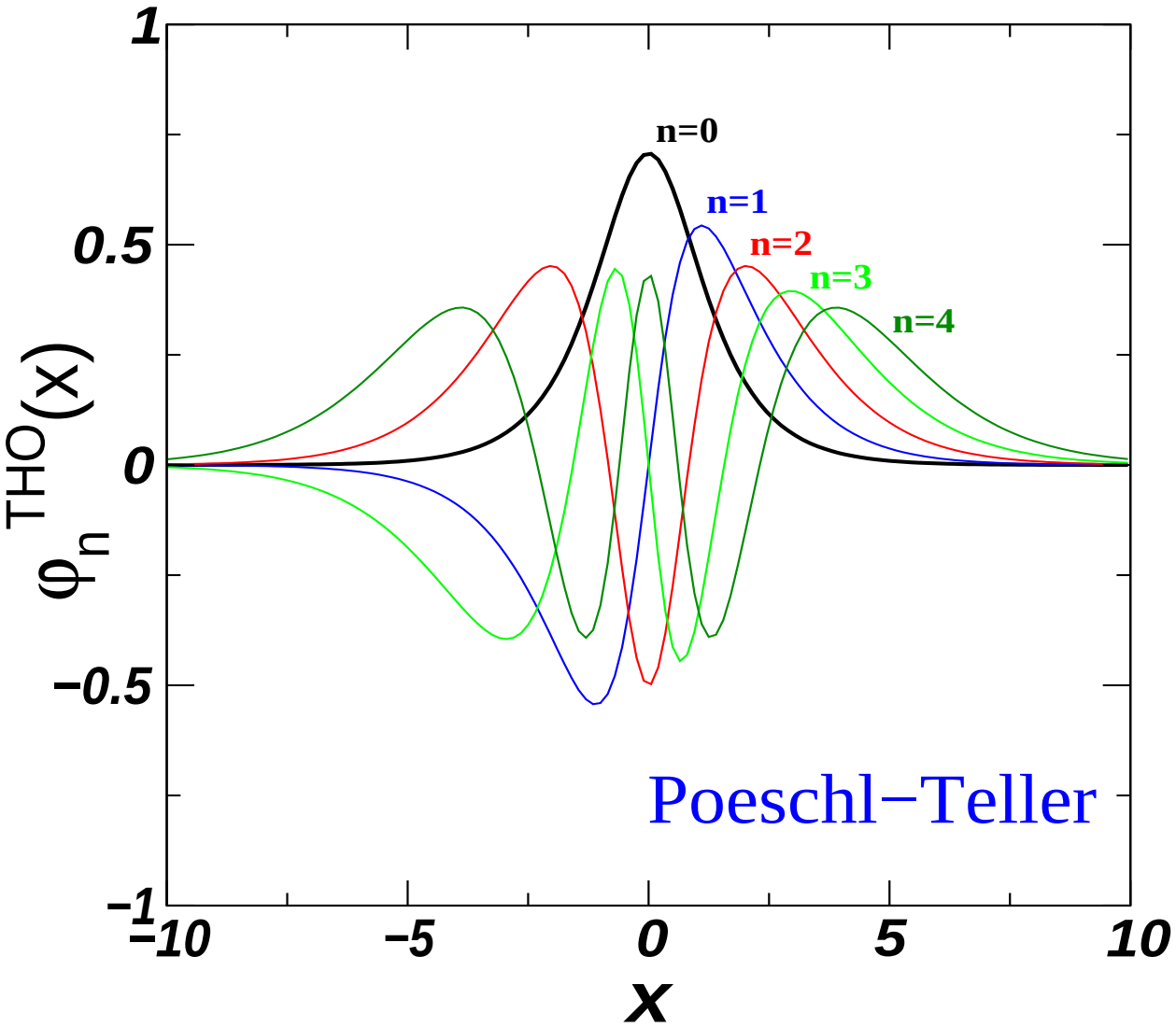
$$\phi_n^{HO}(s) = \mathcal{N}_n H_n(s)\exp(-s^2/2)$$

Orthonormal Basis : $\langle THO, m|\, THO, n\rangle = \delta_{n,m}$

Poeschl-Teller Potential



THO basis



Hamiltonian Diagonalization

$$\langle THO, n|H - E_B|THO, m\rangle = \int dx\, \varphi_n^{THO}(x)(H - E_B)\varphi_m^{THO}(x)$$

$$\langle THO, n|(h - E_B)|THO, m\rangle = \frac{2\hbar^2}{m} n\mathcal{N}_n m\mathcal{N}_m \int ds\ \exp(-s^2) H_{n-1}(s) H_{m-1}(s) \left(\frac{ds}{dx}\right)^2$$

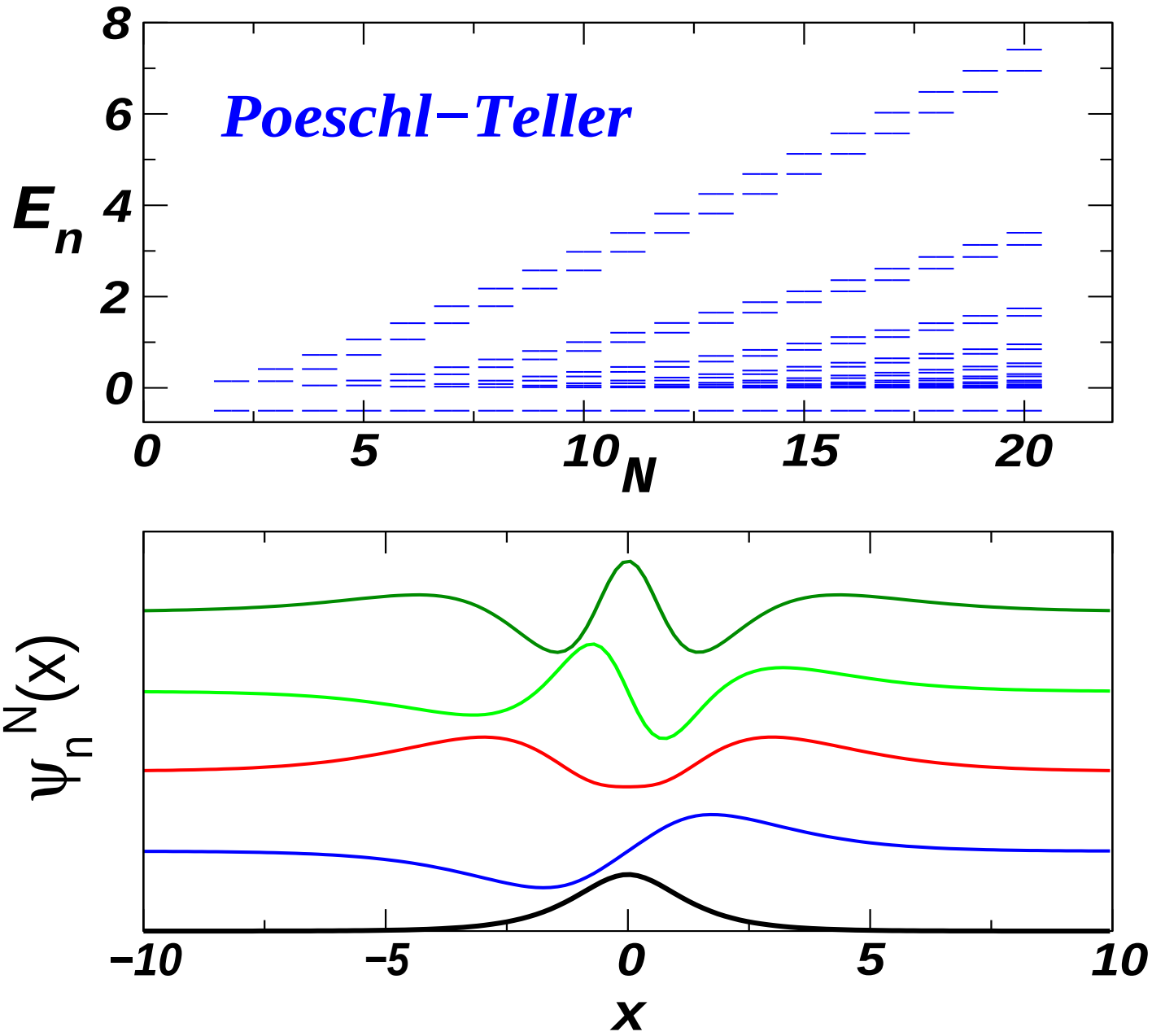
Hamiltonian Eigenstates

$|N,0\rangle = |THO, n=0\rangle \quad \rightarrow \quad$ Eigenstate with eigenvalue E_B.
If dimension of THO basis is restricted to N, we get $N-1$ other states with **positive** energies: $|N,i\rangle\,;\ i=1,\ldots,N-1$.

$$\begin{aligned} |N,0\rangle &= |THO,0\rangle \\ |N,i\rangle &= \sum_{j=1}^{N-1} |THO,j\rangle\langle THO,j|N,i\rangle \end{aligned}$$

$$\langle x|N,i\rangle = \psi_i^N(x) = \pi^{1/4} P_i^{N-1}(s(x))\varphi_0^{THO}(x)$$

$$P_i^{N-1}(s) = \sum_{j=1}^{N-1} \mathcal{N}_j H_j(s)\langle THO,j|N,i\rangle$$


Poeschl−Teller
E_n
N
$\psi_n^N(x)$
x

Checking the THO method: sum rules

Total strength

$$TS(O;N) = \sum_i |\langle N,i|O|N,0\rangle|^2$$

$$TS(O) = TS(O;N\to\infty) = \int dx\, O(x)^2 \varphi_0(x)^2$$

Energy weighted sum rule

$$EW(O;N) = \sum_i (E_i^N - E_B)|\langle N,i|O|N,0\rangle|^2$$

$$EW(O) = EW(O;N\to\infty) = \int dx\, (dO(x)/dx)^2 \varphi_0(x)^2$$

Cuadro: Sum rules results for $O = x$ and the Poeschl-Teller case.

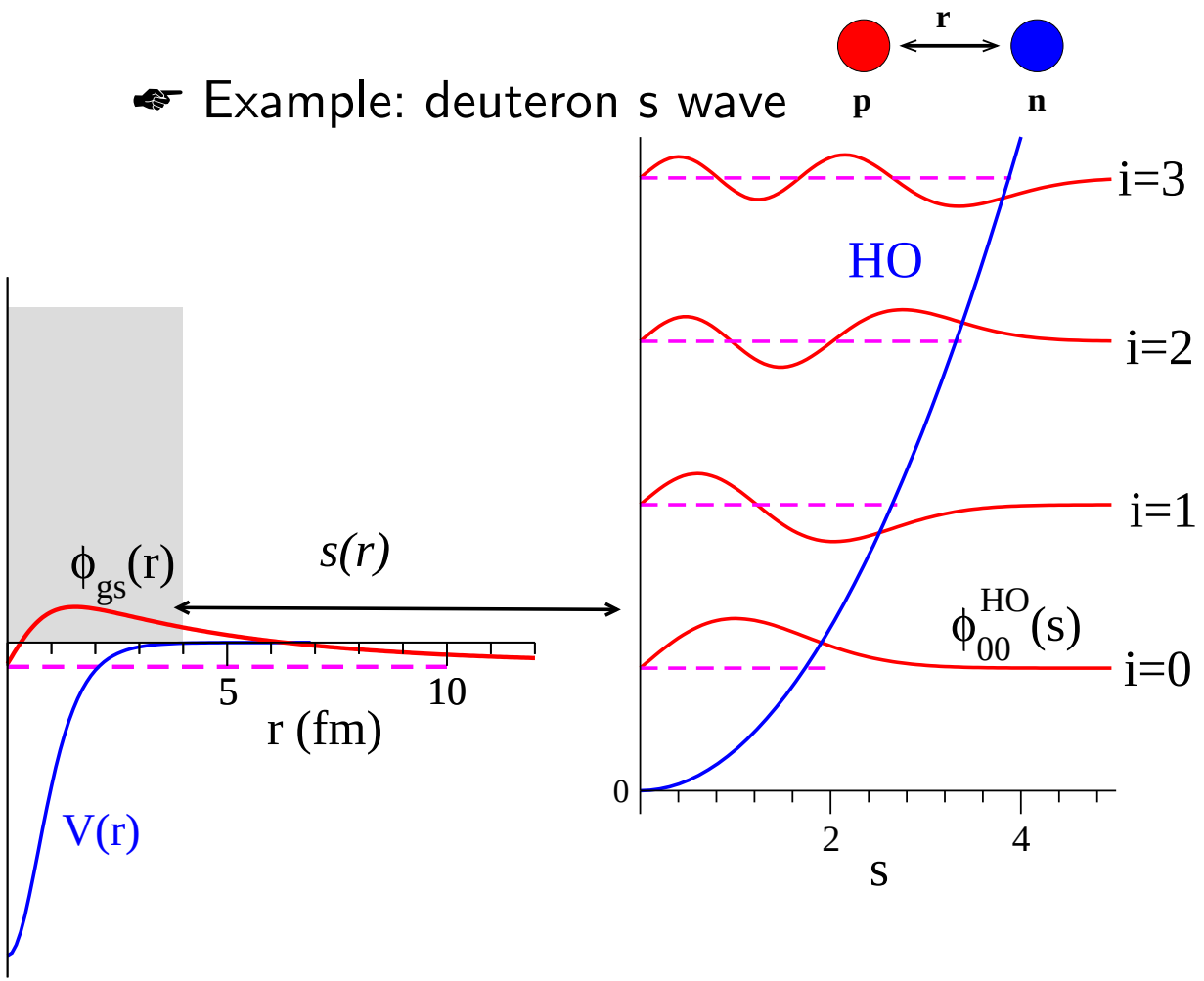
N	$TS(x,N)$	$EW(x,N)$	$PO(x,N)$
3	0,82245	1,05418	1,26254
5	0,822467	1,00068	1,42050
9	–	1,00000	1,42350
	$TS(x)$	$EW(x)$	$PO(x)$
	0,822467	1,00000	1,42350

Cuadro: Sum rules results for $O = V(x)$ and the Poeschl-Teller case.

N	$TS(V,N)$	$EW(V,N)$	$PO(V,N)$
4	0,527628	0,216765	0,0740682
10	0,533187	0,297387	–
16	0,533328	0,304192	–
	$TS(V)$	$EW(V)$	$PO(V)$
	0,533333	0,304762	0,0740741

3D case: THO two-body systems

☛ Example: deuteron s wave



$$\int_0^r dr' |\phi_{gs}(r')|^2 = \int_0^s ds' |\phi_{00}^{HO}(s')|^2$$

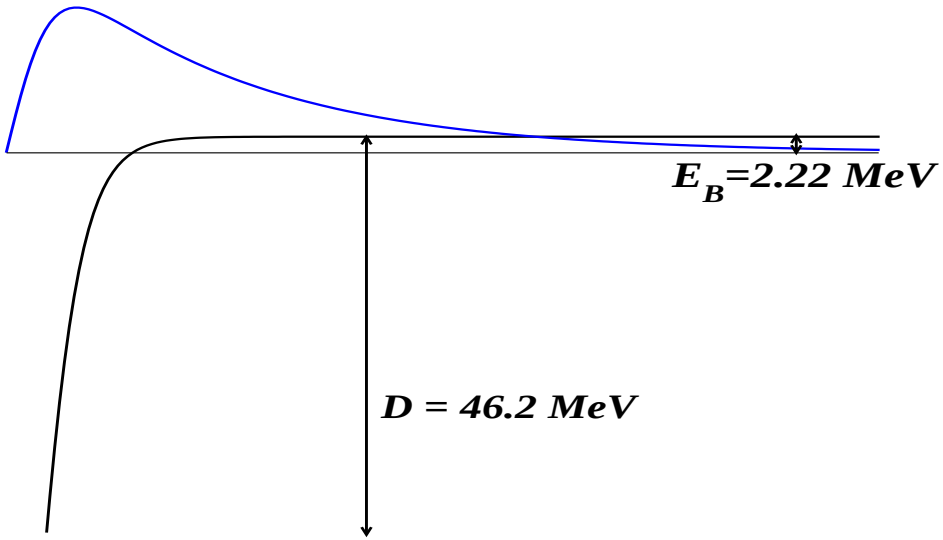
For central potentials the radial Schroedinger equation is:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)+\frac{\ell(\ell+1)\hbar^2}{2mr^2}\right]\varphi_{n\ell}(r)=E_{n\ell}\varphi_{n\ell}(r)$$

Now r goes from 0 to $+\infty$.

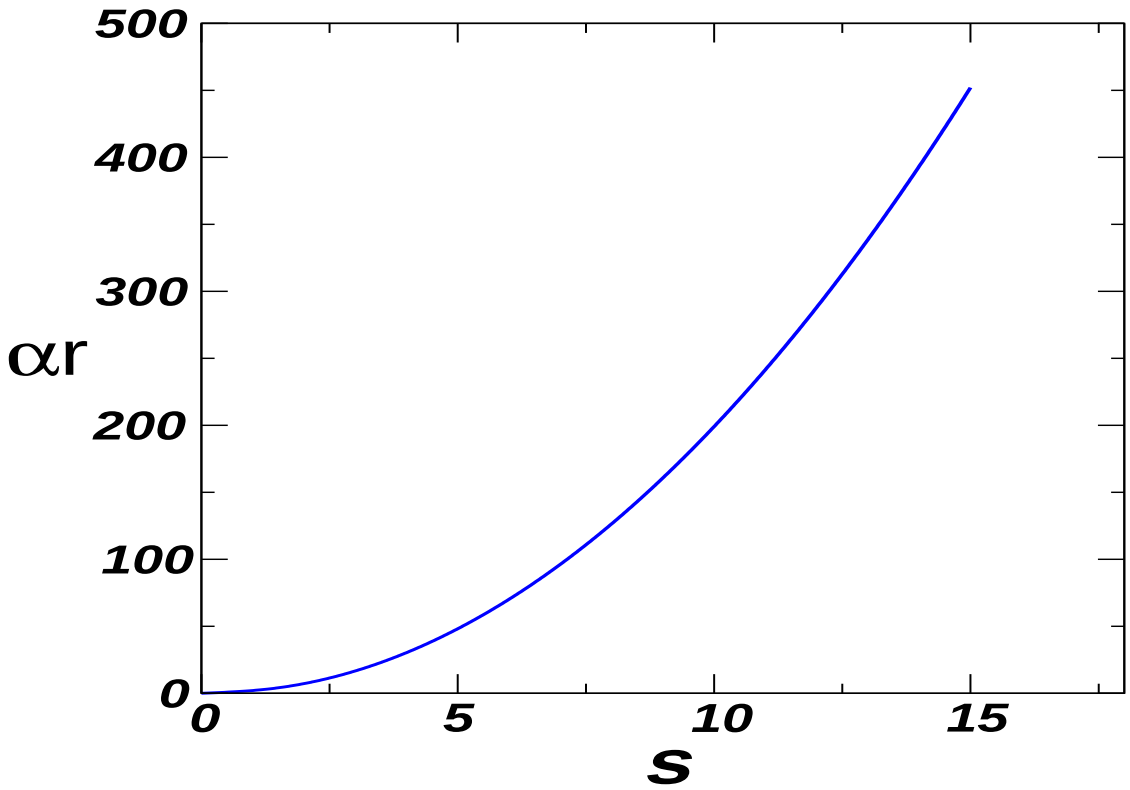
The angular part is given by the spherical harmonics $Y_{\ell,m}(\theta,\phi)$.

- $V(r) = -D\,\frac{1}{\cosh^2(\alpha r)}$; Poeschl-Teller Potential
- $j_D = 1{,}25$; $\alpha = 0{,}941\,fm^{-1}$; $y=\alpha r$
- $\varphi_0(y) = \sqrt{2(j_D-1)\Gamma(2j_D)}P_{j_D}^{-j_D+1}(tanh(y))$

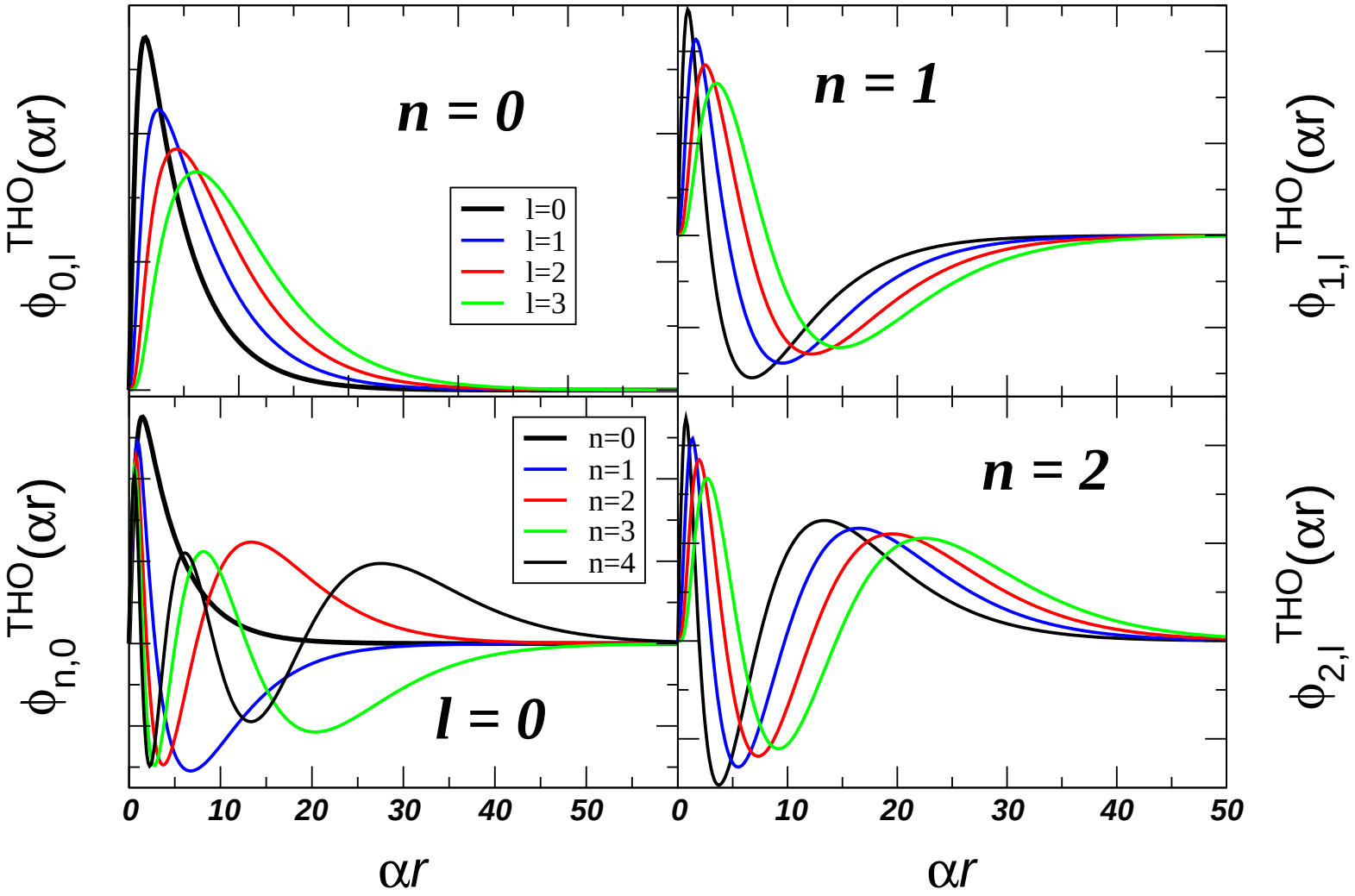


Change of coordinates

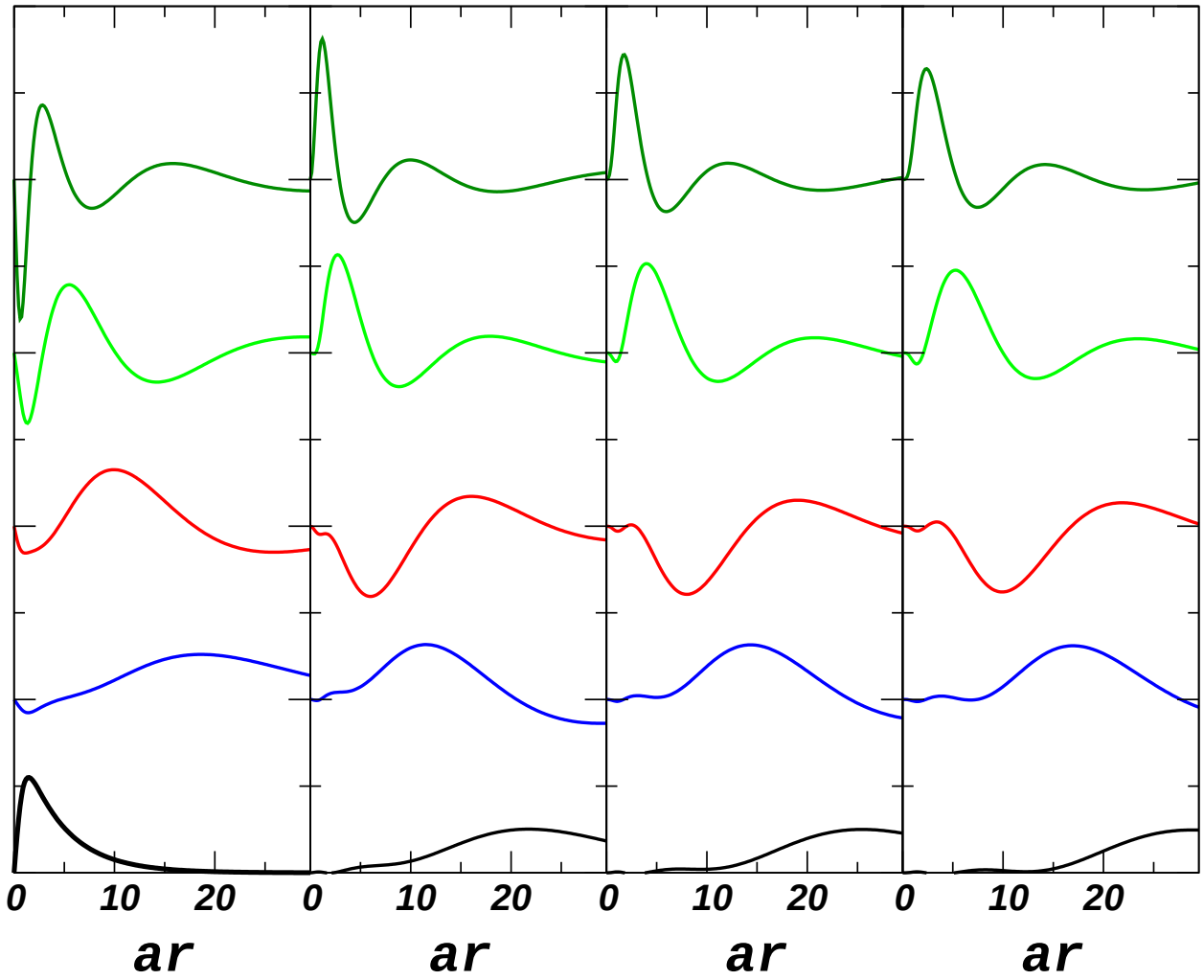
$$1 - \Gamma(2j_D)\,\exp(-2(j_D-1)y) = erf\,(s) - 2s\exp(-s^2)/\sqrt{\pi}$$

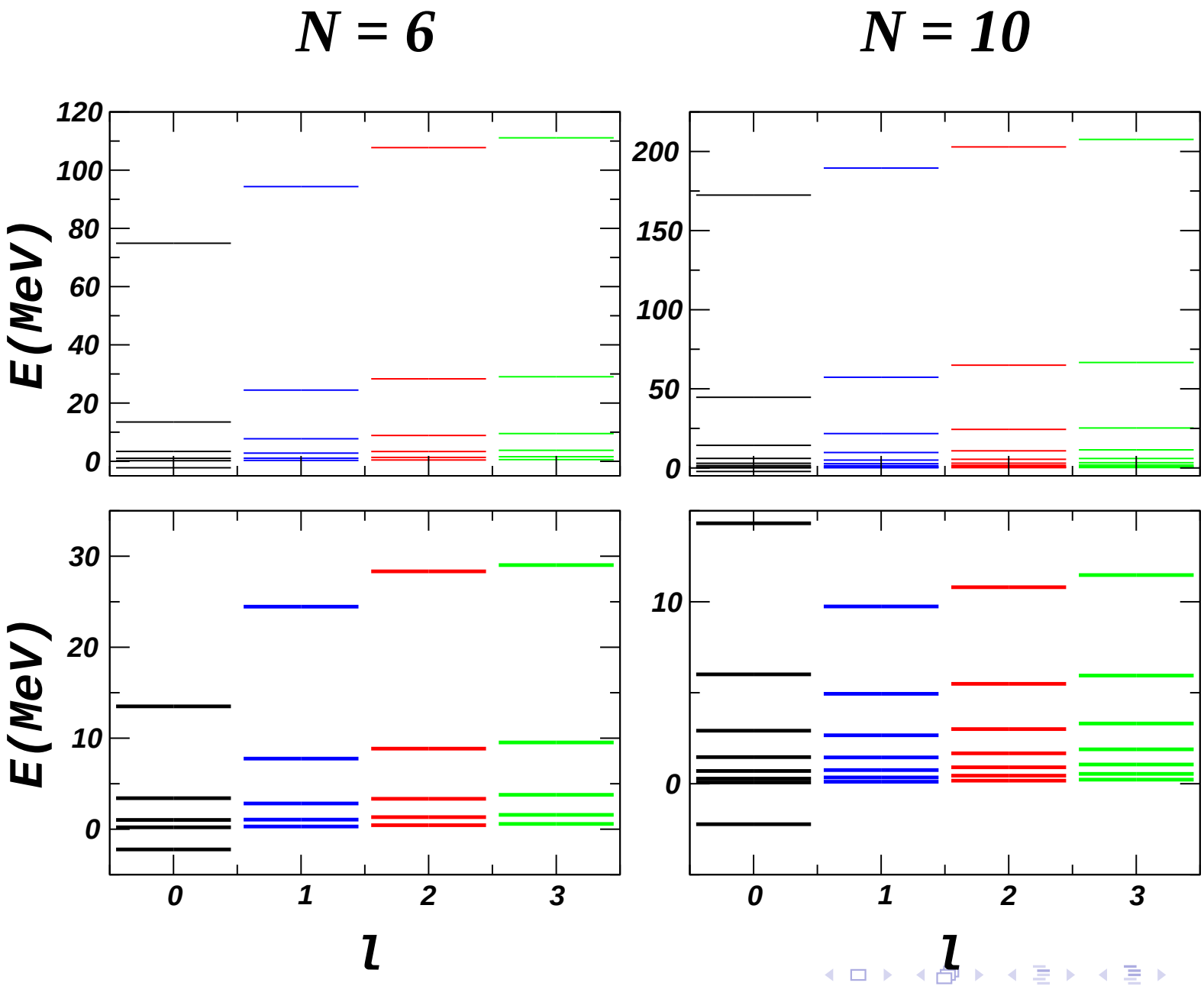


Deuteron THO basis



$\Psi^5_{n0}(ar)$ $\Psi^5_{n1}(ar)$ $\Psi^5_{n2}(ar)$ $\Psi^5_{n3}(ar)$




N = 6
N = 10
E (MeV)
E (MeV)
120
100
80
60
40
20
0
200
150
100
50
0
30
20
10
0
10
0
0
1
2
3
0
1
2
3
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Summary and Conclusions

- We have presented a method capable of an adequate description of the continuum states for both 1D and 3D weakly bound systems, providing a N dimensional orthonormal Transformed Harmonic Oscillator basis.
- The method presented has been applied to two 1D cases (Morse and Poeschl-Teller) and one 3D case (Deuteron as a Poeschl-Teller).
- The convergence of the method has been examined computing for increasing values of N the appropriate sum checks (TS,EWSR,PO) for different operators.
- This method can be envisaged as an alternative to the currently used descriptions for the continuum in coupled channels calculations.