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Exactly Solvable Anharmonic Potentials with Variable Bumps and Depths

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Before We Get Started...

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- What is my research?

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- What is the motivation?

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- What is this about Mathematica Code?

The Schrödinger Equation

1-D Time-Independent Schrödinger Equation:

$$\hat{H}\psi_n(x) = \left(-\frac{\hbar^2}{2m}D_x^2 + V(x)\right)\psi_n(x) = E_n\psi_n(x)\,, \quad n = 0,\,1,\,2,\,\ldots$$

- m is the mass of the particle
- $V(x)$ is the position-dependent potential
- $\langle\psi_m(x)|\psi_n(x)\rangle_{\mathscr{H}} = \delta_{mn}$

Supersymmetric Quantum Mechanics

Now consider the (unitless) Schrödinger equation given by

$$-\psi_0''(x) + V^{(-)}(x)\psi_0(x) = 0\,, \quad \text{where } V^{(-)}(x) \equiv V(x) - E_0\,.$$

The goal is to factor the Hamiltonian. Define two *Hermitian Conjugate Operators*

$$\hat{A} = D_x + \mathcal{W}(x)\,, \qquad \hat{A}^\dagger = -D_x + \mathcal{W}(x)\,,$$

where $\mathcal{W}(x)$ is called the *Superpotential*. Then we have two *Partner Hamiltonians*

$$\hat{H}^{(-)} = \hat{A}^\dagger \hat{A}\,, \qquad \hat{H}^{(+)} = \hat{A}\hat{A}^\dagger\,.$$

Due to the non-zero commutator of $\hat{A}$ and $\hat{A}^{\dagger}$ it is observed that $\hat{H}^{(-)} \neq \hat{H}^{(+)}$ and it should be clear that we have two separate Schrödinger equations defined by the two partner Hamiltonians

$$\hat{H}^{(-)}\psi_n^{(-)}(x) \equiv -D_x^2\,\psi_n^{(-)}(x) + V^{(-)}(x)\psi_n^{(-)}(x) = E_n^{(-)}\psi_n^{(-)}(x)\,,$$
$$\hat{H}^{(+)}\psi_n^{(+)}(x) \equiv -D_x^2\,\psi_n^{(+)}(x) + V^{(+)}(x)\psi_n^{(+)}(x) = E_n^{(+)}\psi_n^{(+)}(x)\,,$$

where the Supersymmetric Partner Potentials are given by

$$V^{(-)}(x) = \mathcal{W}^2(x) - D_x\,\mathcal{W}(x)\,,$$
$$V^{(+)}(x) = \mathcal{W}^2(x) + D_x\,\mathcal{W}(x)\,.$$

The wavefunctions can be related as follows

$$\psi_n^{(+)}(x) = C_n\hat{A}\psi_{n+1}^{(-)}(x)\,, \qquad \psi_{n+1}^{(-)}(x) = C_n\hat{A}^{\dagger}\psi_n^{(+)}(x)\,.$$

Darboux Transformations

The structure of the linear (first-order) differentiable operators $\mathfrak{L}_1 \equiv \hat{A}$ and $\mathfrak{L}_1^\dagger \equiv \hat{A}^\dagger$ establishes an *equivalence* between the approach in supersymmetric quantum mechanics and that of Darboux Transformations through the relations [1-8]

$$\begin{aligned} V^{(+)}(x) &= W^2(x) + D_x W(x) \\ &= W^{(+)}(x) - D_x W(x) + 2D_x W(x) \\ &= V^{(-)}(x) + 2D_x \left(-D_x \log\left[\psi_0^{(-)}(x)\right]\right) \\ &= V^{(-)}(x) - 2D_x^2 \log \psi_0^{(-)}(x)\,, \end{aligned}$$

$$\begin{aligned} \psi_n^{(+)}(x) &= \hat{A}\psi_{n+1}^{(-)}(x) \\ &= \left[D_x + W(x)\right]\psi_{n+1}^{(-)}(x) \\ &= \left[D_x - D_x \log \psi_0^{(-)}(x)\right]\psi_{n+1}^{(-)}(x) \\ &= \left(D_x - \frac{D_x \psi_0^{(-)}(x)}{\psi_0^{(-)}(x)}\right)\psi_{n+1}^{(-)}(x)\,. \end{aligned}$$

$$V^{(+)}(x) = \mathcal{W}^2(x) + D_x\,\mathcal{W}(x) \qquad\qquad V^{(-)}(x) = \mathcal{W}^2(x) - D_x\,\mathcal{W}(x)$$

$$\underbrace{\hat{A}\psi_{0;0}(x) = 0\,, \quad \psi_n^{(+)}(x) = \hat{A}\psi_{n+1}^{(-)}(x)\,, \quad \psi_{n+1}^{(-)}(x) = \hat{A}^\dagger\psi_n^{(+)}(x)\,, \quad n = 0,\,1,\,2,\,\ldots\,,}_{\text{Supersymmetric Formalism}}$$

$$\overbrace{\mathcal{V}(x) = V(x) - 2D_x^2\,\log\psi_0(x)\,, \qquad \Psi_n(x) = \left(D_x - \frac{D_x\psi_0(x)}{\psi_0(x)}\right)\psi_n(x) \equiv \mathfrak{L}_1\psi_n(x)}^{\text{Darboux Transformation Formalism}}\;.$$

The Simple Harmonic Oscillator

We begin with the Schrödinger equation that describes the *Simple Harmonic Oscillator Potential*

$$\hat{H}\psi_n(x) = \left(-\frac{\hbar^2}{2m}D_x^2 + V(x)\right)\psi_n(x) = E_n\psi_n(x)\,, \quad n = 0,\, 1,\, 2,\, \dots\,,$$

where

$$V(x) = x^2\,, \quad E_n = 2n+1\,, \quad \psi_n(x) = C_n\,(-1)^n \exp\left[x^2/2\right] D_x^n \exp\left[-x^2\right]\,.$$

Generalizing the Harmonic Oscillator

With the following change of variables

$$x \to \sqrt{a}z + \frac{b}{\sqrt{a}}\,,$$

for arbitrary constants a and b, it is easy to derive a *Generalized Shifted Non-Linear Oscillator Potential*, where returning to the original change of variables

$$\hat{H}\psi_n(x) = \left(-\frac{\hbar^2}{2m}D_x^2 + V(x)\right)\psi_n(x) = E_n\psi_n(x)\,, \quad n = 0,\, 1,\, 2,\, \ldots\,.$$

Changing back to the original variables for convenience results in:

$$\begin{aligned} V(x) &= (ax+b)^2\ , \\ E_n &= a(2n+1)\,, \\ \psi_n(x) &= C_n\left(-1/\sqrt{a}\right)^n \exp\left[(ax+b)^2/2a\right] D_x^n \exp\left[-(ax+b)^2/a\right]\ . \end{aligned}$$

Applications of the Harmonic Oscillator

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- Phonons on a lattice

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Applications:

- Phonons on a lattice
- Molecular vibrations
- Microresonators
- Quantum field theory
- Basically, anything that doesn't instantly leave your lab

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- In all cases, the energies will remain E_n
- n may end up being restricted on a case-by-case basis

Transformation Key

The Transformation Key:

The *transformation key* $\mathcal{T}$ is a list of non-negative integers

$$\mathcal{T} \equiv \{\mathcal{T}_1; \mathcal{T}_2, \mathcal{T}_3, \ldots\},$$

where $\mathcal{T}_m \in \mathbb{N}$ and $m \in \mathbb{Z}^+$.

Each element of this key, $\mathcal{T}_m$, will correspond to the eigenstate that will be chosen as the seed-function for the m^{th} transformation.

Seed Functions

$$V_1(x) = V_0(x) - 2D_x^2 \log \boldsymbol{\psi_{0;0}(x)},$$

$$\psi_{1;n}(x) = \left(D_x - \frac{D_x \boldsymbol{\psi_{0;0}(x)}}{\boldsymbol{\psi_{0;0}(x)}}\right)\psi_{0;n}(x) \equiv \mathfrak{L}_1 \psi_{0;n}(x)$$

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Example Transformation Key:

$$\mathcal{T} \equiv \{\mathcal{T}_1; \mathcal{T}_2, \mathcal{T}_3, \mathcal{T}_4, \mathcal{T}_5, \mathcal{T}_6\}$$
$$= \{0; 0, 1, 2, 3, 4\}$$

Seed Functions:

- Transformation 1: $\mathcal{T}_1 = 0 \Rightarrow \psi_{0;0}(x)$
- Transformation 2: $\mathcal{T}_2 = 0 \Rightarrow \psi_{1;0}(x)$
- Transformation 3: $\mathcal{T}_3 = 1 \Rightarrow \psi_{2;1}(x)$
- Transformation 4: $\mathcal{T}_4 = 2 \Rightarrow \psi_{3;2}(x)$
- Transformation 5: $\mathcal{T}_5 = 3 \Rightarrow \psi_{4;3}(x)$
- Transformation 6: $\mathcal{T}_6 = 4 \Rightarrow \psi_{5;4}(x)$

We note that the values of $\{\mathcal{T}_2, \mathcal{T}_3, \cdots, \mathcal{T}_m\}$ must be unique from each other.

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State Removal

Standard Darboux transformations remove the ground state on each sequential transformation. However, with our technique this is not necessarily the case. There are two ways that a state may be removed from the spectrum.

First: For a potential that has been transformed m times, the states that become removed are given by the values of $\{\mathcal{T}_2, \mathcal{T}_3, \cdots, \mathcal{T}_m\}$.

Second: Singular potentials remove states $n = 1, 3, 5, \ldots$.

Example Transformation

As an example we will use the transformation key given by

$$\begin{aligned} \mathcal{T} &\equiv \{\mathcal{T}_1;\, \mathcal{T}_2,\, \mathcal{T}_3,\, \mathcal{T}_4,\, \mathcal{T}_5,\, \mathcal{T}_6\} \\ &= \{0;\, 0,\, 1,\, 2,\, 3,\, 4\} \end{aligned}$$

to transform the Generalized Harmonic Oscillator

$$\hat{H}\psi_{0;n}(x) = \left(-\frac{\hbar^2}{2m}D_x^2 + V_0(x)\right)\psi_{0;n}(x) = E_n\psi_{0;n}(x)\,, \quad n = 0,\, 1,\, 2,\, \ldots\,,$$

where

$$\begin{aligned} V_0(x) &= (ax+b)^2\ , \\ E_n &= a(2n+1)\,, \\ \psi_{0;n}(x) &= C_n\left(-1/\sqrt{a}\right)^n \exp\left[(ax+b)^2/2a\right] D_x^n \exp\left[-(ax+b)^2/a\right]\ . \end{aligned}$$

First Transformation

The first transformation, ($m = 1$), is unique. Rather than following standard Darboux methodology, the following differential equation is considered

$$-D_x^2\phi_{0;\mathcal{T}_1}(i[a\,x+b])+V_0(x)\phi_{0;\mathcal{T}_1}(i[a\,x+b]) = \mathcal{E}_{\mathcal{T}_1}\phi_{0;\mathcal{T}_1}(i[a\,x+b])\,, \qquad V_0(x) = (a\,x+b)^2\,,$$

which is obtained by inserting a complex argument into the wavefunctions of the *Generalized Harmonic Oscillator* $\psi_{0;n}([a\,x+b]) \to \phi_{0;\mathcal{T}_1}(i[a\,x+b])$. This simple procedure results in the exact (but nonphysical) solutions given by

$$\begin{aligned}
\phi_{0;\mathcal{T}_1}(x) &\equiv \phi_{0;\mathcal{T}_1}(i[a\,x+b]) \\
&= \exp\left[\frac{(i(a\,x+b))^2}{2\,a}\right] D_x^{\mathcal{T}_1} \exp\left[-\frac{(i(a\,x+b))^2}{a}\right]\,, \\
\mathcal{E}_{\mathcal{T}_1} &= -a(2\,\mathcal{T}_1+1)\,,
\end{aligned}$$

where $\mathcal{T}_1 = 0$ takes place of n.

Algorithm 1: The Initial Transformation

For the first transformation $m = 1$, the generated potential $V_1(x)$ is constructed via

$$V_1(x) = V_0(x) - 2\, D_x^2 \log \phi_{0;\mathcal{T}_1}(x)\,,$$

with corresponding wavefunctions formed by

$$\psi_{1;n}(x) = \left(D_x - \frac{D_x\, \phi_{0;\mathcal{T}_1}(x)}{\phi_{0;\mathcal{T}_1}(x)} \right) \psi_{0;n}(x)\,, \qquad n = 0,\, 1,\, 2,\, \ldots\,,$$

where $\psi_{0;n}(x)$ are the wavefunctions of the original untransformed potential, where the seed-function $\phi_{0;\mathcal{T}_1}(x)$ is their $\mathcal{T}_1^{th}$ state where the complex argument has been inserted.

Application of *Algorithm 1* generates the *Shifted Generalized Harmonic Oscillator* potential, given by

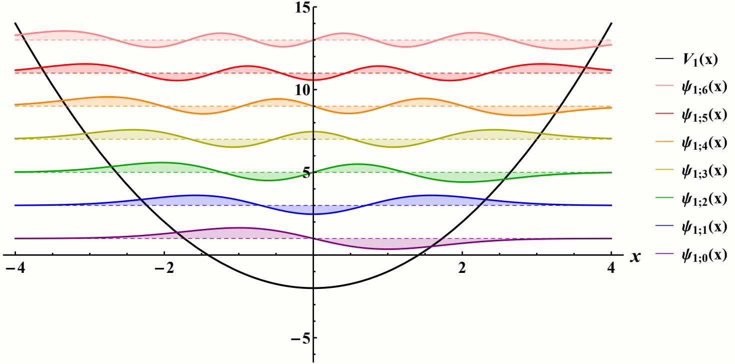
$$\begin{aligned} V_1(x) &= V_0(x) - 2\, D_x^2 \log \phi_{0;\mathcal{T}_1}(x) \\ &= (a\,x + b)^2 - 2a\,, \end{aligned}$$

$$\begin{aligned} \psi_{1;n}(x) &= D_x\, \psi_{0;n}(x) - \frac{D_x\, \phi_{0;\mathcal{T}_1}(x)}{\phi_{0;\mathcal{T}_1}(x)} \psi_{0;n}(x) \\ &= \exp\left[\frac{(a\,x+b)^2}{2\,a}\right] D_x^{n+1} \exp\left[-\frac{(a\,x+b)^2}{a}\right] \,. \end{aligned}$$

where $n = 0,\, 1,\, 2,\, \ldots$.

Shifted Generalized Harmonic Oscillator

$\mathcal{T} = \{0\}$



Algorithm 2: Sequential Transformations

For $m > 1$ the generated potential $V_m(x)$ is defined recursively as

$$V_m(x) = V_{m-1}(x) - 2\, D_x^2 \log \psi_{m-1;\mathcal{T}_m}(x)\,,$$

with corresponding wavefunctions generated by

$$\psi_{m;n}(x) = D_x\, \psi_{m-1;n}(x) - \frac{D_x\, \psi_{m-1;\mathcal{T}_m}(x)}{\psi_{m-1;\mathcal{T}_m}(x)} \psi_{m-1;n}(x)\,.$$

where the seed-function $\psi_{m-1;\mathcal{T}_m}(x)$ is a wavefunctions of the previous potential in the transformation sequence, whose eigenstate is defined by $\mathcal{T}_m$.

Second Transformation

For the second transformation, ($m = 2\,,\ \mathcal{T}_2 = 0$), the seed-function is initiated with

$$\begin{aligned}\psi_{1;\mathcal{T}_2}(x) &= \exp\left[\tfrac{(a\,x+b)^2}{2\,a}\right] D_x^{1+\mathcal{T}_2} \exp\left[-\tfrac{(a\,x+b)^2}{a}\right] \\ &= -2\,(a\,x+b)\exp\left[-\tfrac{(a\,x+b)^2}{2\,a}\right]\,,\end{aligned}$$

and generates a *Generalized Gol'dman and Krivchenkov Potential* [9-11]. given by

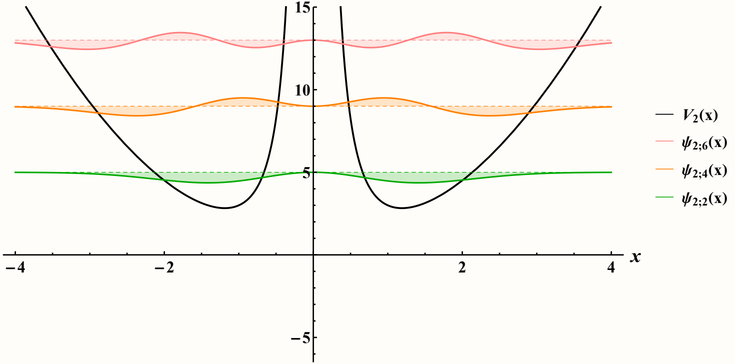
$$\begin{aligned}V_2(x) &= V_1(x) - 2\,D_x^2 \log \psi_{1;\mathcal{T}_2}(x) \\ &= (a\,x+b)^2 + \frac{2\,a^2}{(a\,x+b)^2}\,,\end{aligned}$$

$$\begin{aligned}\psi_{2;n}(x) &= \left(D_x - \frac{D_x\,\psi_{1;\mathcal{T}_2}(x)}{\psi_{1;\mathcal{T}_2}(x)}\right)\psi_{1;n}(x) \\ &= \exp\left[\frac{(a\,x+b)^2}{2\,a}\right]\left(D_x^{n+2} + \frac{2(a\,x+b)^2 - a)}{a\,x+b} D_x^{n+1}\right)\exp\left[-\frac{(a\,x+b)^2}{a}\right]\,,\end{aligned}$$

where n is restricted to $n = 2,\ 4,\ 6,\ \ldots$.

Generalized Gol'dman & Krivchenkov Potential

$\mathcal{T} = \{0; 0\}$



Third Transformation

For the third transformation, ($m = 3\,,\ \mathcal{T}_3 = 1$), the seed-function is initiated with

$$\psi_{2;1}(x) = \frac{2a^2 + 4a(a\,x+b)^2}{a\,x+b}\exp\left[-\frac{(a\,x+b)^2}{2a}\right]\,,$$

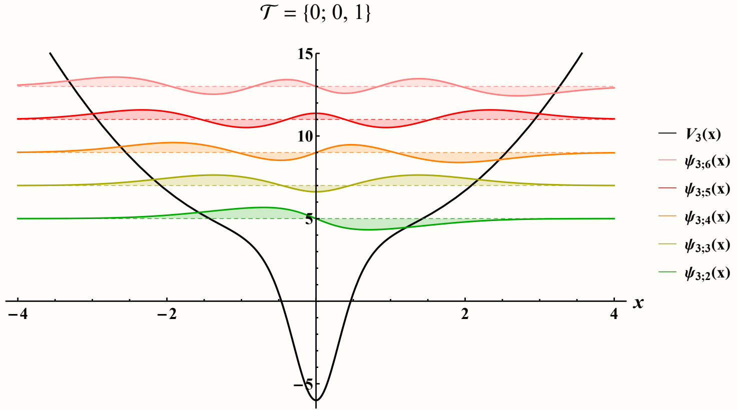
and generates a *Generalized Isotonic Nonlinear Oscillator* [12-20] given by

$$V_3(x) = 2a + (a\,x+b)^2 + \frac{8a^2\left(2(a\,x+b)^2 - a\right)}{\left(a + 2(a\,x+b)^2\right)^2}\,,$$

$$\psi_{3;n}(x) = \exp\left[\frac{(a\,x+b)^2}{2a}\right]\left(D_x^{n+3} + \frac{8(a\,x+b)^3}{a+2(a\,x+b)^2}D_x^{n+2} + \frac{2\left(3a^2+4(a\,x+b)^4\right)}{a+2(a\,x+b)^2}D_x^{n+1}\right)\exp\left[-\frac{(a\,x+b)^2}{a}\right]\,.$$

where n is restricted to $n = 2,\ 3,\ 4,\ \ldots$.

Generalized Isotonic Nonlinear Oscillator



A New Darboux-Like Technique!

It is useful to define an operator $\hat{\mathcal{L}}_m$ as

$$\hat{\mathcal{L}}_m \psi_{m-1;n}(x) = \begin{cases} \left[D_x - \dfrac{D_x[\phi_{0;\mathcal{T}_1}(x)]}{\phi_{0;\mathcal{T}_1}(x)} \right] \psi_{0;n}(x)\,, & m = 1\,, \\ \left[D_x - \dfrac{D_x[\psi_{m-1;\mathcal{T}_m}(x)]}{\psi_{m-1;\mathcal{T}_m}(x)} \right] \psi_{m-1;n}(x)\,, & m > 1\,. \end{cases}$$

Using this operator, the m^{th} wavefunction may be recursively defined for all m as

$$\psi_{m;n}(x) = \hat{\mathcal{L}}_m \psi_{m-1;n}(x) = \hat{\mathcal{L}}_m \, \hat{\mathcal{L}}_{m-1} \, \hat{\mathcal{L}}_{m-2} \, \cdots \, \hat{\mathcal{L}}_2 \, \hat{\mathcal{L}}_1 \, \psi_{0;n}(x)\,.$$

Consequently, the m^{th} potential may be expressed as

$$V_m = \begin{cases} V_0 - 2\, D_x^2 \log \phi_{0;\mathcal{T}_1}(x)\,, & m = 1\,, \\ V_1 - 2 \displaystyle\sum_{i=1}^{m-1} D_x^2 \log \left[\hat{\mathcal{L}}_i \, \hat{\mathcal{L}}_{i-1} \, \hat{\mathcal{L}}_{i-2} \, \cdots \, \hat{\mathcal{L}}_2 \, \hat{\mathcal{L}}_1 \, \psi_{0;\mathcal{T}_{i+1}}(x) \right]\,, & m > 1\,. \end{cases}$$

This formalism permits the expression of a series of transformations using only a transformation key.

Construction of a Potential

To demonstrate our method, we will derive the general form of V_m for the fourth potential generated from our example $\mathcal{T} = \{0;\, 0,\, 1,\, 2,\, 3,\, 4\}$. First we express V_4 in terms of V_3 and a seed-function as

$$\begin{aligned} V_4 &= V_3 - 2\, D_x^2 \log \psi_{3;\mathcal{T}_4}(x) \\ &= V_3 - 2\, D_x^2\, \log \left[\hat{\mathcal{L}}_3\, \hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_4}(x) \right] . \end{aligned}$$

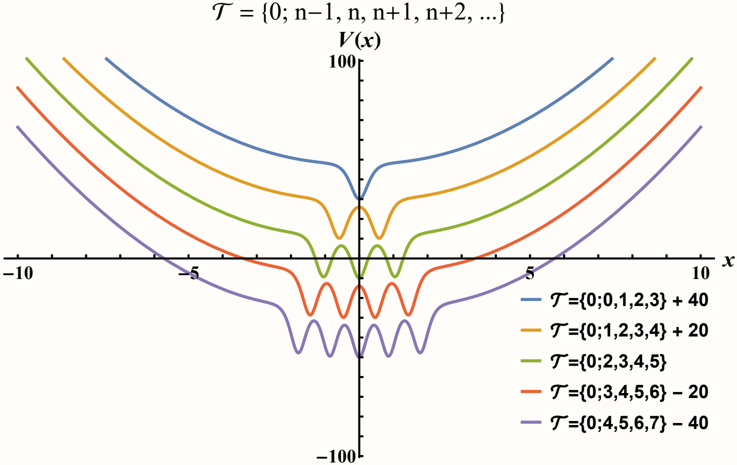
Reapplying the same technique will generate the entire potential

$$\begin{aligned} V_4 &= V_3 - 2\, D_x^2 \log \left[\hat{\mathcal{L}}_3\, \hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_4}(x) \right] \\ &= V_2 - 2\, D_x^2 \log \left[\hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_3}(x) \right] - 2\, D_x^2 \log \left[\hat{\mathcal{L}}_3\, \hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_4}(x) \right] \\ &= V_1 - 2\, D_x^2 \log \left[\hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_2}(x) \right] - 2\, D_x^2 \log \left[\hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_3}(x) \right] - 2\, D_x^2 \log \left[\hat{\mathcal{L}}_3\, \hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_4}(x) \right] \\ &= V_1 - 2 \sum_{i=1}^{3} D_x^2 \log \left[\hat{\mathcal{L}}_i\, \hat{\mathcal{L}}_{i-1}\, \hat{\mathcal{L}}_{i-2}\, \cdots\, \hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;\mathcal{T}_{i+1}}(x) \right] . \end{aligned}$$

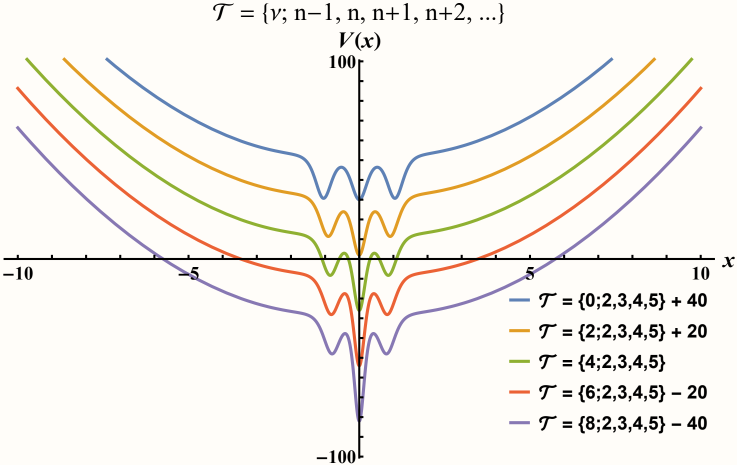
Further, for $m = 4$, the exact solutions associated with the potential $V_4(x)$ may be expressed as

$$\psi_{4;n}(x) = \hat{\mathcal{L}}_4 \psi_{3;n}(x) = \hat{\mathcal{L}}_4\, \hat{\mathcal{L}}_3\, \hat{\mathcal{L}}_2\, \hat{\mathcal{L}}_1\, \psi_{0;n}(x) .$$

n-Bump Anharmonic Family

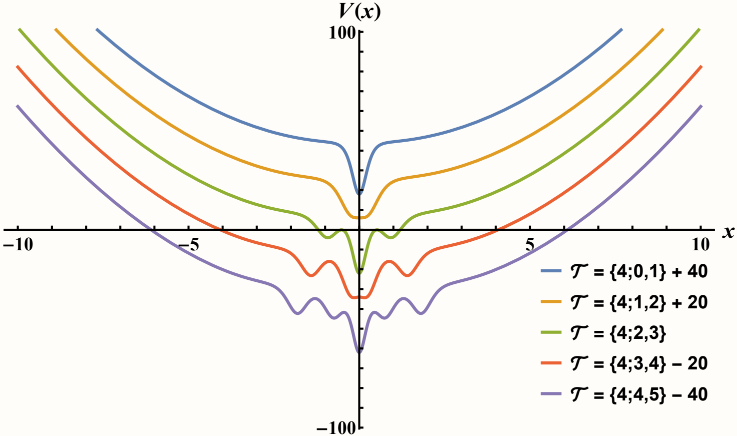


Central-Well n-Bump Anharmonic Family (v1)

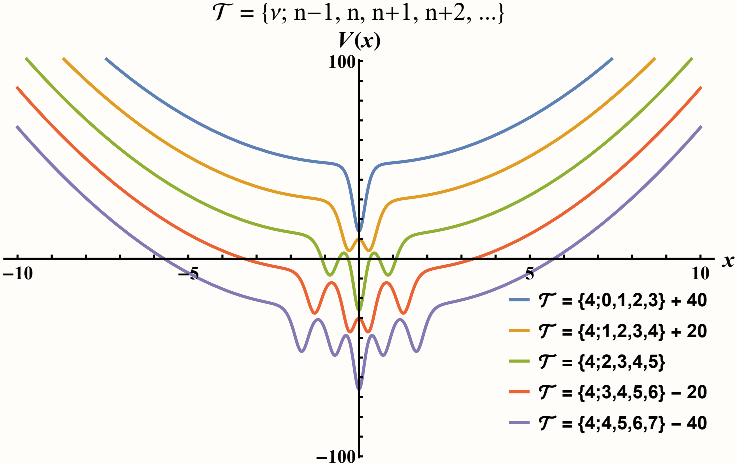


Central-Well n-Bump Anharmonic Family (v2)

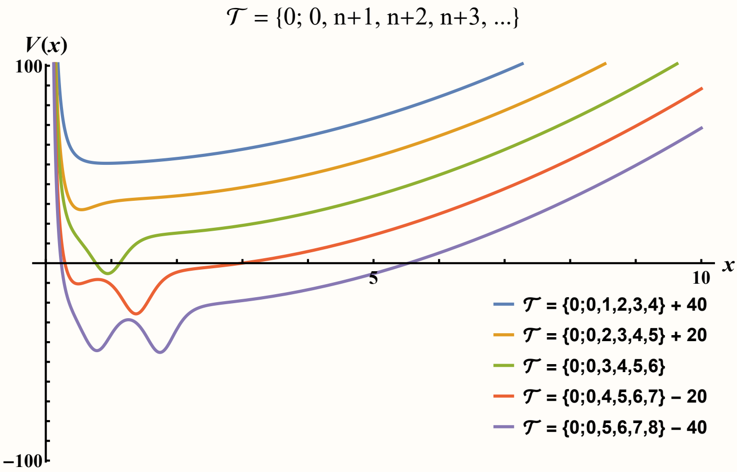
$\mathcal{T} = \{\nu; n-1, n, n+1, n+2, \ldots\}$



Central-Well n-Bump Anharmonic Family (v3)

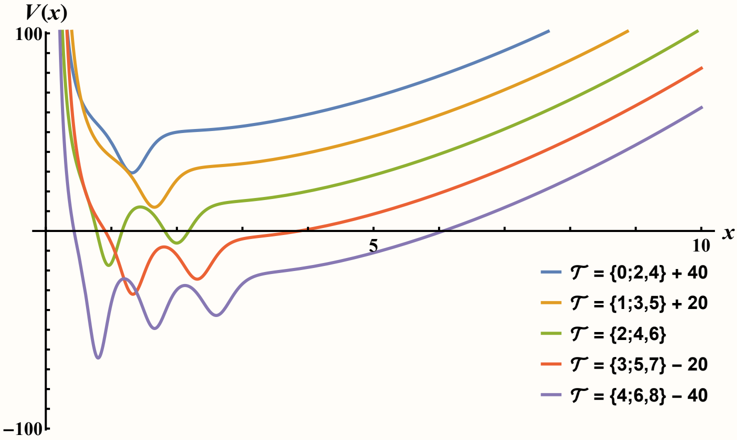


Singular n-Bump Anharmonic Family



Broadened Singular n-Bump Anharmonic Family

$\mathcal{T} = \{n-2; n, n+2, n+4, n+6, \ldots\}$

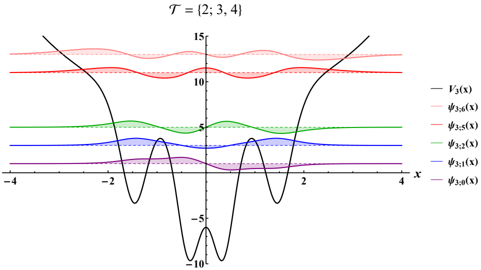


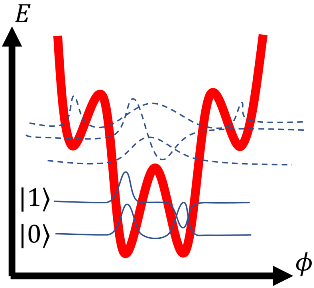
Applications: Generalizing Old Potentials

As we saw earlier, even the most simple case of our transformation key ($\mathcal{T} = \{0;\, 0,\, 1\}$) was able to generalize three highly influential potentials that were already known.

- Generalized Harmonic Oscillator
- Generalized Gol'dman and Krivchenkov Potential
- Generalized Isotonic Oscillator Potential

Applications: Modeling Known Potentials





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