Bound states in the continuum as missing states in Darboux-deformed free particle systems

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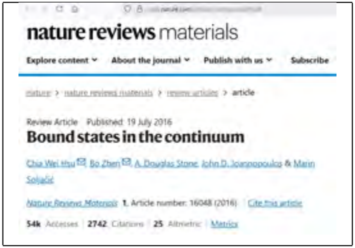
von Neumann and Wigner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Bound states in the continuum

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> Their very existence defies conventional wisdom. Although BICs were first proposed in quantum mechanics, they are a general wave phenomenon and have since been identified in electromagnetic waves, acoustic waves in air, water waves and elastic waves in solids. [1]

[2]

[3]

[1] Mielnik B., and Rosas-Ortiz O. 2009, *Quantum Mechanical Laws*. Eolss Publishers, Oxford, UK. A chapter of Fundamental of Physics - Volume I in Encyclopedia of Life Support Systems. 255-326

[2] Hsu, C. W., Zhen, B., Stone, A. D., Joannopoulos, J. D., & Soljačić, M. (2016). Bound states in the continuum. Nature Reviews Materials, 1(9), 1-13.

[3] M. Kurino, K. Takayanagi. General Theory of Constructing Potential with Bound States in Continuum. Progress of

Darboux transformation and exactly solvable systems in Quantum Mechanics

Initial system

$$\hat{H}_0\psi_n = E_n\psi_n$$

$$\hat{H}_0 = -\frac{d^2}{dx^2} + V_0(x)$$

Transformations

$$V_0(x) \to V_1(x) = V_0(x) - 2\frac{d^2}{dx^2} ln\left[\psi_\epsilon(x)\right]$$

$$\psi_n(x) \to \psi_n^{(1)}(x) = \frac{W\left(\psi_\epsilon(x), \psi_n(x)\right)}{\psi_\epsilon(x)}, \; \psi_\epsilon(x) \neq 0.$$

Deformed system

$$\hat{H}_1\psi_n^{(1)} = E_n\psi_n^{(1)}$$

$$\hat{H}_1 = -\frac{d^2}{dx^2} + V_1(x)$$

4

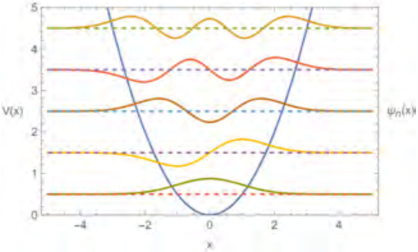
[4] Darboux G 1882 Sur une proposition relative aux ´equations lin´eaires C. R. Acad. Sci. Pa ris 94 1456–9

First Order Darboux Transformation of Harmonic Oscillator

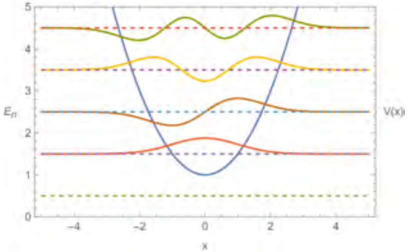
Physical function as seed function (ground state as seed function)

$$V_0(x) = \frac{1}{2}x^2 \rightarrow V_1(x) = V_0(x) - 2\frac{d^2}{dx^2} ln\left[\psi_\epsilon(x)\right] = \frac{1}{2}x^2 + 1$$

$$\psi_n(x) \rightarrow \psi_n^{(1)}(x) = \frac{W\left(\psi_0(x), \psi_n(x)\right)}{\psi_0(x)}, n = 0, 1, 2, ...$$



F3. Initial system



F4. Deformed system by means of the ground state

$\boxed{\text{There are NO missing states}}$

First Order Darboux Transformation

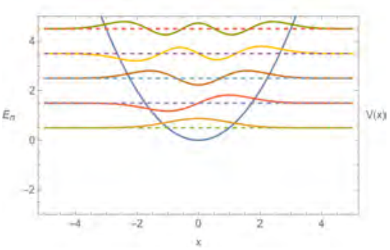
Non-physical seed function (above the grownd state)

General solution of harmonic oscillator

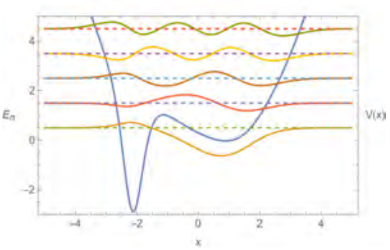
$$\psi_n\left(x;E;A;B\right)=\left[A_1F_1\left(\frac{1-2E}{4};\frac{1}{2};x^2\right)+Bx_1F_1\left(\frac{3-2E}{4};\frac{3}{2};x^2\right)\right]e^{-\frac{x^2}{2}}$$

Seed function

$$\psi_\epsilon\left(x;-\frac{7}{20};1;1\right)$$



F1. Initial system



F2. Deformed system using a non-physical solution as seed function

$\boxed{\text{There are a missing state } \psi_0\left(x\right)}$

Crum Therorem

Initial system

$$\left[-\frac{d^2}{dx^2}+V_0\left(x\right)\right]\psi_n\left(x\right)=E_n\psi_n\left(x\right),$$

N-th transformations

$$V_0\left(x\right)\to V_N\left(x\right)=V_0\left(x\right)-2\frac{d^2}{dx^2}ln\left\{W\left[\psi_{\epsilon_1}\left(x\right),\psi_{\epsilon_2}\left(x\right),...,\psi_{\epsilon_N}\left(x\right)\right]\right\},$$

$$\psi_n\left(x\right)\to\psi_n^{(N)}\left(x\right)=\frac{W\left[\psi_{\epsilon_1}\left(x\right),\psi_{\epsilon_2}\left(x\right),...,\psi_{\epsilon_N}\left(x\right),\psi_n\left(x\right)\right]}{W\left[\psi_{\epsilon_1}\left(x\right),\psi_{\epsilon_2}\left(x\right),...,\psi_{\epsilon_N}\left(x\right)\right]},\ W\left(\psi_{\epsilon_1},\psi_{\epsilon_2}\right)\neq 0.$$

Deformed system

$$\left[-\frac{d^2}{dx^2}+V_N\left(x\right)\right]\psi_n^{(N)}=E_n\psi_n^{(N)}$$

5

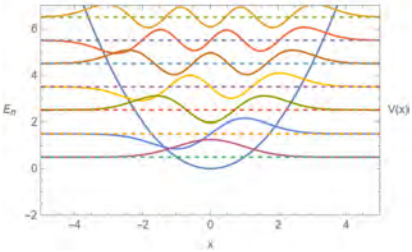
[5] Crum M M 1955 Associated Sturm-Liouville systems Q. J. Math. 6 121–7

Second Order Darboux Transformation

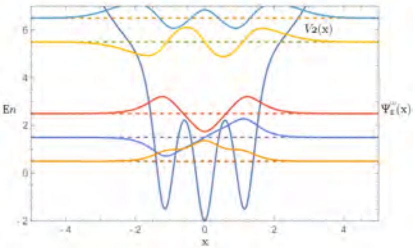
Bound States as Seed Functions

$$V_0(x) \to V_2(x) = V_0(x) - 2\frac{d^2}{dx^2} ln\left\{W\left[\psi_{\epsilon_1}(x), \psi_{\epsilon_2}(x)\right]\right\},$$

$$\psi_n^{(2)}(x) = \frac{W\left[\psi_{\epsilon_1}(x), \psi_{\epsilon_2}(x), \psi_n(x)\right]}{W\left[\psi_{\epsilon_1}(x), \psi_{\epsilon_2}(x)\right]}, \; W\left(\psi_{\epsilon_1}, \psi_{\epsilon_2}\right) \neq 0.$$



F15. Deformed system with 2nd and 3rd exited states



F16. Deformed system with 3rd and 4th exited states

$\boxed{\text{There are NO missing states}}$ [6]

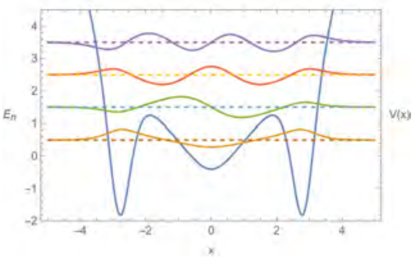
[6] M.G. Krein, DAN SSSR 113 1957 970

Second Order Darboux Transformation

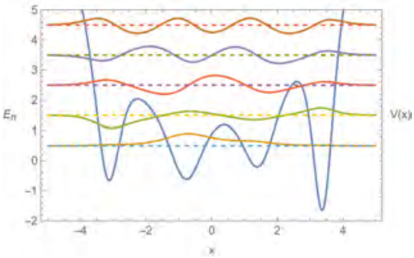
Non-physical seed functions (below the ground state or between two bound states)

$$V_0(x) \to V_2(x) = V_0(x) - 2\frac{d^2}{dx^2} ln\left\{W\left[\psi_{\epsilon_1}(x), \psi_{\epsilon_2}(x)\right]\right\},$$

$$\psi_n^{(2)}(x) = \frac{W\left[\psi_{\epsilon_1}(x), \psi_{\epsilon_2}(x), \psi_n(x)\right]}{W\left[\psi_{\epsilon_1}(x), \psi_{\epsilon_2}(x)\right]},\ W(\psi_{\epsilon_1}, \psi_{\epsilon_2}) \neq 0.$$



F5. Deformed system with non-physical s. f. below the ground state.

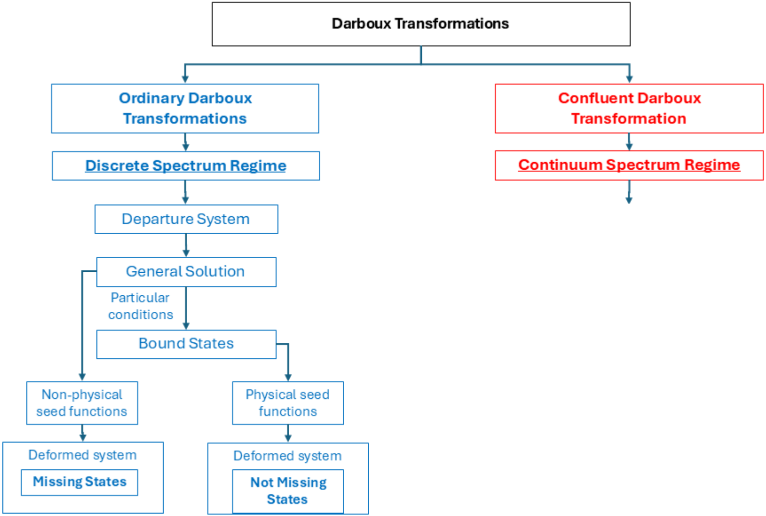


F6. Deformed system with non-physical s. f. between two bound states.

$\boxed{\text{There are two missing states}}$ [7]

[7] Boris F. Samsonov, Physics Letters A 263 (1999) 274-280

Schematic description of the work



Confluent Darboux Transformation

Second Order Ordinary Darboux Transformation

$$V_2(x) = V_0(x) - 2\frac{d^2}{dx^2} ln\left[\psi_\epsilon(x)\right],$$

$$\psi_n^{(2)}(x) = \frac{W(\psi_\epsilon(x), \psi_n(x))}{\psi_\epsilon(x)}, \; \psi_\epsilon(x) \neq 0.$$

Consideration on seed functions

$$\psi_1 = \psi(x, q)$$

$$\psi_2 = \lim_{\alpha \to 0} \psi(x, q + \alpha)$$

Confluent Darboux Transformation

$$V_2(x) = -2\frac{d^2}{dx^2} \ln\left[W(\psi, \partial_q \psi)\right],$$

$$\psi_k^{(2)} = \frac{W(\psi, \partial_q\psi, \psi_k)}{W(\psi, \partial_q\psi)}.$$

8

9

[8] Stahlhofen, A. A. (1995). Completely transparent potentials for the Schrödinger equation. Physical Review A, 51(2), 934;

[9] B. Mielnik, L. M. Nieto, & Rosas-Ortiz (2000). The finite difference algorithm for higher order supersymmetry. Physics

Confluent Darboux Transformation

Darboux-deformed free particle system

Departure system

$$\frac{d^2}{dx^2}\psi_k(x) + k^2\psi_k(x) = 0, \text{ with:} k^2 = \frac{2mE_k}{\hbar^2}.$$

Seed function for a fixed $k^2 = q^2$

$$\varphi(x, q) = \sin[qx + \delta(q)]$$

Deformed potential

$$V_2(x) = 32q^2 \frac{[sin(qx+\delta) - q(x+\gamma_0)cos(qx+\delta)]\,sin(qx+\delta)}{[sin2(qx+\delta) - 2q(x+\gamma_0)]^2}, \text{ with } \gamma_0 = \partial_q\delta$$

Asymptotic behavior of

von Newmann-Wigner type potentials

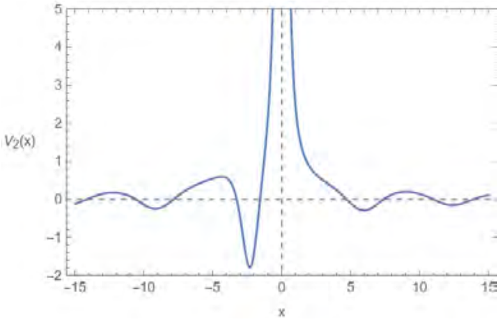
$$V_2(x) = 4q\frac{sin2(qx+\delta)}{x} + O\left(\frac{1}{x^2}\right)$$

Confluent Darboux Transformation

Darboux-deformed free particle system

Deformed potential

$$V_2(x) = 32q^2 \frac{[sin(qx+\delta) - q(x+\gamma_0)cos(qx+\delta)]\,sin(qx+\delta)}{[sin2(qx+\delta) - 2q(x+\gamma_0)]^2}, \text{ with } \gamma_0 = \partial_q \delta$$



F17. Family of deformed potentials $V_2(x)$ with the singularity located at $x=0$, with $q=\frac{1}{2}$, $\gamma_0 = 1$, and $\delta = \frac{\pi}{4} + n$.

Radial potentials with spherical symmetry and $l = 0$

Wave function

$$\Psi(\vec{r}, t) = e^{-i\frac{E}{\hbar}t} Y_l^m(\theta, \phi) \frac{\varphi(r)}{r}$$

Reduced radial Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\varphi_k(r) + V(r)\varphi_k(r) = E_k\varphi_k(r)$$

Additional asymptotic condition

$$\varphi(0) = 0$$

Free particle

$$\frac{d^2}{dx^2}\varphi_k(x) + k^2\varphi_k(x) = 0, \text{ with:} k^2 = \frac{2mE_k}{\hbar^2}$$

Parametric seed function for a fixed $k^2 = q^2$

$$\varphi_q(x) = \sin[qx + \delta(q)]$$

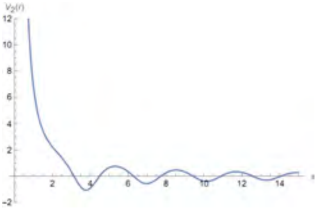


Fig. 18. $q = 1$, $\gamma_0 = 0$, $\delta = \pm n\pi$

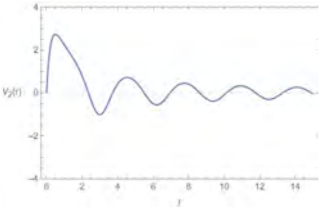


Fig. 19. $q = 1$, $\gamma_0 = 1$, $\delta = \left(\frac{1}{4} + n\right)\pi$

Radial potentials with spherical symmetry and $l = 0$

Fig. 18. $q = 1,\ \gamma_0 = 1,\ \delta = \pm n\pi$

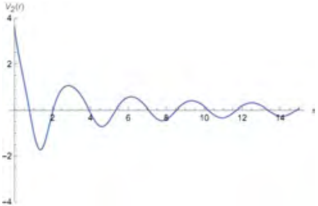


Fig. 19. $\delta = \left(-\frac{1}{4} + n\right)\pi,\ q = 1,\ \gamma_0 = 1.$

Parametric seed function associated with $k^2 = q^2$

$$\varphi_q(x) = \sin\left[qx + \delta\left(q\right)\right]$$

Asymptotic behavior

$$V_2\left(r\right) \sim -4q\frac{\sin 2\left(qr + \delta\right)}{r}$$

von Neumann-Wigner potentials

$$V\left(r\right) \sim a\frac{\sin br}{r}$$

If $\left|a\right| > \left|b\right|$,thus $k^2 = \frac{b^2}{4}$

$$k^2 = q^2$$

Radial potentials with spherical symmetry and $l = 0$

Deformed functions

General solution of initial system:

$$\varphi_k(r) = c_1 e^{ikr} + c_2 e^{-ikr}$$

Initial functions

$$\varphi^{\pm}(k, r) = e^{\pm ikr}$$

Deformed functions

$$\varphi^{\pm}(k, r) = \frac{-\left(k^2 + q^2\right)\sin\left[2\left(qr + \delta\right)\right] + 2q\left(k^2 - q^2\right)\left(r + \gamma_0\right) \pm 4ikq\sin^2\left(qr + \delta\right)}{\sin\left[2\left(qr + \delta\right)\right] - 2q\left(r + \gamma_0\right)} e^{\pm ikr}$$

Asymptotic behavior

$$\varphi_k^{(2)\pm}(r) \sim -\left(k^2 - q^2\right) e^{\pm ikr}$$

Jost solution

$$f^{\pm}(k, r) = \left\{1 + 4q\frac{\left[q\cos\left(qr + \delta\right) \mp ik\sin\left(qr + \delta\right)\right]\sin\left(qr + \delta\right)}{\left(k^2 - q^2\right)\left[\sin 2\left(qr + \delta\right) - 2q\left(r + \gamma_0\right)\right]}\right\} e^{\pm ikr}, \; k \neq q$$

Radial potentials with spherical symmetry and $l = 0$

Deformed functions

General Scattering solution

$$\varphi_s(k,r) = Af^-(k,r) + Bf^+(k,r).$$

Imposing $\varphi_s(k,0) = 0$, we have that

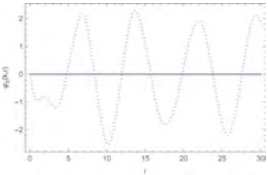
$$B = -A\frac{f^-(k,0)}{f^+(k,0)},$$

Regular scattering solution:

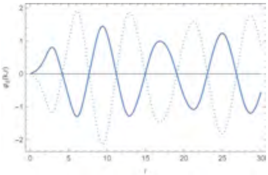
$$\varphi_s(k,r) = A\left[f^-(k,r) - \frac{f^-(k,0)}{f^+(k,0)}f^+(k,r)\right],$$

$$k \neq q.$$

$\boxed{\text{MISSING STATE}}$



F20. RSS: $q = 1$, $k = 0.8$, $\gamma_0 = \delta = n\pi$, $\gamma_0 = 1$



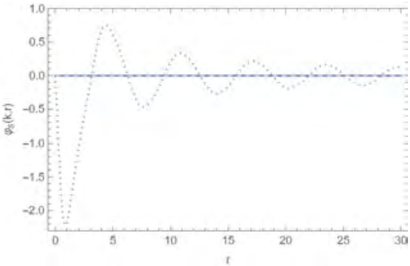
F21. RSS: $q = 1$, $k = 0.8$, $\gamma_0 = 1$,
$\delta = \left(\frac{1}{4} \pm n\right)\pi$, $n = 0, 1, 2, \ldots$

Limit of the Regular Scattering Solution

Bound State in the Continuum

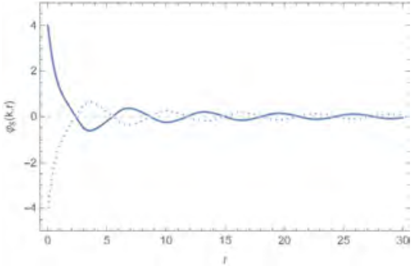
When $k \to q$ we get

$$\lim_{k \to q} \varphi_s(k, r) = 4iA \frac{q\gamma_0 \sin(qr + \delta)}{\sin 2(qr + \delta) - 2q(r + \gamma_0)} e^{i\delta}$$



F22. $q = 1,\ \gamma_0 = 1,\ \delta = n\pi$

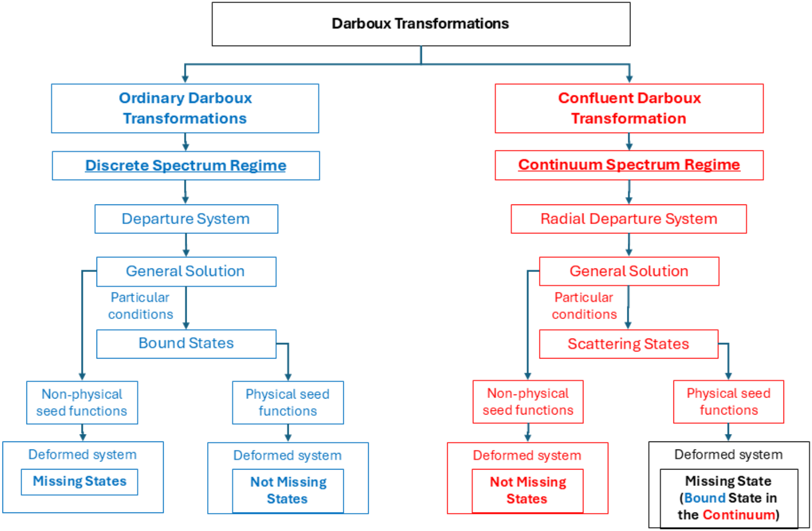
Physical solution
MISSING STATE



F23. $q = 1,\ \gamma_0 = 1,\ \delta = \left(\frac{1}{4} \pm n\right)\pi$

Non-physical solution
NOT MISSING STATE

Schematic description of the beginning of this work



Thanks for your attention.
Spetial grateful to

by its finantial support