A complex-analysis friendly form of Schrödinger equation with a non-vanishing potential

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September 4, 2019

IVP for Schrödinger equation

Given $a(x)$ s.t. $a(x) \neq 0$ for $x > 0$, consider an initial-value problem for the stationary wave equation

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$$u(0) = u_0, \quad u'(0) = u_1.$$

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Classics:

$$u''(x) + a(x)u(x) = 0 \quad \overset{v:=u'/u}{\Longleftrightarrow} \quad v'(x) + v^2(x) + a(x) = 0.$$

(Riccati equation)

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A more interesting tool:

$$u''(x) + a(x)u(x) = 0 \quad \overset{\dots}{\iff} \quad Z'(x) = f(x)\bar{Z}(x).$$

(???)

Some elementary transformations: vectorisation

$$u''(x) + a(x)u(x) = 0 \quad \Longleftrightarrow \quad U'(x) = A(x)U(x),$$

$$U(x) := \begin{pmatrix} \alpha(x)\,u(x) \\ \beta(x)\,u'(x) + \gamma(x)\,u(x) \end{pmatrix}, \qquad \alpha(x),\ \beta(x) \neq 0,$$

$$A(x) := \begin{pmatrix} \dfrac{\alpha'}{\alpha} - \dfrac{\gamma}{\beta} & \dfrac{\alpha}{\beta} \\ \dfrac{\gamma' - \beta a}{\alpha} - \dfrac{\beta' + \gamma}{\alpha\beta}\gamma & \dfrac{\beta' + \gamma}{\beta} \end{pmatrix}(x).$$

Some elementary transformations: mixing

$$U'(x) = A(x)U(x) \quad \overset{V(x)=PU(x)}{\Longleftrightarrow} \quad V'(x) = B(x)V(x),$$

$$A(x) = \begin{pmatrix} \frac{\alpha'}{\alpha} - \frac{\gamma}{\beta} & \frac{\alpha}{\beta} \\ \frac{\gamma' - \beta a}{\alpha} - \frac{\beta' + \gamma}{\alpha\beta}\gamma & \frac{\beta' + \gamma}{\beta} \end{pmatrix}(x),$$

$$B(x) := PA(x)P^{-1} =: \begin{pmatrix} p & r \\ s & q \end{pmatrix}(x),$$

P is a constant invertible matrix.

Less elementary but important transformation

$$V'(x) = B(x)V(x) \quad \overset{W(x)=S(x)V(x)}{\Longleftrightarrow} \quad W'(x) = N(x)W(x),$$

$$B(x) = \begin{pmatrix} p & r \\ s & q \end{pmatrix}(x),$$

$$S(x) := \begin{pmatrix} \exp\left(-\int_0^x p(t)\,dt\right) & 0 \\ 0 & \exp\left(-\int_0^x q(t)\,dt\right) \end{pmatrix},$$

$$N(x) := \begin{pmatrix} 0 & r(x)\exp\left(-\int_0^x (p(t)-q(t))\,dt\right) \\ s(x)\exp\left(\int_0^x (p(t)-q(t))\,dt\right) & 0 \end{pmatrix}.$$

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This is due to:

$$V' - \begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix} V = \begin{pmatrix} e^{\int_0^x p(t)dt} & 0 \\ 0 & e^{\int_0^x q(t)dt} \end{pmatrix} \left(\begin{pmatrix} e^{-\int_0^x p(t)dt} & 0 \\ 0 & e^{-\int_0^x q(t)dt} \end{pmatrix} V \right)'.$$

An observation

$$W'(x) = N(x) W(x), \quad x > 0, \qquad W(0) = W_0,$$

$$N(x) = \begin{pmatrix} 0 & r(x)\, e^{-\int_0^x (p(t)-q(t))dt} \\ s(x)\, e^{\int_0^x (p(t)-q(t))dt} & 0 \end{pmatrix}.$$

Note that if $\quad r(x)\, e^{-\int_0^x (p(t)-q(t))dt} = s(x)\, e^{\int_0^x (p(t)-q(t))dt} =: f(x),$

then $\quad W(x) = (\cosh f(x) I + \sinh f(x) S)\, W_0,$

where $\quad I := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; S := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$

Hint: Write Picard iteration and use $S^{2m} = I$, $S^{2m+1} = S$, $m \in \mathbb{N}$.

Another observation

$$W'(x) = N(x)W(x),$$

$$N(x) = \begin{pmatrix} 0 & r(x)\, e^{-\int_0^x (p(t)-q(t))dt} \\ s(x)\, e^{\int_0^x (p(t)-q(t))dt} & 0 \end{pmatrix}.$$

Second best situation:

$$r(x)\, e^{-\int_0^x (p(t)-q(t))dt} = \bar{s}(x)\, e^{\int_0^x (\bar{p}(t)-\bar{q}(t))dt}$$

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Second best situation:

$$r(x)\, e^{-\int_0^x (p(t)-q(t))dt} = \bar{s}(x)\, e^{\int_0^x (\bar{p}(t)-\bar{q}(t))dt} =: f(x),$$

i.e. if $p(x) - q(x)$ is purely imaginary, we just need $r(x) = \bar{s}(x)$!

Much easy to impose !

Dealing with an interesting matrix

$$W'(x) = N(x)W(x), \quad W(0) = W_0, \qquad N(x) = \begin{pmatrix} 0 & f(x) \\ \bar{f}(x) & 0 \end{pmatrix}.$$

Picard iteration procedure gives a solution representation:

$$W(x) = \begin{pmatrix} C_f(x) & S_f(x) \\ S_{\bar{f}}(x) & C_{\bar{f}}(x) \end{pmatrix} W_0,$$ where

$$\begin{cases} C_f'(x) = f(x)\, S_{\bar{f}}(x), & S_f'(x) = f(x)\, C_{\bar{f}}(x), \\ C_f(0) = 1, & S_f(0) = 0. \end{cases}$$

Final reduction

$$\begin{cases} C_f'(x) = f(x)\, S_{\bar{f}}(x), & S_f'(x) = f(x)\, C_{\bar{f}}(x), \\ C_f(0) = 1, & S_f(0) = 0. \end{cases}$$

These equations can be decoupled:

$$Z_\pm(x) := C_f(x) \pm S_f(x) \quad \Rightarrow \quad \begin{cases} Z_\pm'(x) = \pm f(x)\, \bar{Z}_\pm(x), \\ Z_\pm(0) = 1. \end{cases}$$

Hence it all boils down to solving only one ODE:

$$\begin{cases} Z'(x) = f(x)\, \bar{Z}(x), \\ Z(0) = 1. \end{cases}$$

Example of transformations

$$u''(x) + a(x)u(x) = 0 \quad \Longleftrightarrow \quad U'(x) = A(x)U(x) \quad \overset{V(x)=PU(x)}{\Longleftrightarrow} \quad V'(x) = B(x)V(x)$$

- [1] K. Lorenz, T. Jahnke, C. Lubich, *Adiabatic integrators for highly oscillatory second-order linear differential equations with time-varying eigendecomposition* (2005).

$$U(x) := \begin{pmatrix} \alpha(x)\,u(x) \\ \beta(x)\,u'(x) + \gamma(x)\,u(x) \end{pmatrix} = \begin{pmatrix} u(x) \\ a^{-1/2}(x)u'(x) \end{pmatrix},$$

$$A(x) := \begin{pmatrix} \frac{\alpha'}{\alpha} - \frac{\gamma}{\beta} & \frac{\alpha}{\beta} \\ \frac{\gamma' - \beta a}{\alpha} - \frac{\beta' + \gamma}{\alpha\beta}\gamma & \frac{\beta' + \gamma}{\beta} \end{pmatrix}(x) = \underbrace{\begin{pmatrix} 0 & \sqrt{a(x)} \\ -\sqrt{a(x)} & 0 \end{pmatrix}}_{=\sqrt{a(x)}P^{-1}\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}P} + \begin{pmatrix} 0 & 0 \\ 0 & -\frac{a'(x)}{2a(x)} \end{pmatrix},$$

$$B(x) := PA(x)P^{-1} = \begin{pmatrix} i\sqrt{a} - \frac{a'}{4a} & \frac{ia'}{4a} \\ -\frac{ia'}{4a} & -i\sqrt{a} - \frac{a'}{4a} \end{pmatrix}(x), \qquad P = \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix}.$$

Example of transformations

$$u''(x) + a(x)u(x) = 0 \iff U'(x) = A(x)U(x) \overset{V(x)=PU(x)}{\iff} V'(x) = B(x)V(x)$$

- [2] A. Arnold, N. Ben Abdallah, C. Negulescu, *WKB-based schemes for the Schrödinger equation in the semi-classical limit* (2011).

$$U(x) := \begin{pmatrix} \alpha(x)\,u(x) \\ \beta(x)\,u'(x) + \gamma(x)\,u(x) \end{pmatrix} = \begin{pmatrix} a^{1/4}(x)u(x) \\ \frac{1}{a^{1/4}(x)}u'(x) + \frac{a'(x)}{4a^{5/4}(x)}u(x) \end{pmatrix},$$

$$A(x) := \begin{pmatrix} \frac{\alpha'}{\alpha} - \frac{\gamma}{\beta} & \frac{\alpha}{\beta} \\ \frac{\gamma' - \beta a}{\alpha} - \frac{\beta' + \gamma}{\alpha\beta}\gamma & \frac{\beta' + \gamma}{\beta} \end{pmatrix}(x) = \underbrace{\begin{pmatrix} 0 & \sqrt{a(x)} \\ -\sqrt{a(x)} & 0 \end{pmatrix}}_{=\sqrt{a(x)}P^{-1}\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}P} + \underbrace{\begin{pmatrix} 0 & 0 \\ \frac{a''(x)}{8a^{3/2}(x)} - \frac{5(a'(x))^2}{32a^{5/2}(x)} & 0 \end{pmatrix}}_{=:b(x)},$$

$$B(x) := PA(x)P^{-1} = \begin{pmatrix} i(\sqrt{a} - b) & b \\ b & -i(\sqrt{a} - b) \end{pmatrix}(x), \qquad P = \frac{1}{\sqrt{2}}\begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix}.$$

Example of transformations

$$V'(x) = B(x)V(x) \quad \overset{W(x)=S(x)V(x)}{\Longleftrightarrow} \quad W'(x) = N(x)W(x),$$

In [1] :

$$B(x) = \begin{pmatrix} i\sqrt{a} - \frac{a'}{4a} & \frac{ia'}{4a} \\ -\frac{ia'}{4a} & -i\sqrt{a} - \frac{a'}{4a} \end{pmatrix}(x), \qquad N(x) = \begin{pmatrix} 0 & \frac{ia'(x)}{4a(x)} e^{-2i\int_0^x \sqrt{a(t)}dt} \\ -\frac{ia'(x)}{4a(x)} e^{2i\int_0^x \sqrt{a(t)}dt} & 0 \end{pmatrix}.$$

In [2] :

$$B(x) = \begin{pmatrix} i\left(\sqrt{a} - b\right) & b \\ b & -i\left(\sqrt{a} - b\right) \end{pmatrix}(x), \qquad N(x) = \begin{pmatrix} 0 & b(x)e^{-2i\int_0^x \left(\sqrt{a(t)} - b(t)\right)dt} \\ b(x)e^{2i\int_0^x \left(\sqrt{a(t)} - b(t)\right)dt} & 0 \end{pmatrix},$$

$$b(x) := \frac{a''(x)}{8a^{3/2}(x)} - \frac{5(a'(x))^2}{32a^{5/2}(x)}.$$

Note: in both [1]-[2], we have $N(x) = \begin{pmatrix} 0 & f \\ \bar{f} & 0 \end{pmatrix}(x)$

for some $f(x)$, and hence achieve a reduction to $Z'(x) = f(x)\bar{Z}(x)$.

Some applications of $Z'(x) = f(x)\bar{Z}(x)$

- Efficient hybrid asymptotical-numerical methods for initial-value problems / boundary-value problems (by a "shooting method") in a semi-classical regime for the wave equation ($C(x) \equiv a_0(x) > 0$) / coupled system of oscillators ($C(x)$ is a positive definite matrix), as in [1]-[2],

$$u''(x) + \frac{1}{\epsilon^2} C(x) u(x) = 0, \quad x > 0, \quad 0 < \epsilon \ll 1.$$

After the reduction, no need to trace matrix structure of Picard iterations: the scalar problem yields exactly the same result !

$$\left(\begin{array}{c} \text{Picard iterations for} \quad Z'(x) = f(x)\bar{Z}(x), \quad Z(0) = 1 : \\ Z(x) = 1 + \int_0^x f(t)dt + \int_0^x f(t_2) \int_0^{t_2} \bar{f}(t_1) dt_1 dt_2 + \ldots \end{array} \right)$$

Some applications of $Z'(x) = f(x)\bar{Z}(x)$

$$W'(x) = N(x)W(x), \quad x > 0, \qquad W(0) = W_0.$$

For [2]: $$N(x) = \underbrace{\begin{pmatrix} 0 & \epsilon b_0(x) e^{-\frac{2i}{\epsilon}\int_0^x \left(\sqrt{a_0(t)} - \epsilon^2 b_0(t)\right)dt} \\ \epsilon b_0(x) e^{\frac{2i}{\epsilon}\int_0^x \left(\sqrt{a_0(t)} - \epsilon^2 b_0(t)\right)dt} & 0 \end{pmatrix}}_{=:\bar{f}_0(x)},$$

$$b_0(x) := \frac{a_0''(x)}{8a_0^{3/2}(x)} - \frac{5\left(a_0'(x)\right)^2}{32a_0^{5/2}(x)}.$$

$$\begin{cases} Z_\pm'(x) = \pm\epsilon f_0(x)\bar{Z}_\pm(x), \\ Z_\pm(0) = 1. \end{cases} \Rightarrow \begin{cases} C_{f_0}(x) = \frac{1}{2}\left(Z_+(x) + Z_-(x)\right), \\ S_{f_0}(x) = \frac{1}{2}\left(Z_+(x) - Z_-(x)\right). \end{cases}$$

$$\Rightarrow \quad W(x) = \begin{pmatrix} C_{f_0}(x) & S_{f_0}(x) \\ S_{\bar{f}_0}(x) & C_{\bar{f}_0}(x) \end{pmatrix} W_0.$$

Some alternative reformulations of $Z'(x) = f(x)\bar{Z}(x)$

- Prüfer type equation

Represent $$f = |f|\, e^{i\Phi},\ X = Re^{i\Theta}$$

for some $R = R(x) \geq 0$, $\Phi = \Phi(x)$, $\Theta = \Theta(x) \in \mathbb{R}$. Then:

$$\Theta' = -|f| \sin(2\Theta - \Phi), \quad (\log R)' = \operatorname{Re}\left(f\, e^{-2i\Theta}\right).$$

- Back to a linear 2nd order ODE:

$$\frac{1}{\bar{f}(t)} \frac{d}{dt} \frac{1}{f(t)} \frac{d}{dt} X = X$$

Towards new classes of "integrable" potentials

"Integrable" potentials ($\equiv$ exactly solvable Schrödinger equation)

$$Z'(x) = f(x)\bar{Z}(x), \quad x > 0, \qquad Z(0) = 1.$$

- Consider e.g. $f(x) = e^{-\alpha_0 x}$, $\operatorname{Re}\alpha_0 > 0$.

Take Fourier-Laplace transform ($\hat{F}(k) := \int_0^\infty e^{ikx}F(x)\,dx$):

$$-ik\hat{Z}(k) = \overline{\hat{Z}(-(k+i\bar{\alpha}_0))} + 1, \quad k \in \mathbb{R},$$

$$\Rightarrow \quad -ik\overline{\hat{Z}(-k)} = \hat{Z}(k - i\bar{\alpha}_0) + 1, \quad k \in \mathbb{R},$$

Since $\hat{Z}(k), \overline{\hat{Z}(-k)} \in H_+$ (bounded analytic in the upper half-plane),

$$-i(k+i\bar{\alpha}_0)\overline{\hat{Z}(-(k+i\bar{\alpha}_0))} = \hat{Z}(k) + 1, \quad k \in \mathbb{R},$$

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$$\Longrightarrow \quad \hat{Z}(k) = -\frac{1 + \bar{\alpha}_0 - ik}{1 + k(k + i\bar{\alpha}_0)}.$$

Towards new classes of "integrable" potentials

$$Z'(x) = f(x)\bar{Z}(x), \quad x > 0, \qquad\qquad Z(0) = 1.$$

More generally, one can attempt...

- $f(x) = \sum_{j=1}^{M} c_j e^{-\alpha_j x}, \quad c_j \in \mathbb{C}, \quad \mathrm{Re}\,\alpha_j > 0;$
- $f(x) = \int_0^\infty e^{-px}\psi(p)dp$ for some $\psi(p)$.

...

Summary & Outlook

- We have discussed how IVP for a linear Schrödinger equation with a non-vanishing potential can be reduced in many ways to an equation of an extremely simple form $Z'(x) = f(x)\bar{Z}(x)$.
- Besides the neat look, the obtained equation has advantages for both numerical and theoretical investigation.
- However, it feels like the main advantage of such a reformulation is yet to be understood...
- ... as well as its generalizations.

Thank You!