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Darboux transformations for the Schrödinger equation in three dimensions

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Abstract. We apply Darboux transformations to the Schrödinger equation in three dimensions and derive the general form of the potentials and potential differences which can be treated by these transformations. In particular we establish the existence of a new class of potentials whose solutions are related to each other by these transformations.

1. Introduction

Various analytical methods are available in the literature to solve the time independent Schrödinger equation in three dimensions for some special potentials. In general these procedures require a coordinate system in which the equation is separable and then solve the resulting one-dimensional equations by various techniques which are available to this end. Among these one-dimensional techniques the factorisation method and its generalisations [1, 2] were useful in various physical contexts. However, the extension of this technique to generic problems in higher dimensions (namely, without the assumption of separability) yields non-trivial results only if one uses second-order operators [3]. Still a generalisation of this technique to higher dimensions might be of interest not only in quantum mechanics but also in other physical applications which utilise the Helmholtz equation, e.g. ocean acoustic [4].

In an attempt to find such a generalisation one recalls that the origins of the factorisation method are related to the theory of Darboux transformations [5]. It is therefore of interest to examine the direct application of these transformations to Schrödinger equations in higher dimensions. In this context two recent applications of this technique, to coupled systems in one dimension and supersymmetric models, appeared in the literature [6-8]. In spite of these results the general application of Darboux transformations in higher dimensions remains open. It is therefore our objective in this paper to investigate and give a detailed answer as to when two Schrödinger equations (and consequently their solutions) are related by these transformations. The application of those transformations to non-linear partial differential equations will be deferred to a later publication.

The plan of the paper is as follows. In § 2 we review Darboux transformations in one dimension and then define their counterparts in higher dimensions. We then derive the basic equations which govern these transformations. In § 3 we classify the potential differences which can be related by these transformations in three dimensions. Finally in § 4 we give the general solution to the basic equations of this technique in three dimensions.

2. Darboux transformations in higher dimensions

Darboux transformations for a single ordinary differential equation were defined as follows.

Definition 1. Given the equation

$$\varphi'' = (u(x)+\lambda)\varphi \qquad x \in R \tag{2.1}$$

we say that the transformation

$$\psi = A(x)\varphi + B(x)\varphi' \tag{2.2}$$

is a Darboux transformation if ψ satisfies a differential equation of the form

$$\psi'' = (v(x)+\lambda)\psi. \tag{2.3}$$

When $B=1$ it is easy to show that (2.2) represents a Darboux transformation only if

$$\begin{aligned} &A''+u'+A(u-v)=0 \\ &2A'+u-v=0. \end{aligned} \tag{2.4}$$

Hence we infer that

$$A'-A^2+u=-\nu \tag{2.5}$$

where ν is an integration constant. Linearising equation (2.5) by the transformation $A=-\zeta'/\zeta$ we obtain

$$\zeta'' = (u(x)+\nu)\zeta. \tag{2.6}$$

Thus ζ is an eigenfunction of (2.1) with $\lambda=\nu$. From (2.4) it then follows that

$$v = u - 2(\ln \zeta)'' \tag{2.7}$$

i.e. a Darboux transformations changes the potential function $u(x)$ by $-2(\ln \zeta)''$ where ζ is an arbitrary eigenfunction of (2.1).

In complete analogy to the one-dimensional case we now define Darboux transformations for the Schrödinger equation in higher dimensions.

Definition 2. We say that

$$\psi = A(\boldsymbol{x})\varphi + \boldsymbol{B}(\boldsymbol{x})\cdot\nabla\varphi \qquad \boldsymbol{x}\in R^n \qquad n>1 \tag{2.8}$$

is a Darboux transformation for

$$\nabla^2\varphi = (u(\boldsymbol{x})+\lambda)\varphi \tag{2.9}$$

if ψ satisfies a differential equation of the form:

$$\nabla^2\psi = (v(\boldsymbol{x})+\lambda)\psi. \tag{2.10}$$

Remarks. (i) In the following we consider explicitly equations (2.8) and (2.10) in three dimensions only. However, our approach will apply to other dimensions.

(ii) We observe that Darboux transformations are invertible in one but not in higher dimensions. In fact the inverse of the transformation (2.2) with $B=1$ is

$$\varphi = (A - \mathrm{d}/\mathrm{d}x)\psi.$$

In higher dimensions, however, Darboux transformations are not invertible in general. Thus if

$$\varphi=(C+\boldsymbol{D}\cdot\nabla)\psi \tag{2.11}$$

is an inverse of (2.8) with $\boldsymbol{B}\neq 0$ then by combining (2.8) with (2.11) we infer that

$$B_1D_2+B_2D_1=B_1D_3+B_3D_1=B_2D_3+B_3D_2=0$$

$$B_1D_1=B_2D_2=B_3D_3$$

and

$$A\boldsymbol{D}+C\boldsymbol{B}+(\boldsymbol{B}\cdot\nabla)\boldsymbol{D}=0.$$

Together these equations imply that $\boldsymbol{D}=0$ and $C=0$.

To derive the constraints on A, $\boldsymbol{B}$ which ensure that (2.8) is a Darboux transformation for (2.9) we substitute (2.8) in (2.10) and use (2.9). This yields:

$$\varphi\nabla^2A+2\nabla A\cdot\nabla\varphi+A(u\varphi+\lambda\varphi)+\nabla^2\boldsymbol{B}\cdot\nabla\varphi+\boldsymbol{B}\cdot(\varphi\nabla u+u\nabla\varphi+\lambda\nabla\varphi)+2(\nabla\boldsymbol{B})\cdot\nabla(\nabla\varphi)$$
$$=Av\varphi+\lambda A\varphi+v\boldsymbol{B}\cdot\nabla\varphi+\lambda\boldsymbol{B}\cdot\nabla\varphi.$$

Considering this equation as a polynomial in φ, $\nabla\varphi$, $\partial^2\varphi/\partial x\,\partial y$, etc, and using (2.9) whenever possible we obtain the following systems of equations for A, $\boldsymbol{B}=(B_1,\ldots,B_n)$:

$$\frac{\partial B_i}{\partial x_j}+\frac{\partial B_j}{\partial x_i}=0 \qquad i,j=1,\ldots,n \tag{2.12}$$

$$\frac{\partial B_1}{\partial x_1}=\ldots=\frac{\partial B_n}{\partial x_n}=f(\boldsymbol{x}) \tag{2.13}$$

$$\nabla^2A+A(u-v)+\boldsymbol{B}\cdot\nabla u+2f(u+\lambda)=0 \tag{2.14}$$

$$2\nabla A+\boldsymbol{B}(u-v)=-\nabla^2\boldsymbol{B} \tag{2.15}$$

where $f(\boldsymbol{x})$ is (at the present) an arbitrary function.

In the following sections we solve these equations in full generality in three dimensions and thus give a general classification for the potentials and potential differences which can be related to each other through Darboux transformation.

3. Classification for $u-v$

Since equations (2.12) and (2.13) are independent of A, u, v we can solve them to obtain the general form of $\boldsymbol{B}$ (and hence $f(\boldsymbol{x})$). A long (and interesting) algebra then yields

$$B_1=\tfrac{1}{2}a_5(x^2-y^2-z^2)+a_6xy+a_7xz+a_8x+c_1 \tag{3.1}$$

$$B_2=\tfrac{1}{2}a_6(y^2-x^2-z^2)+a_5xy+a_7yz+a_8y+c_2 \tag{3.2}$$

$$B_3=\tfrac{1}{2}a_7(z^2-x^2-y^2)+a_5xz+a_6yz+a_8z+c_3 \tag{3.3}$$

($\boldsymbol{B}$ can be recognised as the general conformal second-order Killing tensor in Euclidean space).

Although (3.1)-(3.3) give the general solution of (2.12) and (2.13) one can obtain an additional constraint on the coefficients of these solutions from (2.15). In fact by taking the curl of this equation we obtain

$$(u-v)\nabla\times\boldsymbol{B}-\boldsymbol{B}\times\nabla(u-v)=\boldsymbol{0}. \tag{3.4}$$

(This is the integrability condition on (2.15).) Taking the scalar product of this equation with $\boldsymbol{B}$ then yields

$$\boldsymbol{B} \cdot \nabla \times \boldsymbol{B} = 0. \tag{3.5}$$

From (3.1)-(3.3) it then follows that

$$a_5 c_2 = a_6 c_1 \qquad a_5 c_3 = a_7 c_1 \qquad a_7 c_2 = a_6 c_3. \tag{3.6}$$

Using these constraints we can rewrite $\boldsymbol{B}$ as

$$\boldsymbol{B} = f\boldsymbol{x} - \tfrac{1}{2} a \boldsymbol{w} \tag{3.7}$$

where

$$f = \tfrac{1}{3} \nabla \cdot \boldsymbol{B} = a_5 x + a_6 y + a_7 z + a_8 \tag{3.8}$$

$$\boldsymbol{w} = -\nabla^2 \boldsymbol{B} = (a_5, a_6, a_7) \tag{3.9}$$

$$a = \boldsymbol{x} \cdot \boldsymbol{x} - 2c_1/a_5. \tag{3.10}$$

Now that we established the general form of $\boldsymbol{B}$ we proceed to give a general classification for the potential difference $\rho = u - v$ using equation (3.4).

Remark. Motivated by the treatment of the one-dimensional case one could take the scalar product of equation (2.15) with $\boldsymbol{B}$ to obtain

$$v = u + (\boldsymbol{B}/\boldsymbol{B}^2) \cdot (2\nabla A - \boldsymbol{w}). \tag{3.11}$$

Substituting this in (2.14) leads to

$$\nabla^2 A + \boldsymbol{B} \cdot \left(\nabla u - \frac{\nabla(A^2)}{\boldsymbol{B}^2} \right) + \frac{A}{\boldsymbol{B}^2} \boldsymbol{B} \cdot \boldsymbol{w} + 2f(u + \lambda) = 0. \tag{3.12}$$

Since this equation is non-linear it can be solved directly only if $\nabla^2 \boldsymbol{B} = \boldsymbol{0}$, i.e. $\boldsymbol{w} = \boldsymbol{0}$. We shall show however that by solving equation (3.4) one can solve equations (2.14) and (2.15) in full generality.

Since equation (3.6) establishes certain relations between the coefficients of $\boldsymbol{B}$ we carry the classification for ρ by considering several cases.

3.1. $a_5 \neq 0$, $a_6 \neq 0$, $a_7 \neq 0$

Rewriting (3.4) explicitly we obtain

$$B_2 \frac{\partial \rho}{\partial z} - B_3 \frac{\partial \rho}{\partial y} = \rho(2a_6 z - 2a_7 y) \tag{3.13}$$

$$B_3 \frac{\partial \rho}{\partial x} - B_1 \frac{\partial \rho}{\partial z} = \rho(2a_7 x - 2a_5 z) \tag{3.14}$$

$$B_1 \frac{\partial \rho}{\partial y} - B_2 \frac{\partial \rho}{\partial x} = \rho(2a_5 y - 2a_6 x). \tag{3.15}$$

Multiplying these equations by a_5, a_6 and a_7 respectively and adding leads to

$$(a_5 B_2 - a_6 B_1) \frac{\partial \rho}{\partial z} + (a_7 B_1 - a_5 B_3) \frac{\partial \rho}{\partial y} + (a_6 B_3 - a_7 B_2) \frac{\partial \rho}{\partial x} = 0. \tag{3.16}$$

However, we observe from (3.7) that

$$\boldsymbol{w} \times \boldsymbol{B} = f\boldsymbol{w} \times \boldsymbol{x}. \tag{3.17}$$

Hence (3.16) reduces to

$$(a_5 y - a_6 x)\frac{\partial \rho}{\partial z} + (a_7 x - a_5 z)\frac{\partial \rho}{\partial y} + (a_6 z - a_7 y)\frac{\partial \rho}{\partial x} = 0 \tag{3.18}$$

whose general solution is

$$\rho = F(x^2 + y^2 + z^2, a_5 x + a_6 y + a_7 z) \tag{3.19}$$

where F is a general (smooth) function.

Remark. We can obtain equation (3.17) also by multiplying (3.13)-(3.15) by x, y, z respectively and observing that (using (3.7))

$$\boldsymbol{x} \times \boldsymbol{B} = \tfrac{1}{2}a\boldsymbol{w} \times \boldsymbol{x}. \tag{3.20}$$

To see the constraints that have to be imposed on F in equation (3.19) we substitute ρ in (3.13)-(3.15) and obtain

$$a\frac{\partial F}{\partial a} + f\frac{\partial F}{\partial f} + 2F = 0. \tag{3.21}$$

Hence, finally we infer that

$$\rho = \frac{1}{f^2}G\left[\frac{a}{f}\right] = \frac{1}{f^2}G(\alpha) \tag{3.22}$$

where G is an arbitrary smooth function.

We note that the same result for ρ will be obtained if only two of the constants a_5, a_6, a_7 are non-zero. Hence we shall give no special treatment to this case.

3.2. $a_5 = a_6 = a_7 = 0$, $a_8 \neq 0$, $\boldsymbol{c} = (c_1, c_2, c_3) \neq 0$

Equations (3.13)-(3.15) reduce in this case to

$$(a_8 y + c_2)\frac{\partial \rho}{\partial z} - (a_8 z + c_3)\frac{\partial \rho}{\partial y} = 0 \tag{3.23}$$

$$(a_8 z + c_3)\frac{\partial \rho}{\partial x} - (a_8 x + c_1)\frac{\partial \rho}{\partial z} = 0 \tag{3.24}$$

$$(a_8 x + c_1)\frac{\partial \rho}{\partial y} - (a_8 y + c_2)\frac{\partial \rho}{\partial x} = 0. \tag{3.25}$$

Multiplying by x, y and z respectively and adding we obtain

$$(c_2 x - c_1 y)\frac{\partial \rho}{\partial z} + (c_1 z - c_3 x)\frac{\partial \rho}{\partial y} + (c_3 y - c_2 z)\frac{\partial \rho}{\partial x} = 0. \tag{3.26}$$

Hence

$$\rho = F(x^2 + y^2 + z^2, c_1 x + c_2 y + c_3 z) = F(\tilde{a}, b). \tag{3.27}$$

To find the constraints on F we substitute this result in (3.23)-(3.25) to obtain

$$a_8 \frac{\partial F}{\partial b} + 2 \frac{\partial F}{\partial \tilde{a}} = 0. \tag{3.28}$$

Hence

$$F = F(2b - a_8 \tilde{a}). \tag{3.29}$$

We also note that if $\boldsymbol{c} = 0$ then it is easy to show that $F = F(\tilde{a})$. Similarly if $a_8 = 0$ then $F = F(b)$. We also observe that if $\boldsymbol{B} = 0$ then from (2.26), (2.27) it follows that $u - v = 0$.

3.3. Two of a_5, a_6 and a_7 are zero

In the following we treat only one case

$$a_5 \neq 0 \qquad a_6 = a_7 = 0$$

as other possible choices yield symmetric results.

From (3.6) it follows that $c_3 = c_2 = 0$ and therefore equations (3.13)-(3.15) reduce to

$$y \frac{\partial \rho}{\partial z} - z \frac{\partial \rho}{\partial y} = 0 \tag{3.30}$$

$$z(a_5 x + a_8) \frac{\partial \rho}{\partial x} - [\tfrac{1}{2} a_5 (x^2 - y^2 - z^2) + a_8 x + c_1] \frac{\partial \rho}{\partial z} = -2a_5 x \rho \tag{3.31}$$

$$[\tfrac{1}{2} a_5 (x^2 - y^2 - z^2) + a_8 x + c_1] \frac{\partial \rho}{\partial y} - y(a_5 x + a_8) \frac{\partial \rho}{\partial x} = 2a_5 y \rho. \tag{3.32}$$

From these equations it is obvious that without loss of generality we can let $a_5 = 1$. From (3.30) it follows that

$$\rho = F(y^2 + z^2, x) = F(s, x).$$

Substituting this in (3.31) or (3.32) yields

$$(x + a_8) \frac{\partial F}{\partial x} - 2[\tfrac{1}{2}(x^2 - s) + a_8 x + c_1] \frac{\partial F}{\partial s} = -2F.$$

Hence

$$F = \frac{1}{(x + a_8)^2} G\left(\frac{a}{x + a_8}\right). \tag{3.33}$$

Thus although the treatment needed in this case is somewhat different than in § 3.1 the final result is the same, i.e. it can be obtained by substituting $a_6 = a_7 = c_2 = c_3 = 0$ in (3.22).

4. Solutions for *A*

In this section we solve equations (2.14) and (2.15) in full generality for the class of admissible potential differences which were found in the previous section. At the same time we also present the general form of the potentials u which are compatible with the resulting constraints.

As in the previous section we divide our discussion into cases. However we do not treat separately the case $a_6 = a_7 = c_2 = c_3 = 0$ in view of the results of the previous section.

4.1. $w \neq 0$ (assume that at least a_5, $a_6 \neq 0$)

Taking the vector product of (2.15) with $\boldsymbol{w}$ and using (3.7) we obtain

$$(\boldsymbol{w}\times\boldsymbol{x})\cdot\nabla A = 0. \tag{4.1}$$

Hence

$$A = \tilde{h}(\boldsymbol{x}\cdot\boldsymbol{x}, \boldsymbol{w}\cdot\boldsymbol{x}) = h(a, f). \tag{4.2}$$

Substituting this result in (2.15) leads to

$$2\left(2x\frac{\partial A}{\partial a} + a_5\frac{\partial A}{\partial f}\right) + B_1\rho = a_5 \tag{4.3}$$

$$2\left(2y\frac{\partial A}{\partial a} + a_6\frac{\partial A}{\partial f}\right) + B_2\rho = a_6. \tag{4.4}$$

Multiplying (4.3) and (4.4) by a_6 and a_5 respectively and subtracting using (3.7) yields

$$4\frac{\partial A}{\partial a} + f\rho = 0. \tag{4.5}$$

Similarly if we multiply these equations by y and x respectively and subtract we obtain (after using (3.7))

$$4\frac{\partial A}{\partial f} - a\rho = 2. \tag{4.6}$$

From (4.5) and (4.6) it follows then that

$$2a\frac{\partial A}{\partial a} + 2f\frac{\partial A}{\partial f} = f. \tag{4.7}$$

Hence

$$A = \tfrac{1}{2}f - \tfrac{1}{4}F(\alpha) \tag{4.8}$$

where $\alpha = a/f$.

Substituting this result back in (4.5) using (3.22) leads to

$$F' = G. \tag{4.9}$$

Substituting (4.8) and (4.9) in (2.14) yields after somewhat lengthy algebra to

$$(\nu F')' + \tfrac{1}{8}(F^2)' = -f[\boldsymbol{B}\cdot\nabla u + 2f(u+\lambda)] \tag{4.10}$$

where

$$\nu = \tfrac{1}{4}\alpha^2(\boldsymbol{w}\cdot\boldsymbol{w}) + a_8\alpha + c_1/2a_5. \tag{4.11}$$

Hence

$$\nu F' + \tfrac{1}{8}F^2 = -g(\alpha) \tag{4.12}$$

and

$$\boldsymbol{B}\cdot\nabla u+2f(u+\lambda)=g'(\alpha)/f^2 \tag{4.13}$$

where $g(\alpha)$ is some smooth function.

Equation (4.12) is a Ricatti equation which can be linearised through the transformation

$$F=8\nu\sigma'/\sigma \tag{4.14}$$

and we obtain

$$(\nu\sigma')'+\frac{g(\alpha)}{8\nu}\sigma=0. \tag{4.15}$$

Equation (4.13) on the other hand imposes a constraint on the potentials u which are amenable for treatment by Darboux transformations (under the present assumptions). To see how this constraint is satisfied we introduce

$$q=f^2\cdot(u+\lambda). \tag{4.16}$$

Equation (4.13) becomes

$$\boldsymbol{B}\cdot\nabla q+2q\nu'-g'(\alpha)=0. \tag{4.17}$$

To eliminate the middle term in (4.17) we define $q=p/\nu$ and obtain

$$\boldsymbol{B}\cdot\nabla p=g'(\alpha)\nu. \tag{4.18}$$

The general solution of equation (4.18) is the sum of a particular solution of the inhomogeneous equation and the general solution of the homogeneous one. To find a particular solution we let $p=p(\alpha)$ in (4.18) and obtain $p=g/2$. To solve the homogeneous part of (4.18) we make a coordinate transformation to

$$\boldsymbol{\beta}=\boldsymbol{w}\times\boldsymbol{x} \tag{4.19}$$

and obtain

$$\left(\beta_1\frac{\partial}{\partial\beta_1}+\beta_2\frac{\partial}{\partial\beta_2}+\beta_3\frac{\partial}{\partial\beta_3}\right)p=0. \tag{4.20}$$

Hence the general solution for p is

$$p=\frac{g(\alpha)}{2}+\tilde{p}(\beta_2/\beta_1,\beta_3/\beta_1). \tag{4.21}$$

Thus we proved that equation (4.10) is consistent only if $u+\lambda$ is of the form

$$u+\lambda=(1/f^2\nu)[\tfrac{1}{2}g(\alpha)+\tilde{p}(\beta_2/\beta_1,\beta_3/\beta_1)]. \tag{4.22}$$

A is then obtained from equations (4.14) and (4.15). We believe that the results represented by (4.22) and (3.22) are new.

4.2. $\boldsymbol{B}=\boldsymbol{c}$

Since $\boldsymbol{B}=0$ is trivial we can assume without loss of generality that $\boldsymbol{B}^2=1$ and $B_1\neq 0$. To solve equation (2.15) under the present assumptions we take the scalar product of this equation with $\boldsymbol{B}$ and introduce the coordinates.

$$\begin{aligned}&\alpha=B_1x+B_2y+B_2z\\ &\beta=B_1z-B_3x \qquad \gamma=B_1y-B_2x.\end{aligned} \tag{4.23}$$

We obtain using the previous results about this case that

$$\frac{\partial A}{\partial \alpha}+\tfrac{1}{2}\rho=0 \tag{4.24}$$

i.e.

$$A=\tfrac{1}{2}\int \rho(\alpha)\,\mathrm{d}\alpha+\xi(\beta,\gamma). \tag{4.25}$$

However if we substitute this back in (2.15) it follows that ξ must be a constant. Substituting these results in (2.14) leads to

$$A''-(A^2)'+\boldsymbol{B}\cdot\nabla u=0. \tag{4.26}$$

Hence

$$A'-A^2=-g(\alpha) \tag{4.27}$$

and

$$B\cdot\nabla u=g'(\alpha). \tag{4.28}$$

Using the same coordinate transformation as before we infer that

$$u=g(\alpha)+\xi_2(\beta,\gamma) \tag{4.29}$$

where ξ_2 is an arbitrary smooth function. Equation (4.27) can be linearised and solved through the transformation $A=\sigma'/\sigma$.

4.3. $\boldsymbol{B}=a\boldsymbol{x}+\boldsymbol{c}$, $a\neq 0$

When $a\neq 0$ we can let $\boldsymbol{c}=0$ since equations (2.14) and (2.15) are invariant with respect to translations. From the results of the previous section it then follows that $\rho=\rho(r)$ and it is natural to treat this case in spherical coordinates.

Since $B_r=ar$, $B_\theta=B_\varphi=0$ it follows from (2.15) that

$$\frac{\partial A}{\partial \theta}=\frac{\partial A}{\partial \varphi}=0. \tag{4.30}$$

Hence $A=A(r)$ and $\rho=-2A'/ar$. Substituting these results in (2.14) leads to

$$rA''+2A'-\frac{1}{a}(A^2)'+a\frac{\partial}{\partial r}[r^2(u+\lambda)]=0. \tag{4.31}$$

Hence

$$\frac{\partial}{\partial r}[r^2(u+\lambda)]=g'(r) \tag{4.32}$$

and

$$rA'+A-\frac{1}{a}A^2+ag(r)=0 \tag{4.33}$$

where $g(r)$ is an arbitrary smooth function. Thus $u+\lambda$ must be of the form

$$u+\lambda=r^{-2}[g(r)+\xi(\theta,\varphi)]. \tag{4.34}$$

Equation (4.33) is once again a Ricatti equation which can be linearised by the transformation

$$A = -ar\sigma'/\sigma \tag{4.35}$$

which yields

$$(r^2\sigma')' - g(r)\sigma = 0 \tag{4.36}$$

and

$$\rho = u - v = (2/r)[r\sigma'/\sigma]'. \tag{4.37}$$

We observe that equation (2.9) with potentials of the form (4.34) is separable. In fact it is easy to show that the results of this case can be obtained by performing one-dimensional Darboux transformations on the radial part of equation (2.9) with $B = ar$. In view of this result it is important to point out that when $w \neq 0$ equations (4.22) and (3.22) establish the existence of a generic new class of potentials and potential differences in three dimensions whose solutions are related to each other by Darboux transformations.

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