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ORIGINAL PAPER

Two-dimensional Darboux transformations for non-separable angular equations and solvable non-central potentials

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Abstract We construct a two-dimensional Darboux transformation for the angular equation that arises from variable separation of a Schrödinger equation in spherical coordinates. Since we do not assume the angular equation to be further separable, our Darboux transformation allows for the systematic generation of solvable non-central potentials that are not accessible through the usual separation of variables.

Keywords Separation of variables · Angular equation · Non-central potential · Two-dimensional Darboux transformation

1 Introduction

It is well-known that the multivariable Schrödinger equation admits closed-form solutions only in very few cases, the vast majority of which can be found by performing a separation of variables. While the advantage of this process is its simplicity, its applicability is limited to a certain class of potentials per given coordinate system [15,16]. One of the most thoroughly studied cases in this regard is the three-dimensional spherical coordinate system, which applies to many problems in atomic and molecular physics [4]. If the potential is spherically symmetric (central potential), the Schrödinger equation always admits separation of variables, such as in the case of the Coulomb potential in the hydrogen atom. Even if the potential exhibits angular dependence (non-central potential), separability of the Schrödinger equation is not necessarily broken. In many cases, closed-form solutions have been found after a separation of variables, such as in [2,7,12] and references therein. The study of non-central

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potentials is motivated by their high importance in many areas of quantum physics and quantum chemistry. They serve as models for the structure of metallic glasses [9], they describe the quantum dynamics of ring-shaped molecules [8], they are used in the area of nanostructures [10] and scattering theory [11], among others. Clearly, not all non-central potentials that are important in applications render the Schrödinger equation separable, such that usually no closed-form solution can be found. Therefore, the purpose of the present note is to provide a method for solving Schrödinger equations, the potentials of which present non-separable angular dependence. Our method is an adaptation of the recently developed two-dimensional Darboux transformation [13], the one-dimensional counterpart of which [6] became famous in the context of supersymmetry [3,5]. The principal idea is to rewrite the angular part of the Schrödinger equation, such that it takes Schrödinger form itself and allows for the application of our two-dimensional Darboux transformation. In Sect. 2 we briefly summarize basic facts about the two-dimensional Darboux transformation, while Sect. 3 is devoted to the construction of the modified Darboux transformation that applies to the angular part of the Schrödinger equation. In Sect. 4 we present a simple application that illustrates our method.

2 Preliminaries

In [13], the two-dimensional Darboux transformation for time-dependent Schrödinger equations was introduced. The stationary version of this transformation will be needed in this note, such that we review it briefly. Let the following pair of two-dimensional Schrödinger equations be given

$$-(\Psi_{x_1x_1} + \Psi_{x_2x_2}) + V_1\ \Psi = 0 \tag{1}$$

$$-(\Phi_{x_1x_1} + \Phi_{x_2x_2}) + V_2\ \Phi = 0, \tag{2}$$

where the indices stand for partial differentiation. The solutions Ψ, Φ and the potentials V_1, V_2 can each depend on both of the two variables x_1, x_2. For the sake of simplicity, we assume the stationary energy to be zero. Now, let Ψ be a solution of the first Eq. (1) and let $L_1 = l_1 + l\ x_2$ and $L_2 = l_2 + l\ x_1$ for constants $l,\ l_1$ and l_2. Suppose v is a function in one variable that depends on its argument in the following way

$$v\ =\ v\left(\frac{L_1}{l\ L_2}\right), \tag{3}$$

and solves the auxiliary equation

$$-\frac{L_1^2+L_2^2}{2\ L_2^4}\ v'' + \frac{1}{2\ L_2^2}\ v'\ v + \frac{l\ L_1}{L_2^3}\ v' + L_1\ (V_1)_{x_1} + L_2\ (V_1)_{x_2} = 0. \tag{4}$$

Note that the prime denotes differentiation. Now define the Darboux transformation $\mathcal{D}(\Psi)$ of Ψ by

$$\mathcal{D}(\Psi) = \frac{1}{2}\, v + L_1\, \Psi_{x_1} + L_2\, \Psi_{x_2}. \tag{5}$$

Then the function $\Phi = \mathcal{D}(\Psi)$ is a solution of the transformed Schrödinger Eq. (2), where V_2 is related to its counterpart V_1 in (1) via

$$V_2 = V_1 - \frac{1}{L_2^2}\, v'. \tag{6}$$

Thus, the Darboux transformation (5) interrelates the solutions Ψ and Φ of the two-dimensional Schrödinger Eqs. (1) and (2), respectively.

3 The Darboux transformation

It is well known that after separation of variables, the three-dimensional Schrödinger equation in spherical coordinates splits into a one-dimensional radial and a two-dimensional angular part. A Darboux transformation for the radial part has already been constructed, see [14] for details. Usually, the angular part is again separated into a polar and an azimuthal equation, provided the underlying potential admits this separation. Instead of this approach, in the following we set up a Darboux transformation for the fully two-dimensional angular equation. We begin our considerations with a brief review of the variable separation process.

Separation of variables in spherical coordinates. We consider the three-dimensional stationary Schrödinger equation

$$-\left(\Psi_{x_1x_1} + \Psi_{x_2x_2} + \Psi_{x_3x_3}\right) + W_1\, \Psi = E\, \Psi, \tag{7}$$

where the potential W_1 and the solution Ψ can depend on all three spatial variables x_1, x_2, x_3, while the stationary energy E is a real constant. After introduction of the usual spherical coordinates r, θ and φ [1], Eq. (7) renders in the form

$$\Psi_{rr} + \frac{2}{r}\, \Psi_r + \frac{1}{r^2}\, \Psi_{\theta\theta} + \frac{\cos(\theta)}{r^2 \sin(\theta)}\, \Psi_\theta + \frac{1}{r^2 \sin^2(\theta)}\, \Psi_{\varphi\varphi} = (W_1 - E)\, \Psi. \tag{8}$$

We will now separate the radial variable r from the angular variables θ and φ. On setting $\Psi(r, \theta, \varphi) = R(r)\, Y(\theta, \varphi)$, Eq. (8) becomes after some elementary manipulations

$$\frac{R''}{R} + \frac{2\, R'}{r\, R} + \frac{Y_{\theta\theta}}{Y\, r^2} + \frac{\cos(\theta)\, Y_\theta}{Y\, r^2 \sin(\theta)} + \frac{Y_{\varphi\varphi}}{Y\, r^2 \sin^2(\theta)} = W_1 - E. \tag{9}$$

This equation is separable only if the potential W_1 can be written in the form

$$V(r,\theta,\varphi) = U_1(r) + \frac{1}{r^2}\, U_2(\theta,\varphi), \tag{10}$$

for arbitrary functions U_1 and U_2. After separation of variables and introduction of a separation constant λ, we obtain the following two equations:

$$R'' + \frac{2}{r}\, R' - \left(U_1 - E + \frac{\lambda}{r^2}\right) R = 0 \tag{11}$$

$$Y_{\theta\theta} + \frac{\cos(\theta)}{\sin(\theta)}\, Y_\theta + \frac{1}{\sin^2(\theta)}\, Y_{\varphi\varphi} - (U_2 - \lambda)\, Y = 0 \tag{12}$$

The first of these equations is the radial equation, while the second one is the angular equation, which we will focus on in the present work.

Darboux transformation for the angular equation. Our Darboux transformation (5) is not directly applicable to the angular Eq. (12), because it does not match the Schrödinger form (1). In order to fix this problem, we will proceed as follows: first, we use a particular coordinate change that converts (12) into a two-dimensional Schrödinger equation, which admits the Darboux transformation (5). The resulting transformed Schrödinger Eq. (2) is then subject to the inverse coordinate change, reinstalling the initial angular equation's form. This way we have constructed a Darboux transformation between two angular equations of the form (12). Let us apply this scheme by first employing the coordinate change

$$t = \log\left[\tan\left(\frac{\theta}{2}\right)\right], \tag{13}$$

which after substitution of $Y(\theta,\varphi) = \hat{Y}(t,\varphi)$ and replacing $\theta = 2\arctan[\exp(t)]$, converts our angular Eq. (12) into

$$\hat{Y}_{tt} + \hat{Y}_{\varphi\varphi} + \frac{\lambda - U_2}{\cosh^2(t)}\, \hat{Y} = 0. \tag{14}$$

This equation matches the Schrödinger form (1) in the coordinates t and φ, if we multiply by -1 and set the potential V_1 to

$$V_1 = -\frac{\lambda - U_2}{\cosh^2(t)}. \tag{15}$$

We are now ready to construct a Darboux transformation for the angular Eq. (12). To this end, we first apply (5) to the rewritten Eq. (14), and afterwards reinstall its initial form (12) by inverting our coordinate change (13). In the present case, the Darboux transformation for Eq. (14) can be obtained from (5) by renaming $x_1 = t$, $x_2 = \varphi$ and replacing the function Ψ by $\hat{Y}$:

$$\mathcal{D}(\hat{Y}) = \frac{1}{2}\, v + L_1\, \hat{Y}_t + L_2\, \hat{Y}_\varphi, \tag{16}$$

where we assume v to be defined by (3) and to solve the auxiliary Eq. (4) for the potential V_1 as specified in (15). Taking into account the explicit expressions $L_1 = l_1 + l\,\varphi$ and $L_2 = l_2 - l\,t$, the Darboux transformation (16) becomes

$$\mathcal{D}(\hat{Y}) = \frac{1}{2}\, v + (l_1 + l\,\varphi)\, \hat{Y}_t + (l_2 - l\,t)\, \hat{Y}_\varphi. \tag{17}$$

The function $\hat{Z} = \mathcal{D}(Y)$ solves the transformed counterpart of Eq. (14), that is,

$$\hat{Z}_{tt} + \hat{Z}_{\varphi\varphi} - V_2\, \hat{Z} = 0, \tag{18}$$

where V_2 is given by (6), which reads after substitution of (15)

$$V_2 = -\frac{\lambda - U_2}{\cosh^2(t)} - \frac{1}{L_2^2}\, v'. \tag{19}$$

Now, since the Darboux transformation (17) applies to the rewritten version (14) of our angular equation, we will now adjust it, such that it becomes applicable to the initial form (12). To this end, we need to replace the coordinate t by its counterpart θ, using the relation (13). This changes the functions L_1 and L_2 in the Darboux transformation (16) as follows:

$$L_1 \;=\; l_1 + l\,\varphi \qquad L_2 \;=\; l_2 - l\,\log\left[\tan\left(\frac{\theta}{2}\right)\right]. \tag{20}$$

Now, after substitution of $\theta = 2\arctan[\exp(t)]$, $Y(\theta,\varphi) = \hat{Y}(t,\varphi)$ and application of the chain rule, transformation (17) becomes

$$\mathcal{D}(Y) = \frac{1}{2}\, v + (l_1 + l\,\varphi)\, \sin(\theta)\, Y_\theta + \left(l_2 - l\,\log\left[\tan\left(\frac{\theta}{2}\right)\right]\right) Y_\varphi, \tag{21}$$

where according to (3) the function v depends on its arguments in the following explicit way

$$v \;=\; v\left(\frac{L_1}{l\,L_2}\right) \;=\; v\left[\frac{l_1 + l\,\varphi}{l\,\left(l_2 - l\,\log\left[\tan\left(\frac{\theta}{2}\right)\right]\right)}\right]. \tag{22}$$

Now, the function $Z = \mathcal{D}(Y)$ solves Eq. (18) after inverting the coordinate change (13), that is, after substitution of $\theta = 2\arctan[\exp(t)]$ and $Z(\theta,\varphi) = \hat{Z}(t,\varphi)$. Taking into account that v is given by (22), we obtain

$$Z_{\theta\theta} + \frac{\cos(\theta)}{\sin(\theta)} Z_\theta + \frac{1}{\sin^2(\theta)} Z_{\varphi\varphi} - \left[U_2 - \lambda - \frac{v'}{\sin^2(\theta)\left(l_2 - l \log\left[\tan\left(\frac{\theta}{2}\right)\right]\right)^2} \right] Z = 0. \tag{23}$$

This is the transformed angular equation. In summary, if Y is a solution of the angular Eq. (12), then $Z = \mathcal{D}(Y)$ as given in (21) is a solution of the transformed angular Eq. (23).

Solution of the initial Schrödinger equation. Returning to our initial Eq. (7), we can now state the solution of its transformed counterpart, after having performed the Darboux transformation on our angular equation. The transformed equation reads

$$-\left(\Phi_{x_1x_1} + \Phi_{x_2x_2} + \Phi_{x_3x_3}\right) + W_2\, \Phi = E\, \Phi, \tag{24}$$

where the potential W_2 can be obtained by combining (10) and (23):

$$W_2 = U_1(r) + \frac{1}{r^2} U_2 - \frac{v'}{r^2 \sin^2(\theta)\left(l_2 - l \log\left[\tan\left(\frac{\theta}{2}\right)\right]\right)^2}, \tag{25}$$

recall the dependency of v on its argument, see (3). Now, the corresponding solution Φ of Eq. (24) is given by the product $\Phi = RZ$, where R stands for the solution of the radial Eq. (11), and $Z = \mathcal{D}(Y)$ is the Darboux transformation (21):

$$\begin{aligned} \Phi(r,\theta,\varphi) &= R(r)\, Z(\theta,\varphi) \\ &= R(r)\left[\frac{1}{2}\, v\left(\frac{L_1}{l\, L_2}\right) + (l_1 + l\,\varphi)\, \sin(\theta)\, Y_\theta(\theta,\varphi) \right. \\ &\quad \left. + \left(l_2 - l \log\left[\tan\left(\frac{\theta}{2}\right)\right]\right) Y_\varphi(\theta,\varphi)\right]. \end{aligned}$$

The radial solution R has not been modified, as our Darboux transformation only affects the angular part. Therefore, the radial solution can be transformed independently, for example by means of a Darboux transformation, as developed in [14].

4 Application

We will now perform our Darboux transformation on an explicitly given angular equation of the form (12). We take the particular case $U_2 = 0$ and $\lambda = 0$, that is,

$$Y_{\theta\theta} + \frac{\cos(\theta)}{\sin(\theta)} Y_\theta + \frac{1}{\sin^2(\theta)} Y_{\varphi\varphi} = 0.$$

This equation admits the following particular solution:

$$Y(\theta, \varphi) = \log\left[\tan\left(\frac{\theta}{2}\right)\right] + \varphi. \tag{26}$$

Before we can perform our Darboux transformation (21) on the solution (26), we need to solve the auxiliary Eq. (4). Recalling that $V_1 = 0$ according to (15) and the present settings $U_2 = \lambda = 0$, the auxiliary equation reads

$$-\frac{L_1^2 + L_2^2}{L_2^2}\, v'' + v'\, v + \frac{2\, l\, L_1}{L_2}\, v' = 0.$$

This equation is solved by the function

$$\begin{aligned} v &= -\tanh\left[\frac{1}{2\, l}\, \arctan\left(\frac{L_1}{l\, L_2}\right)\right] \\ &= -\tanh\left[\frac{1}{2\, l}\, \arctan\left(\frac{l_1 + l\,\varphi}{l\, l_2 - l^2\, \log\left[\tan\left(\frac{\theta}{2}\right)\right]}\right)\right], \end{aligned} \tag{27}$$

where in the last step we have used the definitions (20), note further that the requirement (3) is fulfilled. Now that we have solved the auxiliary equation, we can proceed with our Darboux transformation (21), which reads in the present case

$$\mathcal{D}(Y) = -\frac{1}{2}\, \tanh\left[\frac{1}{2\, l}\, \arctan\left(\frac{L_1}{l\, L_2}\right)\right] + L_1\, Y_\theta + L_2\, Y_\varphi.$$

For the sake of brevity we have omitted to insert (20) here, that is, the explicit form of L_1 and L_2. After incorporation of our explicit solution as given in (26), the latter Darboux transformation becomes

$$\begin{aligned} \mathcal{D}(Y) = l_1 + l_2 + l\,\varphi - l\, \log\left[\tan\left(\frac{\theta}{2}\right)\right] \\ -\frac{1}{2}\left(\varphi + \log\left[\tan\left(\frac{\theta}{2}\right)\right]\right) \tanh\left[\frac{1}{2\, l}\, \arctan\left(\frac{L_1}{l\, L_2}\right)\right], \end{aligned} \tag{28}$$

where L_1 and L_2 are given by (20). The function $\mathcal{D}(Y) = Z$ is a solution of our transformed angular Eq. (23), which in the present case takes the following form:

$$\begin{aligned} Z_{\theta\theta} + \frac{\cos(\theta)}{\sin(\theta)}\, Z_\theta + \frac{1}{\sin^2(\theta)}\, Z_{\varphi\varphi} \\ -\left(2\, (L_1^2 + L_2^2)\, \sin^2(\theta)\, \cosh^2\left[\frac{1}{2\, l}\, \arctan\left(\frac{L_1}{L_2}\right)\right]\right)^{-1} Z = 0. \end{aligned} \tag{29}$$

Although the functions L_1 and L_2 still have to be substituted from (20), it is immediate to see that Eq. (29) is not further separable, such that we have generated a non-separable angular part of a potential in three dimensions. This potential belongs to the Schrödinger Eq. (24) and can be extracted from the general transformed potential (25) by substituting $U_2 = 0$ and the function v as given in (27):

$$W_2 = U_1(r) + \left(2\, r^2\, (L_1^2 + L_2^2)\, \sin^2(\theta)\, \cosh^2\left[\frac{1}{2\,l}\, \arctan\left(\frac{L_1}{L_2}\right)\right]\right)^{-1},$$

where L_1 and L_2 are given in (20). The corresponding solution Φ of the three-dimensional Schrödinger Eq. (24) is given by $\Phi = RZ$, where $Z = \mathcal{D}(Y)$ is given in (28).

5 Concluding remarks

We have shown that the two-dimensional Darboux transformation can be adapted to the angular equation that results from variable separation of the Schrödinger equation in three dimensions and spherical coordinates. Using our modified Darboux transformation, potentials with non-separable angular part can be generated, together with their corresponding solutions. In the present work we restricted ourselves to spherical coordinates, because they apply to many problems in atomic and molecular physics. In general, though, the two-dimensional Darboux transformation can be applied to any equation that can be linked to a Schrödinger equation.

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