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Pseudopotentials via Moutard Transformations and Differential Geometry

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Abstract. Darboux-like (Moutard) and generalized Moutard transformations in two dimensions are applied to construct families of zero range potentials of scalar and matrix equations of stationary quantum mechanics. The statement about such functionals, defined by closed coordinate curves obtained by Ribokur-Moutard transforms is formulated. Their applications in physics and differential geometry of surfaces are discussed.

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1. Introduction

Quite a number of problems in contemporary physics appear when continuous phenomena are joined with discrete one (discrete-continuous models). This concerns also point particles in quantum theory, mass tensors and Riemannian geometry in gravitation theory. The Dirac delta-function potential on the axis $x \in (-\infty, \infty)$ was first heuristically introduced by Fermi in a one-dimensional model. Its construction in the context of Neumann operator extension theory was understood in [1], see [2] for a review. The concept was realized as the theory of distributions on Schwartz space. A great number of applications of an advanced form of such potentials (zero-range potentials (ZRP) or pseudopotentials) appear in mesoscopic physics. Here it models objects whose dimension is small compared with the de Broglie wavelength of the electron. The generalization to the radial Schrödinger equation on the half-axis $r \in [0, \infty)$, started with a ZRP for s-states which was very successful in the application to scattering problems. From the point of a three-dimensional theory a mathematically rigorous formulation is given in [3]. Introducing the zero-range potential (ZRP) for two-dimensional problems needs special investigations [4].

We shall consider such problems from the point of view of a dressing technique for special cases of the Laplace equation, which allow a dressing procedure [5]. Such cases are known from the pioneering paper of Moutard [6]. More recent E. Ganzha applied it to an equation, equivalent to a Goursat equation [7]. Both equations have a direct link to the two-dimensional Schrödinger and Dirac equations.

As mentioned above, the Moutard and Goursat cases of the Laplace equations allow a kind of covariance statement which appeared already in [6, 8]. This was the starting point of the theory of Darboux transformations (DT). The DT in its original form [8] is a reduction of the Moutard transformation successfully applied by Darboux to the theory of surfaces.

One of the main observations is that the generalized ZRPs of the radial Schrödinger equation for arbitrary orbital quantum number l (GSRP), see, e.g., [3], appear as a result of iterated Darboux transformation in the context of radial Schrödinger equation theory. Such potentials are equivalent to boundary conditions, different for each l [9]. Namely, their three-dimensional description as pseudopotentials is studied in [3].

Two-dimensional ZRPs also may be obtained by DT-type transformations: the Moutard one and the generalized Moutard one for the Goursat case. The important feature of the MT is general for DT: the transform is parameterized by a pair of solutions of the equation and the transform vanishes if the solutions coincide. The Moutard equation (ME) is covariant with respect to the MT. It was studied in connection with central problems of classical differential geometry. More precisely, a chain of derivatives of solutions of the ME solves the system of Lamé equations for the Ribakur transformations [10].

In soliton theory the ME and GE enters the Lax pairs for nonlinear equations such as, for example, the Kadomtsev-Petviashvili and the Veselov-Novikov equation. This fact has important geometrical consequences as "integrable deformations of surfaces" [11].

In Section 2 we explain the general idea on an example of the radial Schrödinger equation along [9]. In Section 3, the Moutard transformation is used to define a chain of ZRP. The last section is devoted to the matrix ZRP problems of one of the two-dimensional two-component Dirac equation. The introduction of a pseudopotential by the generalized MT is traced.

2. General idea of ZRP introduction by dressing procedure

Let us consider a three-dimensional case of a so-called generalized ZRP [9]. Separation of variables yields the radial Schrödinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} + u_l - E\right)\psi_l(r) = 0. \tag{1}$$

where u_l are potentials for the partial waves. The equation (1) describes scattering of a particle with energy $E > 0$ and momentum $k = \sqrt{2E}$. In the absence of a potential, partial shifts $\delta_l = 0$ and partial waves can be expressed via Bessel

functions with half-integer indices. Let us demonstrate how a generalized ZRP (GZRP) can be introduced by the DT. Thus, the spectral problem for GZRP is solved for any value k. On the other hand, the equation (1) is covariant with respect to the DT that yields the corresponding transformations of the potentials

A GZRP is equivalent to a boundary condition at the singularity point $r = 0$

$$\frac{1}{r^{l+1}\psi}\frac{\partial^{2l+1}}{\partial r^{2l+1}}\left(r^{l+1}\psi\right)\Big|_{r=0} = -\frac{2^l l!}{(2l-1)!!}a_l^{2l+1}, \tag{2}$$

where we introduced $a_l^{2l+1} = -\frac{k^{2l+1}}{\tan\eta_l}$, with $s_l = \exp(2i\eta_l)$ being a scattering matrix. Such formulas are obtained by an application of an iterated DT to the zero potential solutions as follows. We start by choosing a spherical Bessel function as the seed solution $\psi_l(r) = Cj_l(kr)$ and apply Nth order Darboux transformation by taking spherical Hankel functions with specific parameters κ_m as prop functions $\varphi_m(r) = Ch_l^{(1)}(-i\kappa_m r)$, $m = 1, \ldots, N$. Crum's formula (e.g., [5]) gives the transformed solution

$$\psi_l^{[N]}(r) = C\frac{W(r\phi_1, \ldots, r\phi_N, r\psi_l)}{rW(r\phi_1, \ldots, r\phi_N)}. \tag{3}$$

The Wronskians can be computed if we consider the asymptotic behavior of the spherical functions at $r \to \infty$, the Wronskians turn into Vandermond determinants V, hence,

$$\psi_l^{[N]} = C\left[(-1)^l\frac{e^{ikr}}{kr}\frac{V(\kappa_1, \ldots, \kappa_N, ik)}{V(\kappa_1, \ldots, \kappa_N)} - \frac{e^{-ikr}}{kr}\frac{V(\kappa_1, \ldots, \kappa_N, -ik)}{V(\kappa_1, \ldots, \kappa_N)}\right]. \tag{4}$$

The Vandermond determinant can be computed by noticing that $k = -i\kappa_m$ (for $m = 1, \ldots, N$) are the roots of the polynomial with respect to k equation. This is obvious from the form of the matrix (replacing $ik \to \kappa_m$ yields that the determinant is zero due to the linear dependencies of the rows). Denoting $s_l = \prod_{m=1}^{N}(\kappa_m - ik)/(\kappa_m + ik)$, we recognize the asymptotics of spherical Hankel functions, hence

$$\psi_l^{[N]}(r) = C\left[s_l h_l^{(1)}(kr) - h_l^{(2)}(kr)\right]. \tag{5}$$

The effective potential corresponding to this solution tends to zero. Due to the asymptotic behaviour, we observe that the Darboux transformation does not change the behavior of the potential at $r \to \infty$, whereas the singular behavior at the origin is changed.

To sum up, the Darboux transformations significantly broaden the range of solvable potentials. In particular, they give a possibility to tune a free-space solution to potential scattering characteristics. Whilst the same transformation of the solution at the origin yields generalized zero-range potentials behavior.

3. Two-dimensional ZRP and Moutard transformation

Let us consider the Moutard equation

$$\psi_{\sigma\tau} + u(\sigma,\tau)\psi = 0\ . \tag{6}$$

The Moutard transformation [6, 5] is a map of Darboux transformation type: it connects solutions and the coefficient $u(\sigma,\tau)$ of the equation (6) so that if φ and ψ are different solutions of it (6), then the solution of the twin equation with $\psi \to \psi[1]$ and $u(\sigma,\tau) \to u[1]$ can be constructed by the system

$$(\psi[1]\varphi)_\sigma = -\varphi^2(\psi\varphi^{-1})_\sigma,$$
$$(\psi[1]\varphi)_\tau = \varphi^2(\psi\varphi^{-1})_\tau.$$

In other words,

$$\psi[1] = \psi - \varphi\Omega(\varphi,\psi)/\Omega(\varphi,\varphi)\ , \tag{7}$$

where Ω is the integral of the exact differential form

$$d\Omega = \varphi\psi_\sigma d\sigma + \psi\varphi_\tau d\tau\ . \tag{8}$$

The transformed coefficient (potential in mathematical physics) is given by

$$u[1] = u - 2(\log\varphi)_{\sigma\tau} = -u + \varphi_\sigma\varphi_\tau/\varphi^2\ . \tag{9}$$

Changing variables by the complex substitution $\sigma = x + iy, \tau = x - iy$ transforms (6) to a two-dimensional Schrödinger equation for x, y for potentials linked by $U(x,y) = -u(\sigma,\tau) + E$

$$-\frac{1}{4}[\psi_{xx} + \psi_{yy}] + U(x,y)\psi = E\psi\ . \tag{10}$$

The transformed potential is obtained via (9).

The explicit form of the ZRP depends on a choice of symmetry. For a cylindric symmetry [3], passing to polar coordinates $x = \rho\cos\phi, y = \rho\sin\phi$ and separating variables $\exp[i\nu\phi]R$ yields either R as solutions of the modified Bessel equation for $E = k^2 > 0$, or the Bessel equation for $E = -\kappa^2 < 0$. The case may be treated almost identically as in Section 2 by means of an iterated (multi-kink) MT, see the Wronskian formulas in [5].

We, however, develop the theory by the MT, extending it to more general symmetry, rewriting the (9) in polar coordinates

$$U[1] = U + \frac{1}{2}\Delta(\log\varphi) = U + \frac{1}{2}[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} + \frac{1}{\rho^2}\frac{d^2}{d\phi^2}](\log\varphi), \tag{11}$$

while $\psi[1]$ is the ψ transform by (7) with

$$\int d\Omega = \frac{1}{2}\int_{0,0}^{\rho,\phi}\left[(\psi\varphi)_\rho - i\ \frac{\varphi^2}{\rho}\left(\frac{\psi}{\varphi}\right)_\phi\right]d\rho + \left[(\psi\varphi)_\phi + i\rho\varphi^2\left(\frac{\psi}{\varphi}\right)_\rho\right]d\phi. \tag{12}$$

For $E = 0$, the Euler equation case in the ρ variable is obtained, and a general solution is $\psi = \sum_{\nu=-\infty}^{+\infty} c_n \exp[i\nu\phi]\rho^\nu$. To demonstrate it by an example, let us substitute the particular solutions $\varphi = \exp[i\nu\phi]\rho^\nu$ into the MT formulas (9). Direct

differentiation prove a potential invariance $U[1] = U$. The same result gives the special case of $\nu = 0$, $\varphi = C \ln \rho + A$. Studying the case $E = 0$, take as ψ typical for scattering problems the free particle state $\psi = \exp[k_x \rho \cos\phi + k_y \rho \sin\phi]$. A choice of an integration curve in (12) yields

$$\int d\Omega = \tfrac{1}{2}(k_x - ik_y)\left(\int_o^\rho \rho^\nu e^{k_x z}\, dz + i\rho^{\nu+1} \int_0^\phi e^{[i(\nu+1)\beta + \rho k_x \cos\beta + \rho k_y \sin\beta]} d\beta\right).$$

Going to a vicinity of $\rho = 0$, approximating the integral and plugging it into the MT (7) gives for $\nu \neq -1$ a continuous function

$$\psi[1] = \exp[k_x \rho \cos\phi + k_y \rho \sin\phi] - \rho e^{-i\nu\phi} \frac{k_x - ik_y}{\nu + 1}\left(e^{i\phi(\nu+1)} + 1\right). \tag{13}$$

Consider the Hilbert space $H = L_2$ and a manifold of continuous functions $\psi \in M \subset H$. Applying Gauss theorem yields for a disk S inside a circumference L of small radius ϵ,

$$\lim_{L\to 0} \int_S \Delta\psi dS + 2\int_S \alpha\delta_2(\rho,\phi)\psi\rho d\rho d\phi = \lim_{L\to 0} \int_L (\vec{n}\cdot\nabla\psi) dL + 2\alpha \int_0^{2\pi} \psi(0,\phi) d\phi, \tag{14}$$

by definition of $\delta_2(\rho, \phi)$.

Generalizing to functions with possible singularity in $\rho = 0$, we arrive at a boundary condition for the solution (6) with zero potential of the form

$$\lim_{L\to 0} \frac{\int_L (\vec{n}\cdot grad\psi)\rho d\phi}{\int_0^{2\pi} \psi(\epsilon,\phi)) d\phi} = 2\alpha. \tag{15}$$

Now we can formulate the approach to ZRP in two dimensions by the following algorithm. It is known that the set of iterated MT has an explicit link to Ribokur transformations. This defines solutions of the Lamé equations for coordinate systems [10], see also [12].

Generalizing (15), let us build a closed curve L as a coordinate line $\exists \epsilon > 0, a = a_0 \in [0, \epsilon], b \in [0, 1]$ by means of such a construction and define the action of $\delta_2(a, b)$ by

Lemma. *The relation* $\int_S \delta_2(a,b)\psi(a,b)dS = \int_0^1 \psi(0,b)db$ *determines a distribution* $\delta_2(a,b) \in D$, *if* L *bounds a domain* S (*interior of* L).

For the proof it is enough to recall the isoperimetric inequality and the Jordan theorem; the functional linearity and continuity is obvious. Going to the set of coordinate systems a_n, b_n, numbered by the MT iteration number yields the

Theorem 1 (Main). *The set of distributions defined by*

$$\lim_{\epsilon\to 0} \frac{\int_0^1 (\vec{n}\cdot grad\psi) db_n}{\int_0^1 \psi(a_n, b_n) db_n} = 2\alpha \tag{16}$$

is dense in a vicinity of 0.

The proof is based on the lemma and the theorem of Ganzha on local completeness of iterated Moutard transformations [10].

4. Goursat equation, matrix ZRP and geometry of surfaces

Let us consider the Laplace equation

$$\psi_{\sigma\tau} + a\,(\sigma,\tau)\,\psi_\sigma + b\,(\sigma,\tau)\,\psi = 0. \tag{17}$$

The system

$$\psi_\sigma = p\chi, \quad \chi_\tau = p\psi, \tag{18}$$

is related directly to the Goursat equation

$$\psi_{\sigma\tau} = \frac{p_\tau}{p}\psi_\sigma + p^2\psi, \tag{19}$$

with the obvious constraint between a, b in (17); see [7], where a covariance with respect to a generalized MT was established. In [13], the matrix form of the problem for $\Psi = \begin{pmatrix} \psi_1 & \psi_2 \\ \chi_1 & \chi_2 \end{pmatrix}$ was introduced in the variables ξ and η as:

$$\partial_\sigma = \partial_\eta - \partial_\xi, \qquad \partial_\tau = \partial_\eta + \partial_\xi,$$

and rewritten (18) in the form of 2x2 Dirac system:

$$\Psi_\eta = \sigma_3\Psi_\xi + U\Psi, \tag{20}$$

where $U = p(\xi,\eta)\sigma_1$. The functions $\psi_k = \psi_k(\xi,\eta)$, $\chi_k = \chi_k(\xi,\eta)$ with k=1,2 are particular solutions of (20) with some $p(\xi,\eta)$, and $\sigma_{1,3}$ are the Pauli matrices. Let $\Psi_1 \neq \Psi$ be a solution of the equation (20). We define a matrix function $\Xi \equiv \Psi_{1,\xi}\Psi_1^{-1}$. The equation (20) is covariant with respect to DT:

$$\Phi[1] = \Phi_\xi - \Xi\Phi, \qquad U[1] = U + [\sigma_3, \Xi]. \tag{21}$$

Let us consider a closed 1-form

$$d\Omega = \Phi\Psi d\xi + \Phi\sigma_3\Psi d\eta.$$

Lemma. *The form is exact if* Ψ *satisfies* (20) *and a* 2×2 *matrix function* Φ *solves the conjugate equation:*

$$\Phi_\eta = \Phi_\xi\sigma_3 - \Phi U. \tag{22}$$

The proof is by direct cross differentiation.

Theorem 2 ([13]). *One can verify by a substitution that* (22) *is covariant with respect to the transform if*

$$\Phi[+1] = \Omega(\Phi, \Psi_1)\Psi_1^{-1}. \tag{23}$$

Now we can alternatively affect U*, by the following transformation:*

$$U[+1,-1] = U + [\sigma_3, \Psi_1\Omega^{-1}\Phi]. \tag{24}$$

Relations (23), (24) we call a binary generalized Moutard transformation (BGMT).

Such a formalism gives a new possibility to define **ZRP for Dirac equation** via Darboux (21) or BGMT (23) transformation. The construction starts from a solution with a matrix potential U which directly relates to the equation (19) with constant p. Therefore we can use the solutions ψ_k of the Schrödinger equation (10)

with $E = p^2$, constructed in the previous section. The matrices Ψ, Φ, are built from solutions ψ_k and $\chi_k = p^{-1}\psi_k$.

As **geometry** is concerned, the original Weierstrass formulas start with two arbitrary holomorphic functions of complex variables $z, \bar{z} \in C$ [12]. They yield an approach for constructing minimal surfaces. Generalization to the arbitrary mean curvature case was given by Kenmotsu [14] and Konopelchenko [11] in complex coordinates as in (6), τ, $\sigma = -\overline{\tau}$. Here p is a real-valued function and ψ or χ as solutions of (18) are complex-valued functions. We define three real-valued functions X_i, $i = 1, 2, 3$ which are the coordinates of a surface in $\mathbb{R}^3$: $X_1 + \imath X_2 = 2\imath \int_\Gamma \left(\overline{\psi^2} d\sigma' - \overline{\chi^2} d\tau'\right), X_3 = -2 \int_\Gamma \left(\overline{\psi}\chi d\sigma' + \overline{\chi}\psi d\tau'\right)$, where Γ is an arbitrary path of integration in the complex plane. The corresponding first fundamental form, the Gaussian curvature K and the mean curvature H yield:

$$ds^2 = 4N^2 d\tau d\sigma \ , \quad K = \frac{1}{N^2}\partial_\tau \partial_\sigma \ln N \ , \quad H = \frac{\sqrt{p}}{N} \ . \tag{25}$$

Here $N = \mid \psi \mid^2 + \mid \chi \mid^2$. Any analytic surface in $\mathbb{R}^3$ can be globally represented by X_i. As it is seen from the solutions nonzero N may yields zero p and hence zero mean curvature on a punctured surface [15].

Remark. Equation (20) is a spectral problem for the Davey-Stewartson (DS) and Boiti-Martina-Leon-Pempinelli (BMLP) equations and produce explicitly invertible Bäcklund auto-transformations. It also induces deformations of the correspondent surfaces following [11, 13].

5. Discussion and conclusion

The importance in applications of the pseudopotentials, introduced as distributions, lies in the possibility to solve multicenter scattering or eigenvalue problems [2]. The dressing procedure also may be applied to such multicenter pseudopotential. This gives additionally ability to approximate real interaction [5]. Technically it is applied to a combination of Green functions of the Schrödinger equation $\psi = \sum C_i G(|\vec{r} - \vec{r}_i|)$ and, next, substituting the result, to boundary conditions in each center ($\vec{r} = \vec{r}_i$). The result is a set of algebraic equations. One of the interesting problems is related to quantum dots, randomly distributed by place and size, and modeled by a generalized ZRP. The theorem about a dense cover of the distribution space in a vicinity of a given point opens a way to developing new representations in potential theory. The problem of the matrix ZRP introduction is solved in an example of a two-dimensional Dirac equation. The idea of a dressing scheme is naturally generalized to other matrix problems as multi-channel scattering [5] or 4×4 matrix Dirac eigenvalue problem [16].

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