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PROPERTIES OF THE SOLUTIONS OF A SYSTEM OF COUPLED SCHRODINGER EQUATIONS

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Abstract
Singularities of solutions for a system of Coupled Schrodinger Equations are studied according to Gantmacher's method for differential matrix equations. Properties of the solutions of Coupled Schrodinger Equations, obtained within this formal frame, are related to basic properties of Scattering Matrix for multichannel system.
Keywords: Coupled Schrodinger Equations, Gantmacher's method

1. Introduction

The Coupled Schrodinger Equations are formal frame for many problems of Quantum Scattering Theory, e.g. [1]. Usually, for practical purposes, a system of coupled Schrodinger equations is solved by numerical approximation methods. There are now methods [2], [3], which provide analytical formulae for the regular and irregular solutions of this system, as well as for their derivatives, [4]. These methods permit an insight into the properties of the solutions of the system. In this paper we present some properties of the solutions of matrix Schrodinger equation which result from their analytical expressions, as well as, from Scattering Matrix symmetry and unitarily.

2. Method and samples

Let us consider the system of *n* coupled Schrodinger equations:

$$\frac{d^2X(x)}{dx^2} = V(x)X(x) \tag{1}$$

where V(x) - potential matrix with the properties:

$$V_{ii} = \frac{\gamma_{i(\gamma_i+1)}}{x^2} + \frac{\beta_i}{x} + V_i(x) \tag{2}$$

$V_i(x \to 0), V_{ik}(x \to 0) = const. (i,k = 1,2,\cdots,n)$

The angular momentum γ_i, the Coulomb parameter β_i and the potentials V_i and V_{ik} are complex quantities. We suppose that the real part of γ_i is a positive number: Re $\gamma_{n-i+1} = m_i + \sigma_i$, $m_i = 0,1,\cdots,n$, and $0 < \sigma_i < 1$.

The system (1) can be transformed [2, 3], into the following first order matrix equation:

$$\frac{dY(x)}{dx} = A(x)Y(x) \tag{3}$$

where

$$Y = \begin{pmatrix} x' \\ x \end{pmatrix}, A = \begin{pmatrix} 0 & V \\ I & 0 \end{pmatrix}, I = \|\delta_{ik}\| \tag{3'}$$

The complete solution of this system is [3]:

$$Y = \begin{pmatrix} X'_r & X'_{ir} \\ X_r & X_{ir} \end{pmatrix} = B^{-1}S^{-1}Gx^M x^{U+\Delta+D} \tag{4}$$

where *r* and *ir* stand for regular and irregular, respectively, and $'$ for derivation with respect to *x*. The explicit forms of solutions are [3, 4]:

$$X_r(x) = TG_{11}(x)x^{M_1}x^{U_{11}+D_1}$$
$$X_{ir}(x) = X_r(x)U_{12}\ln x + TG_{12}(x)x^{M_2}x^{U_{22}+D_2} \tag{5}$$

The same notations as in [3] and [4] were used $\left(\mathrm{M}_1 = |\mathrm{m}_\mathrm{i}\delta_\mathrm{ik}|, \mathrm{D}_1 = |\sigma_\mathrm{i}\delta_\mathrm{ik}|\right)$

$$B_{11} = -B_{22} = \left\| \left(\frac{\beta_i}{2(\gamma_i+1)} + \frac{\gamma_1+1}{x} \right) \delta_{ij} \right\|$$

$$B_{12} = B_{21} = 1$$

$$S_{11} = T; T = \|\delta_{i,n+1-i}\|; S_{12} = S_{21} = 0; S_{22} = I$$

$$\Lambda = \|\lambda_{ij}\|; \lambda_{ij} = (\gamma_{n+1-i})\delta_{ij}; \lambda_{n+i;n+j} = -(\gamma_{n+i,n+j}+1)\delta_{ij}$$

We list here the following properties of U_{11}, U_{12} and $U_{22}, (U_{12} = 0)$, which can be obtained from [3] (formula 18):

$$U_{11} = U_{22} = 0 \; For \; \mathrm{Re}(\gamma_i - \gamma_j) = 1,2,3,\cdots (all\ i\ and\ j)$$
$$U_{12} = 0 \; For \; \mathrm{Re}(\gamma_i - \gamma_j) = 1,2,3,\cdots (all\ i\ and\ j) \tag{6}$$
$$U_{11} = U_{12} = U_{22} = 0 \; For \; \mathrm{Re}\,\gamma_i \neq \frac{n}{2}, (n = 1,2,3,\cdots), (all\ i)$$

T is a constant matrix and $G(x=0)=I$; so the singular terms of the type x^{-m} or $\ln x$ come only from $x^{M_2} = \left| x^{m_{n-i+1}} \delta_{ik} \right|$ and $x^{U+D} = I$ power series in $\left[(U+D)\ln x \right]$,[5]. For $\left(U_{11} + D_1 \right)$ non-diagonal matrix there are the $\ln x$-like terms in the formula of the regular solution. This property is known in another context, e.g.[6], and only for γ_i a real integer. However $X_r(x \to 0) \to 0$, owing to the presence of the matrix x^{M_2}. For $U_{12} = 0$, the first term from X_{ir} formula disappears. The irregular solution X_{ir} has a $\ln x$-like term only for an integer or half-integer real part of the angular momentum γ_i. For $U_{11} = U_{12} = U_{22} = 0$ $\left(\mathrm{Re}\,\gamma_1 \neq \frac{n}{2} \right)$, there are not the $\ln x$-like terms in the formulas (5) for the regular and irregular solutions.

Let us consider as an example the irregular Coulomb function, $X_{ir} = G_\gamma$.

$$G_\gamma = F_\gamma U_{12} \ln x + G_{12} x^{-(\gamma+1)} \tag{7}$$

For $\mathrm{Re}\,\gamma_1 \neq \frac{n}{2}$, $U_{12} = 0$, the first term disappear and remains only the $x^{-(\gamma+1)}$-like singularity for the irregular Coulomb function, [7]. Similar properties hold for derivates also. This approach to study of matrix Schrodinger equations, applied to second-order linear differential equation with finite regular singularity, results into an unitary treatment of some special functions,[8]. The solutions properties, analyzed in this paper, can be verified on Hermite polynomials and parabolic cylinder functions.

3. Results and Discussions

Other properties of the solutions of the system of coupled Schrodinger equations can be obtained from Scattering Matrix symmetry and unitarily for a multichannel reaction system. We define the R-matrix function for a multichannel system by [9]:

$$\begin{aligned} R_r(x) &= X_r''(x) \quad X_r^{-1}(x) = D_x(X_r) \\ R_{ir}(x) &= X_{ir}''(x) \quad X_{ir}^{-1}(x) = D_x(X_{ir}) \\ R(x) &= X'_r(x) \quad X^{-1}(x) = D_x(X) \end{aligned} \tag{8}$$

Here $D_x(X) = X' X^{-1}$, denote the multiplicative Volterra derivative, e.g. [5], and $X = X_{ir} A + X_r B$ (A, B=constant matrices). The R-matrix function for a multichannel system appears as a Volterra derivative of the corresponding matrix radial solution. Now, the matrix [5], $X(x,x_0)$ can be defined by the relation:

$$X(x) = X(x,x_0)\, X(x_0) \tag{9}$$

where x_0 - arbitrary fixed point. Using this concept and the Volterra - derivative property

$$D_x = (X\ A) \quad \textit{(A = constant matrix)} \tag{10}$$

We obtain:

$$R = D_x(X(x,x_0)) \quad (\det .X(x_0) \neq 0) \tag{11}$$

The matrix $X(x,x_0)$ is the solution of the same equation as $X(x)$.

It has the following properties:

$$\begin{aligned} &X(i,k) = X(i,j)X(j,k) \\ &X^{-1}(i,k) = X(k,i) \\ &X(i,i) = I = \|\delta_{ik}\| \end{aligned} \tag{12}$$

We remark that these properties are identical with those of $T(t,t_0)$ - transition operator of quantum dynamics, e.g. [10].

The matrix properties (12) yield to the conditions:

$$X'_r(x_0,x_0) = X_{ir}(x_0,x_0) = I \tag{13}$$

$$X'_{ir}(x_0,x_0) = X_r(x_0,x_0) = 0 \tag{14}$$

Now the R-matrix symmetry $R_r = \tilde{R}_r,\ R_i = \tilde{R}_i,\ R = \tilde{R},$ (the symbol $\sim$ stands for transposition), implies:

$$\tilde{X}'_r(x,x_0)\, X_r(x,x_0) - \tilde{X}_r(x,x_0)\, X'_r(x,x_0) = 0 \tag{15'}$$

$$\tilde{X}'_i(x,x_0)\, X_i(x,x_0) - \tilde{X}_i(x,x_0)\, X'_i(x,x_0) = 0 \tag{15''}$$

$$\tilde{X}'_r(x,x_0)\, X_i(x,x_0) - \tilde{X}_r(x,x_0)\, X'_i(x,x_0) = \tilde{X}'_i(x,x_0)\, X_r(x,x_0) - \tilde{X}_i(x,x_0)\, X'_r(x,x_0) \tag{15'''}$$

The relations (15) have the following matrix form:

$$\tilde{Y}(x,x_0) G\, Y(x,x_0) = G \tag{16}$$

where G is: $$G = \begin{vmatrix} 0 & -I \\ I & 0 \end{vmatrix}_{2n,2n} \tag{17}$$

The relations (16) and (17) tell us that $Y(x,x_0)$ is a symplectic matrix.

Conclusions

The R-matrix symmetry implies the potential matrix symmetry and that the matrix is symplectic. Using the same method we can show that Scattering Matrix unitarily (R = real symmetric matrix [9]) implies $V = \tilde{V}^*$ and

$$Y^*(x,x_0)G\tilde{Y}(x,x_0) = G \tag{18}$$

Also, the reserve assertion, namely $V = \tilde{V}$ (or $V = \tilde{V}^*$) and the relation (16), (or (18)), implies Scattering Matrix symmetry (or unitarily).

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