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EXACT DECOUPLING OF A COUPLED SYSTEM OF TWO STATIONARY SCHROEDINGER EQUATIONS

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Abstract. In this paper we perform the exact decoupling of a coupled system of two 1-dimensional stationary Schroedinger equations that were originally considered by P.L. Christiansen, J.J. Rasmussen and M.P. Sorensen. Based on the characteristics of the uncoupled equations found, we argue that the coupled system of equations is spurious for the problem addressed.

1. Introduction

An interesting topic in the applied version of the theory of differential equations refers to the establishment of approaches and calculation methods that make it possible to solve different types of coupled differential equations, being of particular interest the analytical methods, and among these, those that can reveal, especially, the exact solutions. In some situations, it may be sufficient to have approximate solutions that arise from disregarding the term containing the coupling parameter, if this is relatively small, and if this approach is consistent with some context of the underlying problem; in this situation, it would be inevitable that the approximate solution carries less information[1] than the corresponding exact solution.

In mathematical modeling in physics, coupled differential equations determine, in many cases, the dynamics of several systems of particles. In quantum mechanics, in particular, in the case of the so-called non-ideal Stern-Gerlach effect, which manifests itself through the splitting of a beam of atoms into secondary beams in a plane to which correspond coupled equations for the components of the Pauli spinor, the spatial separation by spin states does not happen[2], otherwise what we have is the simultaneous presence, in each unfolded beam, both of electrons with their spin in the up state, and of electrons with their spin in the down state, as shown in the appendix in [6] through the decoupling of these equations without loss of information, that is, without making any approximation, thus preserving the exact character of the system solutions. The Cauchy problem for matrix factorizations of the Helmholtz equation are considered in papers [11]-[17].

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[1]Note that the information lost, through a specific approach, could be significant for a sector of the problem considered; therefore, it is worth remembering the possibility of making a different approximation if we are interested in disclosing such information.

[2]Contrary to the case with the plane for which the equations are decoupled, which is exclusively presented in textbooks [1] [2] [3] and other references [4] [5].

1.1. The coupled equations by Christiansen-Rasmussen-Sorensen. In an interesting recent work [7], addressing two situations of scattering by singular potentials, for the case of a potential $V(x) = \rho\, \delta(x)$, where ρ is non-negative, a pair of stationary and coupled Schroedinger equations for two wave functions, ψ_a and ψ_b, was proposed. This pair of equations, the one we will be dealing with here, is written as follows,

$$\hat{D}^2\psi_a(x) \ - \rho\, \delta(x)\, \psi_b(x) \ + \ k^2\psi_a(x) \ = \ 0, \tag{1.1}$$

$$\hat{D}^2\psi_b(x) \ - \rho\, \delta(x)\, \psi_a(x) \ + \ k^2\psi_b(x) \ = \ 0, \tag{1.2}$$

where: $\hat{D}^2 \equiv d^2/dx^2$; ρ being the coupling parameter; k the wavenumber and $\delta(x)$ the (what we like to call function) Dirac delta.

In [7] it is noted that the approach generally considered to deal with the Schroedin- ger equation for a quantum wave impinging on a localized potential barrier was equally applied to the case of coupled equations (1.1) and (1.2). It could be expected, however, that before applying this approach, the original equations could have been decoupled and only subsequently apply such treatment to them separately.

2. Mathematical development

In this section, we exactly decouple equations (1.1) and (1.2) without making any approximation, which is possible by imposing an adequate supplementary condition [6]. This supplementary condition may be compatible with a sector of the solution space of this coupled system, with, of course, other solutions of the system that do not fit this condition and which, for this very reason, will not be revealed through the method that will be used here.

The first thing to do is introduce a free parameter, λ, and construct a linear combination of the functions ψ_a and ψ_b as follows,

$$\chi(x) \equiv \psi_a(x) + \lambda\psi_b(x). \tag{2.1}$$

This expression is obtained by multiplying equation (1.2) by λ and adding it to equation (1.1). With this procedure, expression is also obtained[3],

$$\psi_b(x) + \lambda\psi_a(x). \tag{2.2}$$

Then, we consider a second free parameter, β, and it is imposed that,

$$\psi_b(x) + \lambda\psi_a(x) = \beta\chi(x). \tag{2.3}$$

which makes it possible to write the decoupled equation,

$$\hat{D}^2\chi(x) \ - \ \beta\rho\, \delta(x)\chi(x) \ + \ k^2\chi(x) = 0. \tag{2.4}$$

[3]One might expect us to follow, for example, the procedure that Feynman presents in subsection 9-3, in [8], when dealing with certain coupled differential equations, in which, in addition to adding the equations, he also subtracts them to obtain two new equations, which remain coupled. Here we follow another path.

The values of λ and β must be chosen properly, which will be shown later. Now let's consider two distinct functions χ_1 and χ_2, associated with certain distinct values λ_1 and λ_2, respectively; that is, based on (2.1), we write,

$$\chi_1(x) \;=\; \psi_a(x) \;+\; \lambda_1\psi_b(x), \tag{2.5}$$

$$\chi_2(x) \;=\; \psi_a(x) \;+\; \lambda_2\psi_b(x), \tag{2.6}$$

and assume that these are solutions of equation (2.4); accordingly, we write,

$$\hat{D}^2\chi_1(x) \;-\; \beta_1\rho\,\delta(x)\chi_1(x) \;+\; k^2\chi_1(x) = 0, \tag{2.7}$$

$$\hat{D}^2\chi_2(x) \;-\; \beta_2\rho\,\delta(x)\chi_2(x) \;+\; k^2\chi_2(x) = 0, \tag{2.8}$$

β_1 and β_2 being two distinct numbers corresponding, via (2.3), to the numbers λ_1 and λ_2, respectively.

We must invert expressions (2.5) and (2.6) so that functions ψ_a and ψ_b are in terms of functions χ_1 and χ_2, solutions of (2.7) and (2.8). Doing: $\Delta = 1/(\lambda_2 - \lambda_1)$, with $\lambda_2 - \lambda_1 \neq 0$, we write,

$$\psi_a(x) = \Delta\,\Big(\lambda_2\chi_1(x) - \lambda_1\chi_2(x)\Big), \tag{2.9}$$

$$\psi_b(x) = \Delta\,\Big(-\chi_1(x) + \chi_2(x)\Big). \tag{2.10}$$

Then, the function $\psi_a(x)$, as expressed in (2.9), and the function $\psi_b(x)$, as expressed in (2.10), must satisfy equation (1.1), which we reproduce below,

$$\hat{D}^2\psi_a(x) \;-\; \rho\,\delta(x)\psi_b(x) \;+\; k^2\psi_a(x) = 0$$

After making the corresponding substitutions, and sorting them, we find the expression,

$$\lambda_2\;K_1(x) - \lambda_1\;K_2(x) = 0. \tag{2.11}$$

where K_1 and K_2 are given by,

$$K_1(x) \equiv \hat{D}^2\chi_1(x) + \frac{1}{\lambda_2}\rho\,\delta(x)\chi_1(x) + k^2\chi_1(x),$$

$$K_2(x) \equiv \hat{D}^2\chi_2(x) + \frac{1}{\lambda_1}\rho\,\delta(x)\chi_2(x) + k^2\chi_2(x).$$

Note that the values that should be assigned to parameters β_1 and β_2, which are free up to now, will result from requiring that $K_1(x)$ and $K_2(x)$ cancel out simultaneously, thus verifying (2.11). These requirements will lead, by comparison with expressions (2.7) and (2.8), to relations between the parameters λ and β. In this way, it is found,

$$\beta_1 = -\frac{1}{\lambda_2} \qquad \text{and} \qquad \beta_2 = -\frac{1}{\lambda_1}. \tag{2.12}$$

Relations (2.12) are not enough to fix the values of these parameters; however, other independent relations can be obtained, for the same parameters, which will complement these considering that the functions $\psi_a(x)$ and $\psi_b(x)$ must also verify equation (1.2), which we reproduce below,

$$\hat{D}^2\psi_b(x) \;-\; \rho\,\delta(x)\psi_a(x) \;+\; k^2\psi_b(x) = 0.$$

Using (2.9) and (2.10) in (1.2) we obtain, after making the corresponding substitutions and sorting them,

$$-K_3(x) + K_4(x) = 0. \tag{2.13}$$

where K_3 and K_4 are given by,

$$K_3(x) \equiv \hat{D}^2\chi_1(x) + \lambda_2\rho\, \delta(x)\chi_1(x) + k^2\chi_1(x),$$

$$K_4(x) \equiv \hat{D}^2\chi_2(x) + \lambda_1\rho\, \delta(x)\chi_2(x) + k^2\chi_2(x).$$

Under arguments similar to those considered a few lines above, as $K_3(x)$ and $K_4(x)$ cancel out simultaneously, we find a second pair of independent relations between the parameters λ and β, given by,

$$\beta_1 = -\lambda_2 \qquad \text{and} \qquad \beta_2 = -\lambda_1. \tag{2.14}$$

Now we are in a position to determine the specific values that we must assign to each of the parameters λ and β to guarantee the consistency of the equations and the relationships found. Specifically, for equations (2.7), (2.8), (2.11) and (2.13) to be consistent, it must be fulfilled, from (2.12) and (2.14), that,

$$\lambda_2^2 = 1 \qquad \text{and} \qquad \lambda_1^2 = 1, \tag{2.15}$$

generating the possible values: $\lambda_2 = \pm 1$ and $\lambda_1 = \pm 1$. We can choose: $\lambda_2 = 1$; and then, $\lambda_1 = -1$, because, as we have previously assumed, these parameters must have different values. Using (2.14), we have: $\beta_1 = -1$ and $\beta_2 = 1$.

It is important to note the mathematical consistency of the assigned values: $\lambda_1 = -1$, $\lambda_2 = 1$, $\beta_1 = -1$ and $\beta_2 = 1$ with expressions (2.3) and (2.1).

Thus, the previous development allows writing the exact and decoupled version of the coupled equations (1.1) and (1.2) as follows,

$$\hat{D}^2\chi_1 \ + \ \rho\, \delta(x)\chi_1 \ + \ k^2\chi_1 = 0, \tag{2.16}$$

$$\hat{D}^2\chi_2 \ - \ \rho\, \delta(x)\chi_2 \ + \ k^2\chi_2 = 0, \tag{2.17}$$

which are two stationary Schroedinger equations for the functions χ_1 and χ_2, separately. Furthermore, it is worth mentioning that the equivalence between (1.1) & (1.2) and (2.16) & (2.17), which will be verified in the following subsection, is only valid in the case considered in the first paragraph of section 2.

2.1. Verification of equivalence between (1.1) & (1.2) and (2.16) & (2.17). It is simple to check such equivalence. From (2.5) and $\lambda_1 = -1$, we have,

$$\chi_1(x) = \psi_a(x) - \psi_b(x). \tag{2.18}$$

From (2.6) and $\lambda_2 = +1$, we have,

$$\chi_2(x) = \psi_a(x) + \psi_b(x). \tag{2.19}$$

Replacing (2.18) and (2.19) in (2.16) and (2.17), respectively, we have,

$$\hat{D}^2\psi_a(x) - \hat{D}^2\psi_b(x) + \rho\, \delta(x)\psi_a(x) - \rho\, \delta(x)\psi_b(x) + k^2\psi_a(x) - k^2\psi_b(x) = 0, \tag{2.20}$$

$$\hat{D}^2\psi_a(x) + \hat{D}^2\psi_b(x) - \rho\, \delta(x)\psi_a(x) - \rho\, \delta(x)\psi_b(x) + k^2\psi_a(x) + k^2\psi_b(x) = 0. \tag{2.21}$$

Adding (2.20) and (2.21) we find,

$$\hat{D}^2\psi_a(x) - \rho\, \delta(x)\psi_b(x) + k^2\psi_a(x) = 0, \tag{2.22}$$

which coincides with (1.1). Also, subtracting (2.20) from (2.21) we have,

$$\hat{D}^2\psi_b(x) - \rho\, \delta(x)\psi_a(x) + k^2\psi_b(x) = 0, \tag{2.23}$$

which coincides with (1.2), thus demonstrating that the decoupling procedure we have been using is exact.

3. Discussion

1. The exact mathematical solutions ψ_a and ψ_b that can be found for equations (1.1) and (1.2), through expressions (2.9) and (2.10), using the solutions of (2.16) and (2.17), could have no relation to a physical solution if we notice that the decoupled Schroedinger equations contain terms that correspond both to a "well" of potential $V_1(x) = -\rho\delta(x)$, and to a barrier of potential $V_2(x) = +\rho\delta(x)$, separately, an unexpected mathematical fact that has been revealed through the exact decoupling of the original equations. In the considered physical situation, of scattering by a Dirac delta potential, however, there is no "well" of potential; thus, the system of coupled equations (1.1) and (1.2) would be spurious for this problem.

2. The "appearance" of a term corresponding to a potential well is not explicitly perceived in [7] because, in their case, the solutions found for equations (1.1) and (1.2) correspond to two redundant equations for a single independent function, not a coupling situation. According to our development, the redundant case for the coupled system, with $\psi_a = \psi_b$, could not be obtained, because the only way to achieve this, observing expressions (2.9) and (2.10), would be by doing the choice: $\lambda_2 = \lambda_1 = -1$, which is incompatible with the decoupling method considered here, which has these parameters with different values.

4. Conclusion

We have shown that the coupled differential equations (1.1) and (1.2), taken from [7], can be exactly uncoupled, as verified in subsection 2.1. And, based on the characteristics arising from the decoupled equations, we maintain that equations (1.1) and (1.2) are spurious for the problem with a potential barrier of the Dirac delta type. Finally, since the decoupling method we have been using is independent of the nature of the derivatives, it could be useful even when we are considering equations with derivatives of the fractional type [9]-[10].

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