An Application of Gröbner Basis in Differential Equations of Physics

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Z. Naturforsch. **68a,** 646 – 650 (2013) / DOI: 10.5560/ZNA.2013-0044
Received April 9, 2013 / revised May 31, 2013 / published online August 21, 2013

We apply the Gröbner basis to the ansatz method in quantum mechanics to obtain the energy eigenvalues and the wave functions in a very simple manner. There are important physical potentials such as the Cornell interaction which play significant roles in particle physics and can be treated via this technique. As a typical example, the algorithm is applied to the semi-relativistic spinless Salpeter equation under the Cornell interaction. Many other applications of the idea in a wide range of physical fields are listed as well.

Key words: Gröbner Basis; Quantum Mechanics; Ansatz Method.

1. Introduction

The potential model of quantum mechanics, despite being old, is still a challenging topic. In particular, in many cases it leads to differential equations which are not exactly solvable via the common analytical methodologies of mathematical physics such as the supersymmetry quantum mechanics (SUSYQM), pint canonical transformation (PCT), Lie algebras, Nikiforov–Uvarov (NU) technique, series expansion, etc [1]. On the other hand, the analytical approaches are in some aspects superior to their counterpart numerical techniques. For example, they provide a deeper insight into the physics of the problem and are more touchable for graduate and undergraduate students. A very successful approach in these cases is the so-called ansatz approach that has two steps. The first is to find the solution of a corresponding Riccati equation, which is often easily found. The second, and perhaps the more cumbersome step, is solving a consequent system of equations with some unknown parameters. Therefore, if there is a simple way to acquire the explicit solutions of the obtained system of equations, we can have a better understanding of the impact of each parameter in the energy relation and therefore the phenomenological study goes a step forward. In this study, at first the Gröbner basis properties are briefly reviewed. We next apply this method to some present studies on nonrelativistic Schrödinger, semi-relativistic two-body spinless Salpeter, and relativistic Duffin–Kemmer–Petiau (DKP) equations as typical examples. For some interesting points of the ansatz approach, the interested reader can see references [2 – 10], which apply the technique to various equations of quantum mechanics.

A Gröbner basis is a set of multivariate polynomials with desirable algorithmic properties. Using the Buchberger algorithm, every set of polynomials can be transformed into a Gröbner basis [11]. Generally, a Gröbner basis with respect to lexicographic order has an upper triangular structure, and a system with this structure is easy to solve because its first equation has only one variable. So, a usual technique may be applied to extract the root of this one variable polynomial. By obtaining the root of the first equation and substituting in the second equation, which is a two variables polynomial, the solution of the second polynomial equation can be computed and so on.

2. The Two-Body Spinless Salpeter Equation

This semi-relativistic spinless Salpeter equation is the most straightforward generalization of the nonrelativistic Schrödinger equation into the relativistic regime. It originated form the Salpeter equation [12 – 15] by neglecting the spin degrees of freedom and the time evolution. The two-body spinless Salpeter equation under the Cornell potential $V(r) = ar + \frac{b}{r}$ [16] leads to the Schrödinger-like equation [2]

$$\left[\frac{d^2}{dr^2} + \frac{A}{r^2} + \frac{B}{r} + Cr^2 + fr + h\right]\psi_{n,l}(r) = 0\,, \tag{1}$$

where

$$\begin{aligned} A &= -l(l+1) + \frac{\mu b^2}{\hbar^2 \tilde{m}}\,, \quad B = -\frac{2\mu b}{\hbar^2} - \frac{2E_{n,l} b\mu}{\hbar^2 \tilde{m}}\,, \\ C &= \frac{\mu a^2}{\hbar^2 \tilde{m}}\,, \quad f = -\frac{2\mu a}{\hbar^2} - \frac{2\mu E_{n,l} a}{\hbar^2 \tilde{m}}\,, \\ h &= \frac{2\mu E_{n,l}}{\hbar^2} + \frac{\mu E_{n,l}^2}{\hbar^2 \tilde{m}} + \frac{2ab\mu}{\hbar^2 \tilde{m}}\,. \end{aligned} \tag{2}$$

In [2], the authors have proposed the ansatz solution

$$\psi_{n,l}(r) = g_n(r)\exp(y_l(r)) \tag{3}$$

with

$$g_n(r) = \begin{cases} 1\,, & \text{if } n = 0\,, \\ \prod_{i=1}^{n}(r - \alpha_i^n)\,, & \text{if } n \geq 1\,, \end{cases} \tag{4}$$

where, for the nodeless wavefunction,

$$g_n(r) = 1\,, \tag{5a}$$

$$y_l(r) = \delta \ln(r) + \beta r^2 + \gamma r\,. \tag{5b}$$

After equating the corresponding powers on both sides, we get

$$\begin{aligned} &\delta^2 - \delta = -A\,, \; 2\delta\gamma = -B\,, \; 4\beta^2 = -C\,, \\ &4\beta\gamma = -f\,, \; \gamma^2 + 2\beta + 4\beta\delta = -h \end{aligned} \tag{6}$$

which give the energy vs. various parameters engaged.

3. Other Wave Equations of Quantum Mechanics

Within this subsection, we mention other wave equations of quantum mechanics to ensure the wide applicability of the ansatz method. Although we applied the method to other published works such as [5, 10], we avoided including the results due to the huge volume of the calculations. The ansatz approach works well for other equations of quantum mechanics under specific interactions. Some other examples are as follows. We only include the equations to preserve compactness.

3.1. The Nonrelativistic Schrödinger Equation

The Schrödinger equation, despite being old, is still the focus of many studies in various branches of physics and chemistry. In its radial form, the equation is written as [17, 18]

$$\begin{aligned} &\left[\frac{d^2}{dr^2} - \frac{2\mu}{\hbar^2}V(r) - \frac{(D+2l-1)(D+2l-3)}{4r^2}\right. \\ &\left. + \frac{2\mu E_{n,l}}{\hbar^2}\right] R_{n,l}(r) = 0\,, \end{aligned} \tag{7}$$

where r, $\hbar$, μ, $V(r)$, D, l, n, $E_{n,l}$, and $R_{n,l}$ respectively denote the radius, Planck constant, mass, potential (interaction), dimension of problem, orbital quantum number, principal quantum number, energy, and the wave function. The ansatz technique can for example solve the equation under the Killinbeck potential containing linear, quadratic, and inverse (Coulomb) terms.

3.2. Relativistic Dirac Equation in Spin and Pseudo-Spin Symmetry Limits

The Dirac equation describes relativistic spin-$\frac{1}{2}$ particles. In very recent studies, many authors have studied the so-called spin and pseudospin symmetries of the Dirac equation which yield outstanding phenomenological results in hadron and nuclear spectroscopies [19–21]. In these studies, one has to deal with second-order differential equations

$$\begin{aligned} &\left\{\frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r^2} + \frac{2\kappa}{r}U(r) - \frac{dU(r)}{dr} - U^2(r)\right\} F_{n\kappa}(r) \\ &= (M + E_{n\kappa} - \Delta(r))\,(M - E_{n\kappa} + \Sigma(r))\,F_{n\kappa}(r)\,, \end{aligned} \tag{8a}$$

and

$$\begin{aligned} &\left\{\frac{d^2}{dr^2} - \frac{\kappa(\kappa-1)}{r^2} + \frac{2\kappa}{r}U(r) + \frac{dU(r)}{dr} - U^2(r)\right\} G_{n\kappa}(r) \\ &= (M + E_{n\kappa} - \Delta(r))\,(M - E_{n\kappa} + \Sigma(r))\,G_{n\kappa}(r)\,, \end{aligned} \tag{8b}$$

for spin and pseudo-spin symmetries, respectively. As the notation bears,

$$\Delta(r) = V(r) - S(r)\,, \tag{8c}$$

$$\Sigma(r) = V(r) + S(r)\,, \tag{8d}$$

with S and V respectively denoting the scalar and vector interactions. Obviously, the quantum numbers here are n and κ. We see that the ansatz approach works well for the successful Cornell potential in this case.

3.3. Relativistic Klein–Gordon Equation

This relativistic equation investigates spin-0 bosons. In the D-dimensional space, it posses the form [8, 17]

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+E_{n,l}^2+V^2(r)-2E_{n,l}V(r)-m_0^2-S^2(r)\right.\\ \left.-2m_0S(r)-\frac{(D+2l-1)(D+2l-3)}{4r^2}\right]u_{n,l}(r)=0\,. \tag{9}$$

Again, we can use the technique for Cornell, Killingbeck, and Kratzer potentials. The latter contains Coulomb and inverse square terms.

3.4. Relativistic Duffin–Kemmer–Petiau (DKP) Equation

A very challenging equation in quantum mechanics is the DKP equation which governs both spin-0 and spin-1 bosons. In its spin-0 form, and for vanishing scalar interaction, it appears as [10, 22]

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{J(J+1)}{r^2}+(E_{n,J}-V(r))^2\right.\\ \left.-m^2\right)F_{n,J}(r)=0\,, \tag{10}$$

which resembles the Klein–Gordon equation and therefore the same story holds here. It should be mentioned that the DKP equation under a scalar term becomes much more difficult but it has been very recently solved under the coulomb term by the ansatz technique [10].

4. A Worked Example

As a typical example in current physics research, let us now apply the Gröbner basis to solve (6). The given problem is converted to find the zeros of a multivariate polynomials system. As explained in the introduction, using Buchberger algorithm, we can compute the Gröbner basis for the system with respect to lexicographic order. So, the energy of the system is obtained as

$$E=\frac{-ma+\gamma}{m^2a}\,.$$

To see the details, please refer to the Appendix.

5. Conclusion

As already mentioned, there are many differential equations in quantum mechanics which can not be solved by common analytical techniques of mathematical physics. A very economical methodology in dealing with these problems is the quasi-exact ansatz approach which is based on finding the solution of a Riccati equation and solving a set of consequent equations which contain some unknown parameters. Although the story seems simple, solving the obtained equations is somehow difficult. A very efficient methodology for solving these equations (especially for higher nodes) is the Gröbner basis. It should be noted that even with rather high speed computers, we ought to tolerate a relatively long time run. In addition, we wish to emphasize on a very important point; although we included a single example for the sake of conciseness (the solution is many cases tens of pages), the tool and the ansatz approach work well for many differential equations of physics and mathematics. Consequently, the idea works well in many areas of physics such as theoretical nuclear physics, e. g. in the spin and pseudspin symmetry limits of Dirac equation (which find notable applications in hadron and nuclear spectroscopy), theoretical nano and solid-state physics (e. g. in solving the Schrödinger equation for quantum dots and wires, and Dirac equation for Graphene), string theory (e. g. in solving the equations of motion), cosmology (in the problem of quasi-normal modes of black holes and the Wheeler–DeWitt equation), particle physics (for solving Klein–Gordon, Dirac, spinless Salpeter, and DKP equation in meson and baryon spectroscopy, etc.

Appendix

The detailed solution to (6) for various states is

```
> restart;
> E[n,l]:=E:
> with(Groebner):
A:=-l^2-l+m*mu*b^2:
> B:=-2*mu*b-2*m*mu*E[n,l]*b:
> C:=m*mu*a^2:
> F:=-2*mu*a-2*m*mu*E[n,l]*a:
> h:=2*mu*E[n,l]+mu*m*E[n,l]^2
     +2*m*mu*a*b:
> f[1]:=delta^2-delta+A:
```

```
> f[2]:=2*delta*gamma+B:
> f[3]:=4*beta^2+C:
> f[4]:=4*beta*gamma+F:
> f[5]:=gamma^2+2*beta
        +4*beta*delta+h:
> FF:=[f[1],f[2],f[3],f[4],f[5]]:
> vars:=[delta,beta,gamma,l,b,
        E[n,l],a]:
> G:=Basis(FF,plex(delta,beta,gamma,
          l,E[n,l],b,a)); nops(%);
```

$$G := \Big[m^3a^4+\mu a^2, \mu a^2+Em\mu a^2+a^3\gamma m^2, \gamma^4+2\gamma^2\mu E +\gamma a\mu+m\mu Ea\gamma+2\mu^2ba+\gamma^2\mu mE^2+2m^3a^3\mu b, \gamma^3\mu b -\mu^2b^2\gamma^2+\gamma^3\mu bmE+m\mu^2b^2\gamma a+2m\mu^3b^3a+m^2\mu^2 \cdot b^2Ea\gamma+2m^4\mu^2b^3a^3+\gamma^4l^2+\gamma^4l, 2\beta\gamma-\mu a -m\mu Ea, \delta\gamma-\mu b-m\mu Eb\Big]$$

```
> Solve(G,[delta,beta,gamma,l,b,
        E[n,l],a);
```

$$\Big\{\Big[\big[a,\ \gamma^2+2\mu E+\mu mE^2,\ \gamma^2l^2+\gamma^2l+\gamma\mu b+m\mu Eb\gamma -\mu^2b^2,\ \beta,\ \delta\gamma-\mu b-m\mu Eb\big], \mathrm{plex}(\delta,\beta,\gamma,l,b,E,a), \{\}\Big],\ \Big[\big[m^3a^2+\mu,\ \mu+m\mu E+\gamma m^2a,\ -m^2ba+l^2 +l,\ -\mu+2m\beta,\ m^2ba+\delta\big],\ \mathrm{plex}\big(\delta,\beta,\gamma,l,b,E,a\big), \{a\}\Big]\Big\}$$

```
> Solve(a,gamma^2+2mu*E+mu*m*E^2,
  gamma^2*l+gamma^2*l^2+gamma*mu*b
  +gamma*m*mu*E*b-mu^2*b^2,
  beta,delta*gamma-mu*b-m*mu*E*b]);
```

$$\Big\{E=\frac{b\gamma^3}{(\gamma l+\gamma+\mu b)(\gamma l-\mu b)},\ a=0,\ b=b,\ l=l, m=-\frac{(\gamma^2l^2+\gamma^2l+\gamma\mu b-\mu^2b^2)(\gamma l+\gamma+\mu b)(\gamma l-\mu b)}{\gamma^4\mu b^2}, \mu=\mu,\ \beta=0,\ \delta=-\frac{\gamma^2l^2+\gamma^2l-\mu^2b^2}{\gamma^2}\Big\},$$
$$\Big\{E=E,\ a=0,\ b=0,\ l=0,\ m=-\frac{\gamma^2+2\mu E}{E^2\mu}, \mu=\mu,\ \beta=0,\ \delta=0\Big\},\ \Big\{E=E,\ a=0,\ b=0, l=-1,\ m=-\frac{\gamma^2+2\mu E}{E^2\mu},\ \mu=\mu,\ \beta=0,\ \delta=0\Big\}$$

```
> Solve([m^3*a^2+mu,
  mu+m*mu*E+gamma*m^2*a,
  -b*m^2*a+l+l^2,
  2*beta*m-mu,b*m^2*a+delta]);
```

$$\Big\{E=\frac{-ma+\gamma}{m^2a},\ a=a,\ b=\frac{(l+1)l}{m^2a},\ l=l,\ m=m, \mu=-m^3a^2,\ \beta=-\frac{1}{2}m^2a^2,\ \delta=-(l+1)l\Big\},$$
$$\Big\{E=E,\ a=a,\ b=b,\ l=0,\ m=0,\ \mu=0, \beta=\beta,\ \delta=0\Big\},\ \Big\{E=E,\ a=0,\ b=b,\ l=-1, m=0,\ \mu=0,\ \beta=\beta,\ \delta=0\Big\},\ \Big\{E=E,\ a=0, b=b,\ l=0,\ m=m,\ \mu=0,\ \beta=0,\ \delta=0, E=E,\ a=0,\ b=b,\ l=-1, m=m,\ \mu=0,\ \beta=0,\ \delta=0\Big\}$$

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