THE BOUND STATES FOR THE NON POLYNOMIAL POTENTIAL VIA THE GENERALIZED DIFFERENTIAL QUADRATIC METHOD

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ABSTRACT

In a previous work, we have introduced the generalized differential quadratic method (called GDQ) to handle the Schrödinger equation. This paper deals with a particular situation in which an application to the non polynomial potential is considered. The results are compared with some numerical examples for the same potential of interest.

KEYWORDS: Quadratic, bound states, excited states, spectrum.

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RESUME

Dans un récent travail nous avons introduit la méthode quadratique différentielle généralisée pour manipuler l'équation de Schrödinger. Cet article traite une situation particulière dans laquelle une application à un potentiel non polynomial est considérée. Les résultats sont confrontés avec des exemples numériques pour le même potentiel d'intérêt.

MOTS CLES : Quadratique, états liés, états excités, spectre.

1 INTRODUCTION

Several important physical problems require solving the Schrödinger equation for spherical symmetric potential to determine the eigenenergies and the eigenfunctions. It is known that for very limited potentials, Schrödinger equation is exactly solvable.

In fact, many approximate schemas and numerical calculations have appeared in recent years to calculate the eigenspectra of the Schrödinger equation for numerous potential functions [1-8]. The scope of this area remains so far a more active field of numerical schemas.

From general point of view, in the absence of exact analytical solutions, the recourse to approximation techniques to evaluate the spectra of energy is a primary need. Most common approximation methods like phase-integral method, 1/N expansion, perturbational theory, and variational method are often being used for this purpose.

In a recent paper [3], we have formulated a new numerical approach which is based on the generalized differential quadratic method, and applied to the radial Schrödinger equation. This method studies the situation in which the unknown function is identified as the Lagrange polynomial and the interpolating points of the Tchebychev type are used.

2 BRIEF REVIEW OF GENERALIZED DIFFERENTIAL QUADRATIC METHOD

A brief description of generalized differential quadratic method is summarized as follows: the radial Schrödinger equation is written as

$$\left(-\frac{d^2}{dr^2}+w(r)\right)S_{n,l}(r)=\varepsilon S_{n,l}(r) \qquad (1)$$

where $\varepsilon=\frac{2m}{\hbar^2}E$. When the potential is central, the equation (1) is identified as the reduced Schrödinger equation, $w(r)=\frac{2m}{\hbar^2}V(r)+\frac{l(l+1)}{r^2}$ is the effective potential where l denotes the angular momentum quantum number, and the radial function $R_{n,l}(r)$ is linked to $S_{n,l}(r)$ by the relation

$$S_{n,l}(r)=rR_{n,l}(r) \qquad (2)$$

We can construct the solution $S_{n,l}(r)$ by making the following transformation

$$S(x) = S_{as}(x)x^{\rho}\phi(x) \tag{3}$$

where we have now dropped the "n,l" subscript for simplicity.

When we plug (3) into (1), it can be verified that the function $\phi(x)$ must satisfy the equation

$$h\phi(x) = 0 \tag{4}$$

where the differential operator h is defined by

$$h = -F(x)\frac{d^2}{dx^2} - 2A(x)\frac{d}{dx} + B(x) \tag{5}$$

So, the term $[h\phi(x)]$ can be expressed as a constant coefficient eigenfunction combination at all discrete points in the domain of the variable x as

$$[h\phi]_i = \sum_{j=1}^{N} \beta_{ij}\phi(x_j) \text{ for } i = 1,...,N \tag{6}$$

where $\{x_j\}$, $1 \le j \le N$, are the sequences of the x - variable.

we can extract β_{ik} as

$$\beta_{ik} = B(x_i)\alpha_{ik}^{(0)} - 2A(x_i)\alpha_{ik}^{(1)} - F(x_i)\alpha_{ik}^{(2)} \tag{7}$$

the superscripts 0, 1 and 2 in parentheses do not indicate powers, but merely identify the derivatives of the Lagrange's polynomial with which the quantities α_{ik} are associated.

$$\alpha_{ik}^{(j)} = \frac{d^j P_{N,k}(x_i)}{dx^j} \tag{8}$$

Now one can accurately solve the following matrix equation and therefore the original problem (1)

$$[\beta]\phi = 0 \tag{9}$$

3 NON - POLYNOMIAL POTENTIAL

It has been widely handled in atomic and optical physics [5, 6, 7, 9, 10, 13, 14], and has the following form

$$V(A,B,k,b;x) = \frac{A}{x^2} + Bx^2 + \frac{kx^2}{x^2+b}$$

where A , B and k are parameters with.

$$A = \left(\alpha + \frac{\beta b}{2} + 1\right)\left(\alpha + \frac{\beta b}{2}\right) \text{ and } B = \frac{\beta^2}{4}.$$

Consider the radial part of Schrödinger equation for the above potential under consideration and apply the previous developments to it together with [3] we obtain,

$$U^{(2)}(x) - U^{(1)}(x)\left(\frac{2\alpha + \beta(x^2+b)}{x}\right) + U(x)\left(E + D - \frac{kx^2}{x^2+b}\right) = 0 \tag{10}$$

where we have replaced S(x) by

$$S(x) = x^{-\left(\alpha + \frac{\beta b}{2}\right)} e^{-\frac{\beta x^2}{4}} U(x) \tag{11}$$

Alternately, we may identify all quantities as

$$\begin{cases} F(x) = -1 \\ S_{ab} = e^{-\frac{\beta x^2}{4}} \\ A(x) = \dfrac{2\alpha + \beta(x^2+b)}{2x} \\ B(x) = E + D - \dfrac{kx^2}{x^2+b} \\ \rho = -\left(\alpha + \dfrac{\beta b}{2}\right) \end{cases} \tag{12}$$

It is not difficult to check that, from these expressions, the operator h keeps invariant the space of polynomials at most of degree $\le N$.

4 RESULTS AND DISCUSSION

For comparison, we have reported in table 1, the first three energy levels obtained by the (GDQ) method, the B-spline method and the exact method by the introduction of an ansatz for the state-function, similar to the power series expansion method [5]. We observe essentially that these results are very close with those of ref. [5]. As an illustration, the figure 1 shows graphically the three wave-function solutions R(x) as a function of x for the case n°3 of table 1. We can underline from these shapes, a good performance is obtained and the behavior of the wavefunction is very well outlined and preserved for the three states of interest.

We have introduced the GDQ method in order to determine the bound-state eigenvalues and the associated eigenfunctions for a specific non polynomial potential.

In order to enlarge the field of applications of this method would be also interesting to examine the case where the solution cannot be handled analytically with the usual techniques. This subject is in preparation and will be done in a sequel of this paper.

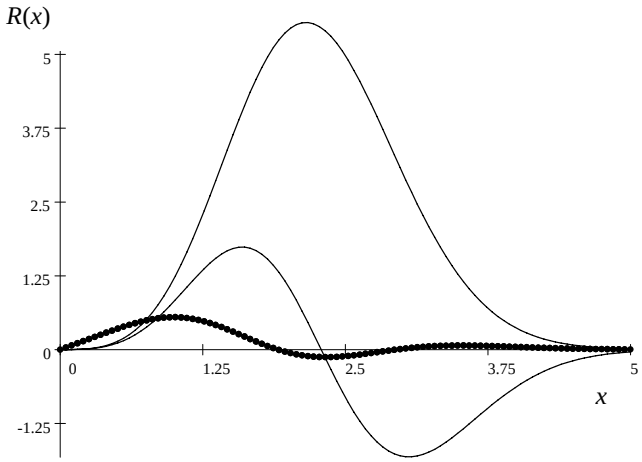

Figure 1 : Representation of bound states R(x) for the case n° 3 (Table 1). Solid line: ground state, dash line: first excited state, and dot-dash line: second excited state.

Table 1 : Eigenenergies E_0, E_1, and E_2 obtained for the ground, first, and second excited states respectively. Comparison with exact result [5] and B-spline results [11]

				E_0			E_1			E_2		
Case	α	b	β	*exact*	*step (0,5) (GDQ)*	*step (0,2) B-spline*	*exact*	*step (0,5) (GDQ)*	*step (0,2) B-spline*	*exact*	*step (0,5) (GDQ)*	*step (0,2) B-spline*
1	*-3/2*	*1*	*1*	*-4,5*	*-4,5001*	*-4,439*	*-3,472*	*-3,5715*	*-3,172*	*-2,611*	*-2,6098*	*-1,1397*
2	*-3*	*1*	*2*	*-5*	*-4,9997*	*-4,9667*	*-2,566*	*-2,6098*	*-2,455*	*-0,062*	*-0.0617*	*0,1853*
3	*-4*	*1*	*2*	*-7*	*-7*	*-6,998*	*-4,295*	*-4,295*	*-4,281*	*-1,547*	*-1,5473*	*-1,4241*
4	*-2*	*1*	*2*	*-3*	*-1*	*1,125*	*-2,997*	*-1,012*	*1,154*	*-2,984*	*-0,764*	*2,3635*
5	*-4*	*1*	*4*	*0*	*5,247*	*10,716*	*0,0001*	*4,25*	*10,781*	*-0,001*	*5,2411*	*10,73*

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