Variationally Improved Spectral Method as an extremely accurate technique for solving time-independent Schrödinger equation

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Abstract

We introduce three distinct, yet equivalent, optimization procedures for the Fourier Spectral Method which increase its accuracy. This optimization procedure also allows us to uniquely define the error for the cases which are not exactly solvable, and this error matches closely its counterpart for the cases which are exactly solvable. Moreover, this method is very simple to program, fast, extremely accurate (*e.g.* an error of order 10^{-130} is usually obtainable as compared to the exact results), very robust and stable. Most importantly, one can obtain the energies and the wave functions of as many of the bound states as desired with a single run of the algorithm. We first thoroughly test this method against an exactly solvable problem and then apply it to two problems which are not exactly solvable, all for finding the bound states of the time-independent Schrödinger equation. We present a detailed comparison between the results obtained by this method and some of the more routine methods.

1 Introduction

Eighty years after the birth of quantum mechanics [1], the Schrödinger's famous equation still remains a subject for numerous studies, aiming at extending its field of applications and at developing more efficient analytic and approximation methods for obtaining its solutions. There has always been a remarkable interest in studying exactly solvable Schrödinger equations. At this point, we have to state that traditionally the term "exactly solvable" has been used

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in a well-defined mathematical sense, meaning that the eigenvalues and eigenfunctions of the Hamiltonian under consideration may be expressed in an explicit and closed form [2]. In this sense, the exact solubility has been found for only a very limited number of potentials, most of them being classified already by Infeld and Hull [3] on the basis of the Schrödinger factorization method [4], which in turn appeared to be a rediscovery of the formalism stated nearly 120 years ago by Darboux [5]. However, a vast majority of the problems of physical interest do not fall in the above category when we formulate a more or less realistic model for them. Then we have to resort to approximation techniques which can be analytic or numeric. Examples of approximate analytic techniques would be the usual perturbation method, the semiclassical or WKB approximation, and the variational method [6, 7]. In the perturbation method the problem is divided into two segments. The main segment is supposed to be exactly solvable. The second segment is supposed to modify the solution obtained in the main segment only very slightly. This modification can be obtained analytically for any desired degree of accuracy. On the other hand, the numeric solutions could be either perturbative in nature or completely numeric. Indeed, the relevant Schrödinger equation can always be solved numerically, and in view of the immensely increased computational power, this numerical solution could be extremely accurate. Such solutions could serve the dual purpose of being a substitute for the exact solution and being used as a comparison with experimental results, when applicable, whose accuracy are also rapidly on the rise. The need for such methods have stimulated development of more sophisticated integration approaches, *e.g.* embedded exponentially-fitted Runge-Kutta [8] and dissipative Numerov-type [9] methods, as well as interesting techniques, such as a relaxational approach [10] based on the Henyey algorithm [11], an adaptive basis set using a hierarchical finite element method [12], and an approach based on microgenetic algorithm [13], which is a variation of a global optimization strategy proposed by Holland [14]. To be more specific, Amore [15] has used the variational sinc collocation method to obtain the bound state solutions for a Schrödinger equation and has obtained accuracies of order 10^{-42}. Also Jentschura [16] has used the Instanton method for

similar kind of problems and obtained accuracies of order 10^{-180}. Problems which consist of systems of coupled ODE's with multiple delta function potentials can be solved by, for example, the method of shooting to multiple fitting points and implementing the delta functions as boundary conditions at those points [17]. Moreover, problems involving moving singularities are always are difficult to handle. However a few algorithm have been recently introduced to solve these problems (see for example [18]). However, even in this simplest case, the success of applying any direct numerical integration method depends on the quality of initial guesses for the boundary conditions and energy eigenvalues. Moreover, one usually encounters difficulties with the intrinsic instabilities of typical problems, and rarely with the existence of actual solutions which posses rapid oscillation.

Here we discuss an alternative technique for finding the bound states of the time-independent Schrödinger equation, applicable for any potential which supports such states. This method has the following seven distinct advantages: It is very simple, fast, can be extremely accurate, does not have the aforementioned difficulties with the choice of boundary conditions. It is very robust and stable, *i.e.* it does not have the instability problems due to the usual existence of divergent solutions of most physical problems. These problems usually produce difficulties for the spatial integration routines such as Finite Difference Method (FDM). Moreover, we have encountered problems in quantum cosmology whose exact solutions posses very rapid oscillations [19] which prevent any successful application of more routines such as FDM, and we were able to solve this problem using our alternative technique with ease [20]. Here, our main goal is to improve this method by an optimization procedure which first of all allows us to define the errors uniquely and secondly decrease them drastically. This method can also easily handle cases with mild moving singularities, which also occurred in the aforementioned problem. Finally, and perhaps most importantly, we can obtain the wave functions and energies of as many of the bound states as desired with a single run of the algorithm. This method, which was first introduced by Galerkin over 90 years ago, consists of first choosing a complete orthonormal set of eigenstates of a, preferably relevant, hermitian operator to be

used as a suitable basis for our solution. For this numerical method we obviously can not choose the whole set of the complete basis, as these are usually infinite. Therefore we make the approximation of representing the solution by a superposition of only a finite number of the basis functions. By substituting this approximate solution into the differential equation, a matrix equation is obtained. The energies and expansion coefficients of these approximate solutions could be determined by the eigenvalues and eigenfunctions of this matrix, respectively. This method has been called the Galerkin Method, and is a subset of the more general Spectral Method (SM) [21, 22, 23]. Spectral methods generally fall into two broad categories. The interpolating, and the noninterpolating method. In the first category, which includes the Pseudospectral and the Spectral Element Methods, one divides the configuration space into a set of grid points. Then one demands that the differential equation be satisfied exactly at a set of points known as the collocation or interpolation points. Presumably, as residual function is forced to vanish at an increasingly larger number of discrete points, it will be smaller and smaller in the gaps between the collocation points. The noninterpolating category includes the Lanczos tau-method and the Galerkin method, mentioned above. The latter is the method that we use and, in conformity with the usual nomenclature, we shall simply refer to it as the Spectral Method. The interesting characteristic of this method is that it is completely distinct from the usual spatial integration routines, such as FDM, which concentrate on spatial points. In SM the concentration is on the basis functions and we expect the final numerical solution to be approximately independent of the actual basis used. Moreover in this method, the refinement of the solution is accomplished by choosing a larger set of basis functions, rather than choosing more grid points, as in the numerical integration methods. We should note that we are implicitly assuming that the true solution is expandable in any complete orthonormal basis such as the Fourier basis. However, first of all this requirement is usually satisfied for cases of physical applications, secondly we have found that when this requirement is not satisfied the method does not fail, but we loose overall accuracy.

In this paper we concentrate on the Fourier basis and refine SM by introducing three distinct

optimization methods. Then we show that these three procedures, perhaps surprisingly, yield identical results which we shall henceforth call the Variationally Improved Spectral Method (VISM). This refinement adds two particularly important advantages to SM: first we find a unique method to define the error for the cases which are not exactly solvable, and when tested on the exactly solvable cases matches closely with the standard definition of the error. Second, This refinement, as we shall show, usually improves the accuracy drastically. Then we show an application of this amazingly powerful method to the problem of finding the bound states of the time independent Schrödinger equation.

The remainder of this paper is organized as follows. In Section 2, we present the underlying theoretical bases for the formulation of the SM in connection with the problems of quantum nature. Then we introduce our optimization procedures to obtain VISM. In Section 3, we first use this method for the Simple Harmonic Oscillator (SHO), which is an exactly solvable problem for three important reasons: first to illustrate the method, second to show that the three distinct optimization procedures yield the same results, and third to test the method thoroughly. We then apply this method to two perturbed harmonic oscillators, the first with quartic anharmonic term, and second with a rapidly oscillating trigonometric anharmonic term. Neither problem is exactly solvable, and are particularly chosen to illustrate some of the powerful features of this method. We compare the results for the earlier case with those obtained by the usual first order perturbation theory method, the conventional and a variationally improved Sturmian approximation method [24], and a highly accurate method [25]. The latter, though in principle an approximate method, can determine rather precisely the energy levels for this problem from the quantization of an angle variable with an accuracy of order 10^{-90}. The trigonometric anharmonic problem has some very interesting physical and mathematical aspects which we shall point out. In Section 4, we state our conclusions and some final remarks.

2 The Spectral Method

Let us consider the time-independent one-dimensional Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x), \tag{1}$$

where m, $U(x)$, and E stand for the reduced mass, potential energy, and energy, respectively. Throughout this paper, we only examine the bound states of this problem, i.e. the states which are the square integrable. Therefore the general ODE that we want to solve is a linear one that can be written in the form,

$$-\frac{d^2\psi(x)}{dx^2} + \hat{f}(x)\psi(x) = \varepsilon\,\psi(x), \tag{2}$$

where,

$$\hat{f}(x) = \frac{2m}{\hbar^2}\,U(x), \qquad\qquad \varepsilon = \frac{2m}{\hbar^2}\,E. \tag{3}$$

As mentioned before, any complete orthonormal set can be used for the SM. We use the Fourier series basis as an example. That is, since we need to choose a finite subspace of a countably infinite basis, we restrict ourselves to the finite region $-L < x < L$. This means that we can expand the solution as,

$$\psi(x) = \sum_{i=1}^{2}\sum_{m=0}^{\infty} A_{m,i}\;\; g_i\left(\frac{m\pi x}{L}\right), \tag{4}$$

where,

$$\begin{cases} g_1\left(\frac{m\pi x}{L}\right) = \frac{1}{\sqrt{LR_m}}\sin\left(\frac{m\pi x}{L}\right), \\ g_2\left(\frac{m\pi x}{L}\right) = \frac{1}{\sqrt{LR_m}}\cos\left(\frac{m\pi x}{L}\right), \end{cases} \qquad R_m = \begin{cases} 2 & \text{m=0,} \\ 1 & \text{otherwise.} \end{cases} \tag{5}$$

In the above choice of the basis we are implicitly assuming periodic boundary condition. It is interesting to note that since we are interested only in the bound states, we could choose only the sine series but with the shifted problem $x \to x - L$. Our shifted domain will be $0 < x < 2L$ and the potential function is shifted accordingly. That is our new basis functions and the differential equation are

$$g\left(\frac{m\pi x}{2L}\right) = \frac{1}{\sqrt{L}}\sin\left(\frac{m\pi x}{2L}\right), \qquad \text{and} \qquad -\frac{d^2\psi(x)}{dx^2} + \hat{f}(x-L)\psi(x) = \varepsilon\,\psi(x), \tag{6}$$

For simplicity we shall refer to this alternate approach the confinement boundary condition. Now going back to our original formulation we can also make the following expansion,

$$\hat{f}(x)\psi(x) = \sum_i \sum_m B_{m,i} \;\; g_i \left(\frac{m\pi x}{L}\right), \tag{7}$$

where $B_{m,i}$ are coefficients that can be determined once $\hat{f}(x)$ is specified. By substituting Eqs. (4,7) into Eq. (2) and using the differential equation of the Fourier basis we obtain,

$$\sum_{m,i} \left[\left(\frac{m\pi}{L}\right)^2 A_{m,i} + B_{m,i}\right] g_i \left(\frac{m\pi x}{L}\right) = \varepsilon \sum_{m,i} A_{m,i}\, g_i \left(\frac{m\pi x}{L}\right). \tag{8}$$

Because of the linear independence of $g_i(\frac{m\pi x}{L})$, every term in the summation must satisfy,

$$\left(\frac{m\pi}{L}\right)^2 A_{m,i} + B_{m,i} = \varepsilon\, A_{m,i}. \tag{9}$$

It only remains to determine the matrix B. Using Eq. (7) and Eq. (4) we have,

$$\sum_{m,i} B_{m,i} g_i \left(\frac{m\pi x}{L}\right) \;\; = \sum_{m,i} A_{m,i} \hat{f}(x) g_i \left(\frac{m\pi x}{L}\right). \tag{10}$$

By multiplying both sides of the above equation by $g_{i'}(\frac{m'\pi x}{L})$ and integrating over the x-space and using the orthonormality condition of the basis functions, one finds,

$$B_{m,i} = \sum_{m',i'} A_{m',i'} \int_{-L}^{L} g_i \left(\frac{m\pi x}{L}\right) \;\; \hat{f}(x) \;\; g_{i'} \left(\frac{m'\pi x}{L}\right) \;\; dx = \sum_{m',i'} A_{m',i'} C_{m,m',i,i'} \;, \tag{11}$$

Therefore we can rewrite Eq. (9) as,

$$\left(\frac{m\pi}{L}\right)^2 A_{m,i} + \sum_{m',i'} C_{m,m',i,i'} \;\; A_{m',i'} = \varepsilon\, A_{m,i}. \tag{12}$$

Where the coefficients $C_{m,m',i,i'}$ are defined by Eq. (11). It is obvious that the presence of the operator $\hat{f}(x)$ in Eq. (2), leads to nonzero coefficients $C_{m,m',i,i'}$ in Eq. (12), which in principle could couple all of the matrix elements of A. Therefore we have to resort to a numerical solution. In general the number of basis elements are at least countably infinite. The aforementioned coupling of terms in the main matrix Eq. (12) forces us to make the approximation of using a finite basis. It is easy to see that the more basis functions we

include, the closer our solution will be to the exact one. By selecting a finite subset of the basis functions, *e.g.* choosing the first $2N$ which could be accomplished by letting the index m run from 1 to N in the summations, equation (12) can be written as,

$$D\,A = \varepsilon\,A, \tag{13}$$

where D is a square matrix with $(2N) \times (2N)$ elements. Its elements can be obtained from Eq. (12). The eigenvalues and eigenfunctions of the Schrödinger equation are approximately equal to the corresponding quantities of the matrix D. That is the solution to this matrix equation simultaneously yields $2N$ sought after eigenstates and eigenvalues. The only problem which remains is to solve the eigenvalue problem Eq. (13), and to control the round-off errors. This is often a serious issue for the usual spatial integration method using double precision. However, we can easily overcome this problem and obtain an extremely high precision. This is possible if the following conditions are satisfied. First, the potential energy and its derivatives should be smooth. Second, the programming language (such as MATHEMATICA, MAPLE, etc) should be capable of keeping the desired number of significant digits. Third, when the integrations involved in the calculations (Eq. 11) can be done analytically the coefficients in the matrix equation (Eq. 12) become exact and the accuracy increases. This also reduces the computational time drastically. At this point it is worth mentioning that when the Hamiltonian commutes with the parity operator, we can simplify our task of solving Eq. (13) by separating the search for the positive and negative parity solutions.

Now we can introduce our optimization procedure. We are free to adjust two parameters: $2N$, the number of basis elements used and the length of the spatial region, $2L$. This length should be preferably larger than spatial spreading of all the sought after wave functions. However, if $2L$ is chosen to be too large we loose overall accuracy. As we shall show, the error decreases extremely rapidly as the number of basis elements is increased. However, it is important to note that for each N, L has to be properly adjusted. This is in fact an optimization problem and is not a trivial task and requires some further analysis. We shall

denote this optimal quantity by $\hat{L}(N)$. We have come up with three methods to determine this quantity. These are based on the minimization of any of the eigenvalues (usually chosen to be those of the ground state), its error, or the error of the corresponding eigenfunction. For the minimization of the energy we proceed as follows. For a few fixed values of N we compute $E(N, L)$ which invariably has an inflection point in the periodic boundary condition and a minimum in the confinement boundary condition. Interestingly enough this points exactly coincide. Therefore, all we have to do is to compute the position of these inflection or minimum points and compute an interpolating function for obtaining $\hat{L}(N)$. Obviously the more points we choose the better our results will be. We shall explain the other two optimization methods in section 3. Once $\hat{L}(N)$ is computed, we can use the method described above to compute the eigenvalues and eigenfunctions. The necessary program is usually about 15 lines. As we shall see, the addition of this refinement to SM can have dramatic consequences. Throughout this paper we use VISM.

Computation of the relative error in the exactly solvable cases is straightforward. For example for computing the relative error of the eigenvalue, denoted by δ_E, we only need to find the absolute value of the difference between the result and the exact one and divide by the latter. For cases which are not exactly solvable, we compute the difference between the eigenvalues for a given N and those obtained with $N + 1$, both lying on the $\hat{L}(N)$ curve. We shall denote the error computed by this procedure $\hat{\delta}_E$. We have computed $\hat{L}(N)$ for all cases, and subsequently computed the eigenfunctions, eigenvalues and their errors using this method, and checked their validity in the exactly solvable case of SHO. Obviously to obtain consistent results we have to keep the same precision throughout the calculations.

At this point we should mention that the only weakness of this method that we have found is that, like most other routines, the more discontinuous the potential or its derivatives, the less accurate our solution will be. This is due to the fact that these discontinuities would induce associated discontinuities in the wave functions or their derivatives via the Schrödinger equation. In these cases we would need more basis functions, in particular high frequency ones,

to reproduce these features of the wave functions.

3 Some applications of the Spectral Method

In this section, for illustrative purposes, we first apply VISM to find the bound states of a Simple Harmonic Oscillator (SHO) which is an exactly solvable case, for the reasons stated at the end of the Introduction section. Briefly, the purpose is to readily check the validity of our three distinct optimization procedures, which includes our prescriptions for finding $\hat{L}(N)$, and compare them. We can also check the overall accuracy of our results. We then apply this method to two perturbed harmonic oscillators, the first with quartic anharmonic term, and second with a rapidly oscillating trigonometric anharmonic term. Neither problem is exactly solvable. We compare our results for the earlier case with some other reported results.

a. Simple Harmonic Oscillator

The Schrödinger equation for a SHO is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+\frac{1}{2}m\omega^2x^2\psi(x)=E\psi(x), \tag{14}$$

where ω is the natural frequency of the oscillator. Dividing both sides by $\hbar\omega/2$, we convert this differential equation into the following dimensionless form,

$$-\frac{d^2\psi(x')}{dx'^2}+x'^2\psi(x')=E'\psi(x'), \quad \text{where} \quad x'=\sqrt{\frac{m\omega}{\hbar}}x, \quad E'=\frac{2}{\hbar\omega}E. \tag{15}$$

This differential equation is exactly solvable and its eigenvalues and eigenfunctions, which are all bound states, can be easily found analytically and are well known,

$$E_n=(n+\frac{1}{2})\hbar\omega, \qquad \psi_n(x)=\left(\frac{\omega}{\pi}\right)^{1/4}\frac{H_n(\sqrt{\omega}x)}{\sqrt{2^n n!}}e^{-\omega x^2/2}, \qquad n=\{0,1,2,...\}, \tag{16}$$

where $H_n(x)$ denote the Hermite polynomials. Using VISM we can calculate approximately the energy levels and the corresponding eigenfunctions of this Hamiltonian. The computation of the errors of the wave functions are analogous to that of the energy. We divide the configuration space into M grid points. Then, we average the square of the absolute value of the difference

between the exact solution and that obtained by the VISM on the grid points,

$$\delta_{E_n} = \frac{|E_n^{\rm exact} - E_n^{SM}|}{E_n^{\rm exact}}, \qquad\qquad \delta^2_{\psi_n} = \frac{\sum_{i=1}^{M} |\psi_n^{\rm exact}(i) - \psi^{(N)}(i)|^2}{\sum_{i=1}^{M} |\psi_n^{\rm exact}(i)|^2}. \tag{17}$$

In the left part of figure 1 we show the ground state energy computed using SM for the fixed value of the $N = 5$ as a function of L using periodic boundary condition. In the right part of figure 1 we show the corresponding quantity computed using confinement boundary condition. Note the existence of the inflection and minimum points which exactly correspond to each other in the figure. These points determine $\hat{L}(5)$. We repeat this procedure for a few other values of N. After plotting these values we can obtain an interpolating function $\hat{L}(N)$. Our second optimization method is based on the minimization of the error of the eigenvalue (δ_{E_0}), and to proceed we first exhibit a semi-log plot of the square of the exact error for the ground state energy using SM in terms of N and L in Fig. 2. Note the existence of a valley in this figure indicating the optimal quantity $\hat{L}(N)$, which can gives us the best values for the eigenvalues and eigenfunctions using VISM. Our third optimization method is based on the minimization of the error of the wave function (δ_{ψ_0}), and proceeds analogously to the previous method. In Fig. 3 we show our results for $\hat{L}(N)$ obtained using the three aforementioned methods and their interpolating function. Having determined $\hat{L}(N)$, we can proceed to compute the bound states. We have checked the validity of our results for the eigenvalues and their errors, and the eigenfunctions using this method as compared to the corresponding exact values. Table 1 shows the results for the first 10 eigenfunctions for $N = 100$. Note the outstanding accuracy of $\delta_E \approx 10^{-130}$ and $\delta_{\psi_0} \approx 10^{-70}$. The values for $\hat{\delta}_E$ are also shown in Table 1. The values for $\hat{\delta}_{\psi_0}$ could similarly be calculated, but are not shown here. Now we want to exhibit explicitly the errors of the ground state wave function, whose value is shown in Table 1 for $N = 100$, for some other values of N. The left part of Figure 4 shows the exact and approximate ground state wave functions for $N = \{3, 5, 7\}$ using SM with fixed un-optimized $L = 10$. The right part of the same figure shows the exact and approximate ground state wave functions for $N = \{1, 2\}$ using VISM with optimized $\hat{L} = \{2.52479, 3.04635\}$, respectively. Note that in the

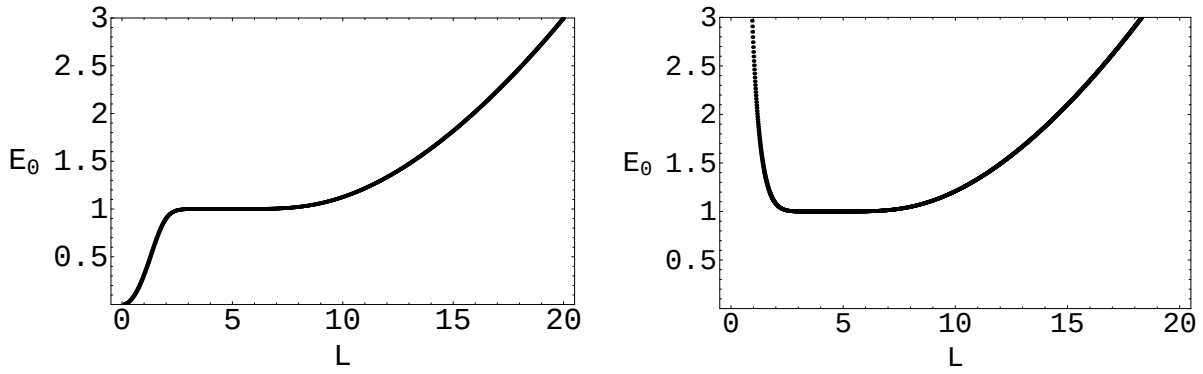

Figure 1: Ground state energy for SHO versus L for $N = 5$, using SM in units where $\hbar\omega = 2$. In the left part the results using periodic boundary condition are shown and on the right using confinement boundary condition.

un-optimized case (SM) for $N \geq 7$ the exact and approximate wave functions are practically indistinguishable on the graph, while in the optimized case (VISM) this occurs for $N \geq 2$. This clearly shows the significance of our variational improvement to SM. Here, we can report that, using VISM, $\hat{\delta}_{E_0} = \{2 \times 10^{-4}, 4 \times 10^{-6}, 9 \times 10^{-9}, 2 \times 10^{-13}\}$ for $N = \{2, 3, 5, 7\}$, respectively. Extrapolating from this, our minuscule errors for $N = 100$ are easily justified. In the left part of Fig. 5 we show a semi-log plot of the error for the ground state energy, obtained using VISM, in terms of N. As can be extrapolated from the figure significantly smaller errors are easily obtainable. The interesting feature of this graph is that the error decreases exactly exponentially and, interestingly enough, the error of the simple Fourier expansion of smooth functions has exactly the same behavior. We interpret this as a strong signal that our procedure works well.

In Fig. 5 we show a semi-log plot of the corrected computation time versus N. Note that the curvature of this plot is negative and considering this together with the plot of $\ln(\delta_E)$ shows how the effective efficiency of our program increases with N.

b. Anharmonic Oscillator with a quartic term

Now we apply this method to an anharmonic oscillator which has a quartic term. This is probably one of the most famous problem in quantum mechanics which is not exactly solvable

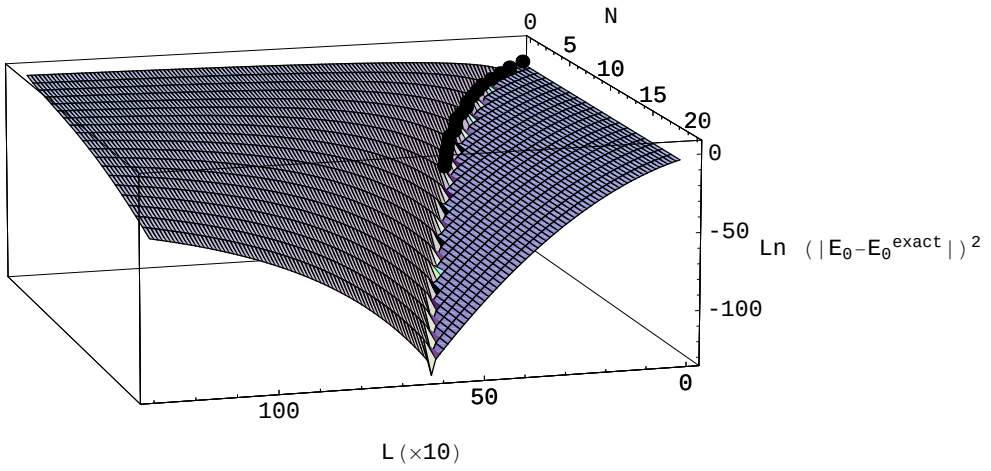

Figure 2: Semi-log plot of the square of the error of the ground state energy of SHO (in units where $\hbar\omega = 2$) versus N and L using SM. Superimposed on top of the figure is the $\hat{L}(N)$ obtained from this figure, which indicates the direction of the valley.

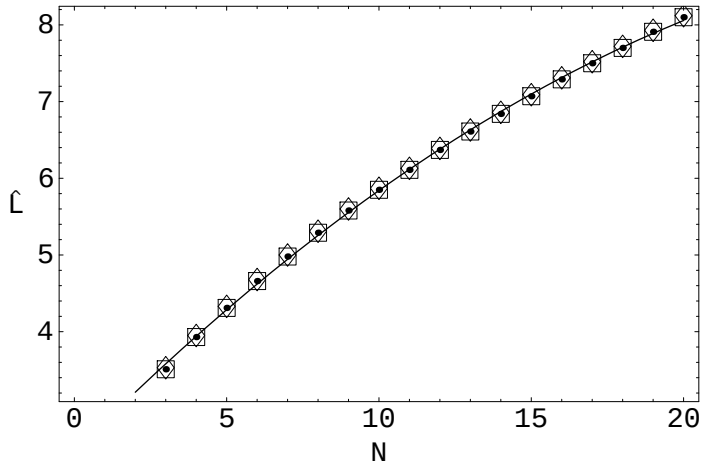

Figure 3: $\hat{L}$ versus N computed by our optimization methods involving minimization of E_0 in confinement boundary condition (boxes), minimization of δE_0 (circles), as shown in Fig. 2, and minimization of δ_{ψ_0} (diamonds). Also shown in the figure is the interpolating function $\hat{L}(N)$.

n	E_n^{exact}	E_n^{SM}	δ_E	$\hat{\delta}_E$	δ_ψ
0	1.	1.	2.6×10^{-139}	2.5×10^{-139}	7.3×10^{-70}
1	3.	3.	1.1×10^{-133}	1.1×10^{-133}	3.5×10^{-68}
2	5.	5.	5.9×10^{-134}	5.7×10^{-134}	3.1×10^{-67}
3	7.	7.	7.5×10^{-129}	7.2×10^{-129}	7.9×10^{-66}
4	9.	9.	2.2×10^{-129}	2.1×10^{-129}	6.2×10^{-65}
5	11.	11.	1.5×10^{-124}	1.4×10^{-124}	1.0×10^{-63}
6	13.	13.	3.1×10^{-125}	3.1×10^{-125}	6.8×10^{-63}
7	15.	15.	1.3×10^{-120}	1.3×10^{-120}	9.5×10^{-62}
8	17.	17.	2.4×10^{-121}	2.3×10^{-121}	6.1×10^{-61}
9	19.	19.	7.1×10^{-117}	6.8×10^{-117}	6.8×10^{-50}

Table 1: The results for the first 10 eigenvalues and eigenfunctions of the SHO in units where $\hbar\omega = 2$. E_n^{SM} are values obtained using VISM with $N = 100$. The values of δ_E and δ_ψ refer to the difference between the quantities computed using VISM and the corresponding exact quantities as given by Eq. (17). Note the good correspondence between $\hat{\delta}_E$ and δ_E shows the consistency of our method. Obviously we could not display all the digits of E_n^{SM} due to insignificant errors. The total computation time was about 50 seconds on a typical Pentium 2.4 GHz machine for obtaining the first 200 eigenvalues and eigenfunctions, which were all obtained with a same single run of the algorithm. It is worth mentioning that choosing N=30 we obtain $\delta_E \approx 10^{-15}$ with computational time of 0.5 Sec.

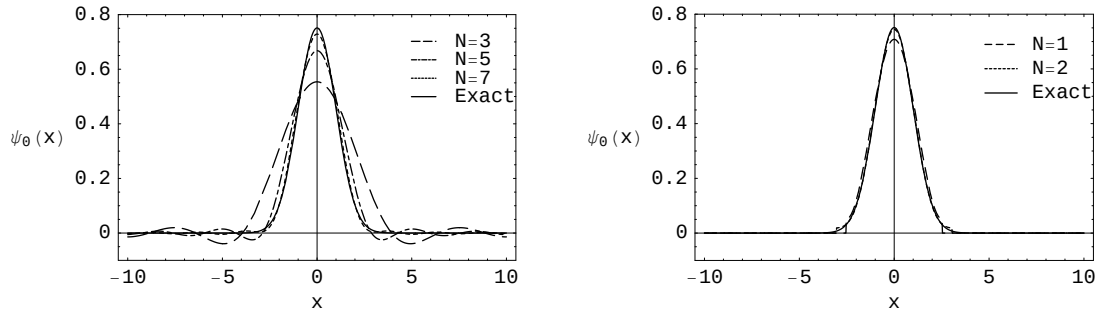

Figure 4: Left, the exact and approximate ground state wave functions of SHO for $N = \{3, 5, 7\}$ using SM with fixed un-optimized $L = 10$. Note that for $N \geq 7$ the exact and approximate wave functions are almost indistinguishable on the graph. Right, the exact and approximate ground state wave functions of SHO for $N = \{1, 2\}$ using VISM with optimized $\hat{L} = \{2.52479, 3.04635\}$, respectively. Note that for $N \geq 2$ the exact and approximate wave functions are practically indistinguishable on the graph. Also note the drastic effect of our optimization procedures.

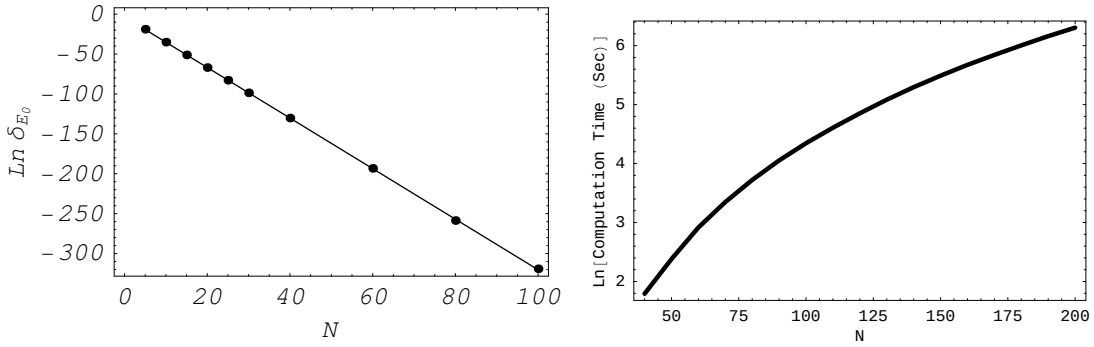

Figure 5: Left, semi-log plot of the error for the first eigenvalue of the SHO obtained by VISM using various number of basis functions ($2N$ equals the number of basis functions used). Right, semi-log plot of the computation time versus N for the ground state of SHO.

and is used as at least as a toy model. The Schrödinger equation for this model is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+\left(\frac{1}{2}m\omega^2x^2+\epsilon x^4\right)\psi(x)=E\psi(x). \tag{18}$$

Using VISM we can find the bound states energy spectrum and the corresponding eigenfunctions of this Hamiltonian. The results that we have obtained using $N = 100$ are extremely accurate ($\delta_{E_0} \approx 10^{-120}$) (Table 2). We have also compared our method and results with some other more or less routine methods such as the zero and first order perturbation theory (Table 2), the conventional Sturmian approximation of Ref. [26], the zero, first and second order variational sturmian approximation of Ref [24], and the highly accurate values of Ref. [25]. The results of these comparisons is that the seven advantages of our method mentioned in the introduction are clearly justified. We just have to mention that the reported accuracy in Ref. [25] was only 90 significant digits. The accuracy of the other methods were even lower, that is not better than $\mathcal{O}(10^{-4})$.

c. Harmonic Oscillator perturbed by rapid oscillations

Now we want to solve an example which exhibits another less explored and powerful feature of VISM. As mentioned in the introduction this method can easily handle problems whose solutions exhibit rapid oscillations, in sharp contrast to the spatial integration methods. A rather interesting example that we have constructed for this purpose is a harmonic oscillator

n	E_n^{SM}	SD	$E_n^{(0)}$	$\frac{\lvert E_n^{(0)}-E_n^{SM}\rvert}{E_n^{SM}}$	$E_n^{(1)}$	$\frac{\lvert E_n^{(1)}-E_n^{SM}\rvert}{E_n^{SM}}$
0	1.06528550954371768885709162878909308430448641781 89	124	1	0.061	1.075	0.009
1	3.30687201315291350712812168469286904959465520975 16	121	3	0.032	3.450	0.043
2	5.74795926883356330473350311847713127888097606639 13	120	5	0.13	5.975	0.039
3	8.35267782578575471215525773464369770539510526050 59	118	7	0.16	8.875	0.063
4	11.09859562263304301108645874929740325062183128234 8	118	9	0.19	12.08	0.088
5	13.96992619774279930097343395684213396114071363429 5	116	11	0.21	15.58	0.11
6	16.95479468614415133769261650881713437554998725836 1	114	13	0.23	19.38	0.14
7	20.04386360418846123364142110738511157057226690582 6	115	15	0.25	23.48	0.17
8	23.22955217993928907064708743432331824353493859948 7	112	17	0.27	27.88	0.20
9	26.50555475253661741746950300673872367605793218954 2	110	19	0.28	32.58	0.23

Table 2: The first 10 energy levels of the Schrödinger equation (Eq. (18)) whose dimensionless form is $(-d^2/dx'^2 + x'^2 + \epsilon' x'^4)\psi(x') = E'\psi(x')$. We have chosen the parameter $\epsilon' = 4\epsilon/(m\omega^4) = 1/10$ and exhibited the results for the energies in units where $\hbar\omega = 2$. E_n^{SM} are the values obtained using VISM with $N = 100$, and SD denotes the significant digits. For space limitations only the first 50 significant digits are displayed. $E_n^{(0)}$ and $E_n^{(1)}$ denote the energy eigenvalues obtained using zero and first order perturbation theory, respectively. Obviously the accuracy of these methods are far inferior compared to VISM.

perturbed by rapid oscillations whose precise Schrödinger equation is given by,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \left(\frac{1}{2}m\omega^2x^2 + \alpha\cos(\beta\pi x)\right)\psi(x) = E\psi(x), \tag{19}$$

where ω is the natural frequency of the oscillator and α and β are arbitrary constants. This differential equation is not exactly solvable and for high frequency perturbations β the spatial integration routines like FDM would have serious difficulties in these situations. They should consider many spatial points for overcoming the rapid oscillations of the potential which increases the time and round off errors of the routine and decreases the efficiency and stability of the method. However, this is not a case for the VISM which can also handle these type of potentials very easily. For large β the behavior of the potential is very oscillatory and centered around the curve $\frac{1}{2}m\omega x^2$. As expected all the eigenstates of this problem are bound states. The results for the ground state are shown in the Fig. 6. In the left part of the figure we show the full potential $U(x)$, the ground state wave function ($\psi_0(x)$), and a zoomed box highlighting the fine structural behavior of the wave function. In the right part of the figure we show the ground state energy E_0 versus N. Note for N smaller than $\beta\hat{L}$ (100 here) VISM is not sensitive enough to respond to the rapidly oscillating part of the potential and the results are very

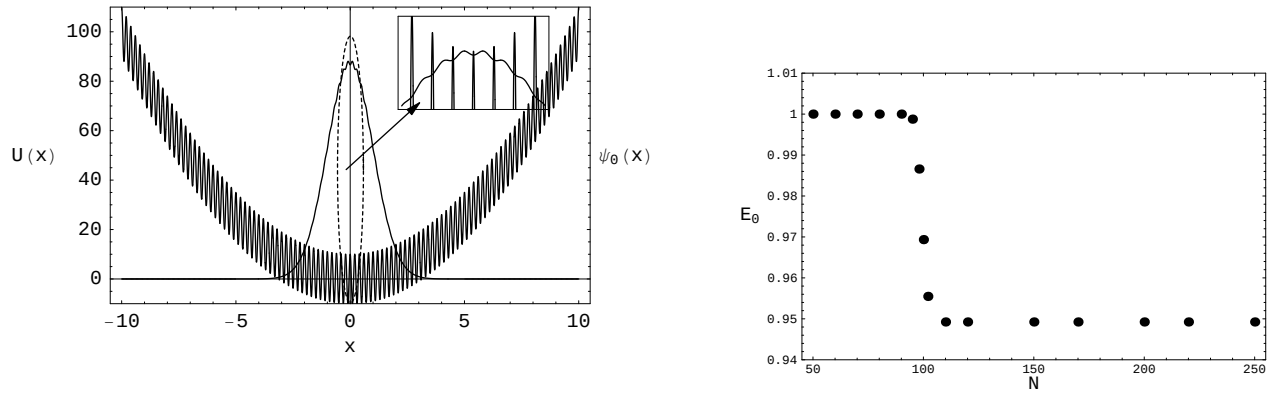

Figure 6: Left, the potential of the harmonic oscillator perturbed by rapid oscillations, whose Schrödinger equation (Eq. (19)) in dimensionless form is $(-d^2/dx'^2+x'^2+\alpha'\cos(\beta'\pi x'))\psi(x') = E'\psi(x')$. We have chosen the parameters $\beta' = \sqrt{2/m}\beta/\omega = 10$, and $\alpha' = (2/\hbar\omega)\alpha = 10$ and exhibited the results for the energies in units where $\hbar\omega = 2$. Superimposed on the same graph is the ground state wave function calculated using VISM with $N = 150$. The zoomed box exhibits the behavior of the wave function and the potential for $-0.7 < x < 0.7$. Right, the ground state energy versus N for the same parameters as in the left figure.

close to those of the (unperturbed) SHO. As is apparent from the figure, for N even slightly larger than $\beta\hat{L}$, the VISM easily incorporates the rapidly oscillating part of the potential and rapidly approaches the exact energy eigenvalue as N increases. This explains the sharp drop in the graph of $E_0(N)$. In particular for $N = 150$ we obtain $\hat{\delta}_{E_0} \approx 10^{-50}$. The physics of this phenomenon is very clear: When the set of basis functions is large enough to include those whose frequencies are at least as large as the ones induced in the wave function by the oscillations or discontinuities in the potential, via the Schrödinger equation, VISM can easily finds the accurate eigenfunctions and the corresponding eigenvalues. the fine structure of the ground state energy exhibited in the left part of the figure is also very interesting. The slight ripples in the wave function are produced by the conflicting tendencies of the wave function to accumulate in the rapidly occurring wells of the perturbed part of the potential and that of the second derivative operator to smooth out the wave function.

4 Conclusions

We have introduced three distinct yet equivalent variational improvements for the Fourier Spectral Method and used them as an extremely accurate method for obtaining the energies and wave functions of the bound states of the time-independent Schrödinger equation. In this method a finite basis is used for approximating the solutions. Our variational improvement of the method is to calculate an optimized spatial domain for a given number of basis elements, denoted by $\hat{L}(N)$. The three optimization procedures are based on minimizing the eigenvalues, the error of the eigenvalues, and on minimizing the error of the eigenstates. Our refinement schemes usually improve the accuracy of SM drastically, as can be seen in Fig. 4, for example. This improvement increases rapidly with N. In particular, when the problem is not exactly solvable there does not seem to be any other canonical way to fix L and the errors. We applied this method to an exactly solvable problem and easily found an extraordinarily good agreement with the exact solutions (errors of order 10^{-130}). In the quartic anharmonic oscillator case which is not exactly solvable, the accuracy of this method is much higher than some of the more conventional methods such as the perturbation method, the conventional sturmian approximation, and the variational sturmian approximation. In the problem of SHO perturbed by trigonometric anharmonic term, we observed how easily and accurately VISM handles problems involving potentials with very rapid oscillations. To summarize, this method is very simple, fast, extremely accurate in most cases, very robust and stable, can easily handle solutions with rapid oscillations and moving singularities, and there is no need to specify the boundary conditions on the slopes. Most importantly, one can obtain the energies and the wave functions of as many of the bound states as desired with a single run of the algorithm. The main sources of error are using too few number of basis elements and having potentials with major discontinuities. When the latter dose not exist we can obtain extraordinary good results, *e.g.* 130 significant digits, by choosing appropriate parameters. This method can be easily extended to D dimensional Schrödinger equation. For example, We have solved 2-D

Harmonic Oscillator $V(x,y) = x^2 + y^2$ and QCD potential $V(x,y) = x^2y^2$ using VISM and found extremely highly accurate results [27]. In 2-D SHO case the accuracy with 15 significant digits can be easily obtained with only 22 basis functions, and this shows the efficiency of VISM.

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