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Scaling, generator coordinate method and the eigensolutions of the Schrödinger equation

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Abstract. An extremely simple (approximate) variational method for the study of the eigensolutions of the one-dimensional Schrödinger equation is introduced, based upon the idea of employing scaled eigenstates of the harmonic oscillator as generating functions for the generator coordinate method. The approach is successfully applied to a variety of situations.

1. Introduction

It is well known that Schrödinger's equation, even in the one-particle, one-dimensional case, rarely possesses an exact (analytical) solution.

The eigensolutions of even the simplest (one-dimensional) Hamiltonian

$$\hat{H} = \hat{p}^2/2m + U(\hat{x}) \tag{1.1}$$

may deserve careful scrutiny, in view of the prevailing belief that they may lead, in many instances, to a fuller understanding of 'equivalent' models in field theory (Bozzolo and Plastino 1981a).

In a recent effort (Bozzolo and Plastino 1981b), an extremely simple variational method was presented, designed so as to study the solutions for the anharmonic oscillator $U(\hat{x}) = m\omega^2\hat{x}^2/2 + \lambda V(\hat{x})$, where V is an even function. The idea of the corresponding approach is that of finding the eigenstates $|J\rangle$ of (1.2) starting with the eigenstates $|j\rangle$ of the harmonic oscillator. The states $|J\rangle$ and $|j\rangle$ are necessarily connected by means of a unitary transformation of the form

$$|J\rangle = \exp(i\hat{F})|j\rangle \tag{1.2}$$

and the question is then that of finding $\hat{F}$, which is tackled by recourse to the variational principle. It is easy to show that a first-order approach to $\hat{F}$ (let us call the approximate operator $\hat{F}_1$) is tantamount to a scaling operation on any function $g(x)$ of the coordinate, i.e.,

$$\exp(i\hat{F}_1(x))g(x) = \sqrt{\alpha}\, g(\alpha x) \qquad \alpha \text{ real.} \tag{1.3}$$

Consequently, minimisation of expectation values of $\hat{H}$ with respect to the scaling factor α allows for a quite simple method that yields rigorous upper bounds to both the ground state (GS) and the first excited state (FES) of (1.2) (the latter for reasons of symmetry).

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The purpose of the present work is two-fold: on the one hand, we wish to deal with Hamiltonians of the type (1.1), which are of a more general form than (1.2). On the other one, we would like to find rigorous upper bounds to *all* the eigenvalues of (1.1). These goals will be achieved by recourse to the generator coordinate method (GCM), to be described in the following section.

2. The generator coordinate method

The generator coordinate method (Hill and Wheeler 1953, Griffin and Wheeler 1957) is an approach of great physical appeal based on the following ansatz for the wavefunction one is interested in

$$\Psi(x) = \int \mathrm{d}\alpha f(\alpha)\phi(\alpha, x), \tag{2.1}$$

where $\phi(\alpha, x)$ is called the generating function, α the generator coordinate and $f(\alpha)$ the weight function. The latter is to be determined by the variational principle

$$\delta(\langle\Psi|\hat{H}|\Psi\rangle/\langle\Psi|\Psi\rangle) = 0. \tag{2.2}$$

As shown by Hill and Wheeler (1953) and Griffin and Wheeler (1957), the variational principle (2.2) leads to the Hill-Wheeler equation

$$\int \mathrm{d}\beta f(\beta)(\mathcal{H}(\alpha, \beta) - E\mathcal{O}(\alpha, \beta)) = 0 \tag{2.3}$$

with

$$\mathcal{H}(\alpha, \beta) = \langle\phi(\alpha, x)|\hat{H}|\phi(\beta, x)\rangle \qquad \text{and} \qquad \mathcal{O}(\alpha, \beta) = \langle\phi(\alpha, x)|\phi(\beta, x)\rangle. \tag{2.4}$$

which, after discretisation, can be solved by recourse to diagonalisation techniques (see Faessler and Plastino 1973, and references therein).

3. Scaling and the GCM

In order to obtain approximate expressions for the eigenvalues of (1.10) (we will restrict $U(x)$ to be an even function), and according to the ideas outlined in § 1, it seems rather natural to employ as generating functions the eigenstates of the harmonic oscillator, *scaled* according to (1.4), and with α as the generator coordinate. Indeed, this is the *basic idea* that underlies the present effort. The ansatz (2.1) will thus be cast as

$$\phi(\alpha, x) = \exp(\mathrm{i}\hat{F}_1(\alpha))g(x) \qquad \Psi(x) = \int \mathrm{d}\alpha f(\alpha)\sqrt{\alpha}g(\alpha, x) \tag{3.1}$$

where $g(x)$ is the wavefunction corresponding to the GS (FES) of the 'unperturbed' (harmonic oscillator h_0) Hamiltonian, which in suitable units reads

$$\hat{h}_0 = \mathrm{d}^2/\mathrm{d}x^2 + x^2. \tag{3.2}$$

According to the parity (even or odd) we have, for example

$$g(\alpha x) \equiv \phi_{\text{even}}(\alpha, x) = \pi^{-1/4}\sqrt{\alpha}\exp(-\alpha^2 x^2/2), \tag{3.3}$$

and a similar expression holds for $\phi_{\text{odd}}(\alpha, x)$.

In solving the Hill-Wheeler equation (2.3) we will face (after discretisation of the generator coordinate α) a generalised diagonalisation problem of the form

$$\sum_{\beta} (\mathcal{H}_{\alpha\beta} - E\mathcal{O}_{\alpha\beta}) f_{\beta} = 0. \tag{3.4}$$

If the integral (2.3) is discretised by replacing it with a sum over N points, the diagonalisation of (3.4) yields N eigenvalues, which we shall take as approximations to the first N even (first N odd) eigenstates of $\hat{H}$. The approximate wavefunctions are of the form

$$\Psi_m = \sum_{i=1}^{N} f_m(\alpha_i)\phi(\alpha_i, x), \qquad m = 1, \ldots, N. \tag{3.5}$$

If the $\phi(\alpha_i, x)$ are linearly independent, we are in a position to argue that the eigenvalues E_m arising from (3.4) are upper bounds to the corresponding eigenvalues of $\hat{H}$ (Hylleraas and Undheim 1930). The linear independence of the generating functions $\phi(\alpha, x)$ is guaranteed as long as one eigenvalue of the overlap matrix (α, β) is different from zero.

A final point to be discussed is that of the discretisation of (2.1). In other words, how are we to choose the N points α_i in that equation so as to reduce the Hill-Wheeler equations to the form (3.4). An appealling choice is that of setting $\alpha = \sqrt{\omega}$. In this way, we could select a particular value of ω, say ω_0, as a 'fundamental' frequency, and the remaining $(N-1)$ values as 'overtones' of that frequency, i.e., $\omega_n = n\omega_0$, $n = 1, \ldots, N$. We can regard ω_0 as an additional degree of freedom which is fixed by the variational principle.

4. Simple applications

We shall now deal with specific applications of the formalism introduced in the present work. This entails dealing with typical potentials $U(x)$, as specific instances of the general Hamiltonian (1.1).

In our case we need, first of all, expressions for the overlap $\mathcal{O}(\alpha, \beta)$, and, for each $U(x)$, the kernel $\mathcal{H}(\alpha, \beta)$. This task is to be separately performed for both even (e) or odd (o) states, and one easily finds

$$\mathcal{O}_{\text{even}}(\alpha, \beta) = \left(\frac{2\alpha\beta}{\alpha^2+\beta^2}\right)^{1/2} \qquad \mathcal{O}_{\text{odd}}(\alpha, \beta) = \left(\frac{2\alpha\beta}{\alpha^2+\beta^2}\right)^{3/2}. \tag{4.1}$$

4.1. The generalised anharmonic oscillator

This is a problem of permanent interest for a variety of reasons. A vast amount of literature is available, for instance, Chaudhuri and Mukherjee (1984, and references therein) and Flessas and Whitehead (1984). The Hamiltonian is (in suitable units)

$$\hat{H} = -\frac{d^2}{dx^2} + \hat{x}^2 + \sum_{i=2}^{N} \lambda_i \hat{x}^{2i}, \tag{4.2}$$

so that (see equation (2.4))

$$\mathcal{H}_{\text{even}} = \mathcal{O}_{\text{even}}(\alpha, \beta)\left(\frac{\alpha^2\beta^2+1}{\alpha^2+\beta^2} + \sum_{i=2}^{N} \frac{\lambda_i (2i-1)!!}{(\alpha^2+\beta^2)^i}\right). \tag{4.3}$$

We have performed calculations for $N=2$ for a wide range of coupling constants λ (between 1 and 40 000). Our results are to be compared with the 'exact' ones of Biswas *et al* (1973) based on the Hill determinant method. We have used seven points in discretising the corresponding secular equation ((7×7) matrices to be separately diagonalised for even and odd states). The agreement between our results and those of Biswas *et al* (1973) is excellent (seven digits for the GS). Notice that we deal just with 7×7 matrices, while Biswas *et al* (1973) have to tackle matrices of the order 50×50.

4.2. Double minimum potential

This is a potential of the form (Bozzolo *et al* 1984)

$$U(\hat{x}) = -\hat{x}^2 + \lambda \hat{x}^4 \tag{4.4}$$

that exhibits a double minimum and a 'barrier' at the origin. Here we have

$$H_e(\alpha,\beta) = \mathcal{O}_{even}(\alpha,\beta)\left(\frac{\alpha^2\beta^2-1}{\alpha^2+\beta^2}+\frac{3\lambda}{(\alpha^2+\beta^2)^2}\right). \tag{4.5}$$

Our treatment yields rather satisfactory results. As an example, we mention that for $\lambda = 5.0$ an 8-point GCM mesh is able to reproduce the figures obtained by means of a 25×25 diagonalisation (in a harmonic oscillator basis) up to seven digits for the GS and the FES.

4.3. Razavy potential (Razavy 1980)

The motion of a particle in the presence of two centres of force is approximately described by double-well potentials, as, for instance,

$$U(\hat{x}) = \tfrac{1}{8}m^2(\cosh(4\hat{x})-1) - m(n+1)\cosh(2\hat{x}), \tag{4.6}$$

n,m being free parameters. An exact analytical solution exists for the first $(n+1)$ levels. In our case we have

$$\mathcal{H}_e(\alpha,\beta) = \mathcal{O}_{even}(\alpha,\beta)\left(\frac{\alpha^2\beta^2}{\alpha^2+\beta^2}+\frac{m^2}{8}\{\exp[8/(\alpha^2+\beta^2)]-1\}\right.$$
$$\left. - m(n+1)\exp[2/(\alpha^2+\beta^2)]\right). \tag{4.7}$$

We have compared 10 GCM mesh point results with the exact ones. The agreement is excellent. We have taken $n=1$ and $n=2$ with m ranging from $m=1$ up to $m=50$. If we define $\varepsilon = |(E_{exact}-E_{GCM})/E_{exact}|$, ε ranges between 2.10×10^{-4} and 1.0×10^{-10} for the GS, with slightly worse results for excited states. As this is by no means a trivial $U(x)$, we believe these results will prove to be hard to match by other approximations.

4.4. Square well

Let $U(x)=\beta$ for $|x|>\alpha$. This simple potential poses a rather stringent test for our approach, since $U(x)$ does not look at all like an anharmonic oscillator potential. We have taken, as an example, $\alpha=0.2$ and $\alpha=0.5$ and $\beta=0.2$, 0.5 and 1.0. Only one bound state exists in these circumstances and

$$\mathcal{H}_e(\alpha,\beta) = \mathcal{O}_{even}(\alpha,\beta)\left(\frac{\alpha^2\beta^2}{\alpha^2+\beta^2}+\beta\ \mathrm{erf}\{\alpha[\tfrac{1}{2}(\alpha^2+\beta^2)]^{1/2}\}\right). \tag{4.8}$$

The present scheme reproduces the exact results (up to three significant digits) with a 9-point mesh.

4.5. Interaction of the type $\lambda x^2/(1+gx^2)$

Let us consider the Hamiltonian (Biswas *et al* 1973)

$$\hat{H} = -\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \lambda x^2/(1+gx^2) \tag{4.9}$$

with the interaction in the last term characterised by two free parameters λ and g (we have chosen $\lambda = 50$ and $\lambda = 100$, with g ranging from 0.1 up to 100.0).

This Hamiltonian is not exactly solvable. Approximation schemes must be used, based usually either on variational or on perturbation methods. An elegant approach has been formulated by Mitra (1978), who employs the Ritz variational method in conjunction with the Givens-Householder algorithm. Sophisticated numerical techniques guarantee the accuracy of these results. More recent studies were done by Chaudhuri and Mukherjee (1983) and Cohen (1984)

$$\mathscr{H}_e(\alpha,\beta) = \mathscr{O}_{even}(\alpha,\beta)\left\{-\frac{\alpha^2\beta^2}{\alpha^2+\beta^2}+\frac{\lambda}{g}\left[1-\left(\frac{\pi(\alpha^2+\beta^2)}{2g}\right)^{1/2}\right]\right.$$
$$\left.\times\exp\left(\frac{\alpha^2+\beta^2}{2g}\right)\operatorname{erf}\left[\left(\frac{\alpha^2+\beta^2}{2g}\right)^{1/2}\right]\right\}. \tag{4.10}$$

Our results for the first three eigenvalues of (4.9) with nine points reproduce exactly those published by Mitra (1978).

5. Conclusions

A simple, approximate variational procedure for the study of the one-dimensional Schrödinger equation (with the potential an even function of the coordinate) has been presented. The approach is based upon the idea of extending, by recourse to the GCM with the scaling parameter as generating coordinate, the well known scaling (of the wavefunction) method, widely employed in order to obtain upper bounds to the GS.

Our approach thus yields upper bounds not only to the GS, but to excited states as well. The use of a scaled wavefunction is just a particular instance of the present algorithm, for which one just takes a single point in the discretisation scheme (and minimises the expectation value of $\hat{H}$ with respect to the scaling parameter).

The present technique leads to an extremely simple numerical problem (diagonalisation of matrices of the order 10×10), which is to be contrasted with the sophisticated algorithms employed by other authors with reference to the anharmonic oscillator problem. Moreover, our approach is quite general while it is not so easy to see how these latter formalisms could be applied to problems different from the one posed by the anharmonic oscillator.

As a further advantage of the present approximation, it should be pointed out that the (in some cases) quite difficult evaluation of matrix elements is entirely bypassed here. All one needs is just the integral of the $U(x)$ times a Gaussian (available, in general, from suitable tables).

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References

Biswas S N, Datta K, Saxena R P, Srivastava P K and Varma V S 1973 *J. Math. Phys.* **14** 1190
Bozzolo G and Plastino A 1981a *KINAM* **3** 347
—— 1981b *Phys. Rev.* D **24** 3113
Bozzolo G, Esebbag C and Plastino A 1984 *KINAM* **6** 11
Chaudhuri R N and Mukherjee B 1983 *J. Phys. A: Math. Gen.* **16** 4031
—— 1984 *J. Phys. A: Math. Gen.* **17** 277
Cohen M 1984 *J. Phys. A: Math. Gen.* **17** 2345
Faessler A and Plastino A 1973 *Z. Phys.* **260** 305
Flessas G P and Whitehead R R 1984 *J. Math. Phys.* **25** 923
Griffin J J and Wheeler J A 1953 *Phys. Rev.* **108** 381
Hill D L and Wheeler J A 1953 *Phys. Rev.* **89** 1102
Hylleraas E A and Undheim B 1930 *Z. Phys.* **65** 759
Mitra A K 1978 *J. Math. Phys.* **19** 2018
Razavy M 1980 *Am. J. Phys.* **48** 285