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Linear variational approximation to the gx^{2n} anharmonic oscillator

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Abstract. An approximate, variational method for the study of the gx^{2n} anharmonic oscillator is presented. The idea of the method is to introduce into the unperturbed oscillator states the correlations originated by the presence of the anharmonic term via a unitary operator $\exp(iF)$ which is expanded up to second order in F. The variational principle determines F and one is led to a linear system of equations. The whole unperturbed basis is employed.

1. Introduction

The anharmonic oscillator poses a problem which has been the subject of much work, both from the analytical and the numerical point of view. During the last decade the corresponding literature has been greatly enriched (Banerjee *et al* 1978, Boyd 1978, Fung *et al* 1978, Gillespie 1976, Graffi and Grecchi 1973, Halliday and Suranyi 1980), the interest in this type of investigation arising from the belief that the nature of the solutions of the corresponding Hamiltonian may lead to a fuller understanding of an equivalent one-dimensional model Hamiltonian in field theory (Boyd 1978). Moreover, the knowledge of the exact eigenvalues of an x^4-anharmonic oscillator is of particular interest in molecular physics. More specifically, we are talking about quantum mechanical systems defined by Hamiltonians of the form

$$\hat{H} = \hat{H}_0 + \lambda \hat{V} \tag{1.1}$$

where $\hat{H}_0$ is the harmonic oscillator and $\hat{V}$ is a polynomial of even degree. In order to evaluate the eigenvalues and eigenvectors of (1.1) several approximation procedures have been applied, such as WKB techniques (Bender and Wu 1969, Lu *et al* 1973), Hill determinant (Biswas *et al* 1971), approximate canonical transformation (Halpern 1973), Borel–Padé methods (Graffi *et al* 1970, 1971), etc.

In the present work we shall restrict ourselves to the one-dimensional case,

$$\hat{H} = \hat{p}^2/2m + \tfrac{1}{2}m\omega^2\hat{x}^2 + g\hat{x}^{2m}, \tag{1.2}$$

m integer, and present a simple variational procedure which allows one to obtain an approximation to the eigenvalues and eigenfunctions of the Hamiltonian (1.2).

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The method yields expressions that are very simple to compute. The corresponding formalism is developed in § 2 and specific applications are made in § 3. The results are discussed in § 4.

2. Formalism

2.1. The mapping operator

In appropriate units our problem is that of looking for the spectrum of the differential operator

$$-\mathrm{d}^2/\mathrm{d}x^2 + x^2 + gx^{2m} \qquad m = 1, 2, \ldots . \tag{2.1}$$

Introducing the creation and destruction operators

$$\hat{a}^\dagger = \hat{p} + \mathrm{i}\hat{x} \qquad \hat{a} = \hat{p} - \mathrm{i}\hat{x} \tag{2.2}$$

such that $\{\hat{a}, \hat{a}^\dagger\} = 2$, we can find an Hermitian operator $\hat{B}$ according to

$$\hat{B} = -\mathrm{i}(\hat{a}^\dagger - \hat{a}) \tag{2.3}$$

and rewrite our Hamiltonian as

$$\hat{H} = \hat{a}^\dagger\hat{a} + \hat{1} + g\hat{B}^{2m}2^{-2m}. \tag{2.4}$$

We denote by $|j\rangle$ the eigenstates of

$$\hat{H}_0 = \hat{a}^\dagger\hat{a} + \hat{1} \tag{2.5}$$

whose eigenvalues will be called E_j. The method to be proposed is based on the idea of relating the eigenstates $|j\rangle$ of $\hat{H}_0$ to those $|J\rangle$ of $\hat{H}$ by means of a mapping operator $\hat{F}_j$

$$|J\rangle = \exp(\mathrm{i}\hat{F}_j)|j\rangle \tag{2.6}$$

of the general form

$$\hat{F}_j = \mathrm{i}\sum_{k=1}^{\infty} h_j^{(k)}(\hat{a}^{\dagger 2k} - \hat{a}^{2k}). \tag{2.7}$$

The approximate procedure to be proposed here proceeds as follows. One expands the exponential in equation (2.6) up to second order

$$\exp(\mathrm{i}\hat{F}_j) \simeq \hat{1} + \mathrm{i}\hat{F}_j - \tfrac{1}{2}\hat{F}_j^2 \equiv e_2^{\mathrm{i}F_j} \tag{2.8}$$

and then determines the quantities $h_j^{(k)}$ $(k = 1, \ldots,)$ of equation (2.7) by minimisation of (keep terms up to second order only)

$$E_J = \langle j|e_2^{-\mathrm{i}\hat{F}_j}\hat{H}e_2^{\mathrm{i}\hat{F}_j}|j\rangle. \tag{2.9}$$

It is worthwhile pointing out that, according to this prescription, (i) one is working *with the whole unperturbed basis* (see equation (2.7)) and (ii) the $h_j^{(k)}$ arise as the solution of a *linear* system of inhomogeneous equations

$$\delta E_J/\delta h_r^{(k)} = 0 \qquad r = 1, 2, \ldots . \tag{2.10}$$

The method to be developed can be applied to any excited state of $\hat{H}$. However, only in the case of the ground state (GS) and that of the first excited state, does it provide us with an upper bound to the corresponding energies (in the latter case for reasons of symmetry).

2.2. Expectation values

The general expression for the approximate energy of the jth excited state can be written in a compact form if we are willing to introduce some definitions. We shall need a scalar quantity b^n_{jk}, two column vectors $\boldsymbol{C}$ and $\boldsymbol{h}$ and a matrix M, as given below.

$$b^n_{jk} = \langle j|\hat{B}^n|k\rangle \tag{2.11}$$

$$\|\boldsymbol{C}\|_p = 2^{p+1}\gamma\{[j!/(j-2p)!]^{1/2}b^{2n}_{j-2p,j} - [(j+2p)!/j!]^{1/2}b^{2n}_{j,j+2p}\} \tag{2.12}$$

$$\|\boldsymbol{h}_j\|_p = h^{(j)}_p \tag{2.13}$$

and

$$\begin{aligned}\|M_j\|_{m,k} = {} & m2^{2m+3}\{[j!/(j-2m)!] - [(j+2m)!/j!]\}\delta_{mk} \\ & - 2^{k+m}\gamma[\![2\{[(j+2k+2m)!/j!]^{1/2}b^{2n}_{j,j+2k+2m} \\ & + j!^{-1/2}\{[(j+2k)!(j+2m)!]/j!\}^{1/2}b^{2n}_{j+2k,j+2m} \\ & + [j!/(j-2k-2m)!]^{1/2}b^{2n}_{j-2k-2m,j} - 2[(j+2k)!/(j-2m)!]^{1/2}b^{2n}_{j+2k,j-2m} \\ & + j!/((j-2m)!(j-2k)!)^{1/2}b^{2n}_{j-2m,j-2k}\} \\ & - 2\{[j!(j-2m+2k)!]^{1/2}/(j-2m)!\}b^{2n}_{j+2k-2m,j} \\ & - 2(j+2k)!/[(j-2m+2k)!j!]^{1/2}b^{2n}_{j,j+2k-2m}]\!].\end{aligned} \tag{2.14}$$

The expectation value we are looking for is (see appendix for details of the calculations)

$$E_J = \langle J|\hat{H}|J\rangle = \langle j|\hat{H}|j\rangle + \gamma b^{2n}_{jj} + \boldsymbol{C}\cdot\boldsymbol{h} - \tfrac{1}{2}\boldsymbol{h}_j^t M_j \boldsymbol{h}_j. \tag{2.15}$$

The column vector $\boldsymbol{h}$ is the solution of the system (2.10) which leads to

$$M_j\boldsymbol{h}_j = \boldsymbol{C}_j \tag{2.16}$$

which involves an infinite number of equations. In a practical calculation one is forced to truncate the system for a given finite number N of equations, i.e.

$$\sum_{k=1}^{N} (M_j)_{pk}h^{(j)}_k = (C_j)_p \qquad p = 1, \ldots, N. \tag{2.17}$$

The scheme here proposed can be easily generalised in order to study polynomial perturbations to H_0. As an example, if the anharmonicity is given by $\lambda x^n + \mu x^m$ it is enough to redefine the quantities b^n_{ab} introducing instead

$$b^{nm}_{ab} = \langle a|\lambda B^n + \mu B^m|b\rangle. \tag{2.18}$$

3. Numerical example

The first point to be investigated concerns the 'size' of the system given by equation (2.10), which lead to the infinite linear system (2.16). In truncating it, as is done in (2.17), how large should N and, correspondingly, k be? This question can be discussed with reference to table 1, which illustrates the situation that arises in the case gx^4 for $g = 0.1$. The table displays the quantities $h^{(k)}_0$ for different values of N (along the vertical). The index k runs along the horizontal, and it is seen that (i) $h^{(k)}$ decreases rapidly as k increases and (ii) for a given k, the corresponding value of h converges very quickly as N grows, attaining afterwards stable values. Thus the linear system of

Table 1. Values of $h_0^{(k)}$ for different sizes (N) of the linear system given by (2.17), corresponding to the anharmonicity given by $0.1x^4$.

N \ k	1	2	3	4	5	6
2	$-0.139\,22 \cdot 10^{-1}$	$0.394\,14 \cdot 10^{-3}$				
3	$-0.139\,24 \cdot 10^{-1}$	$0.414\,21 \cdot 10^{-3}$	$0.775\,35 \cdot 10^{-5}$			
4	Stable	$0.414\,37 \cdot 10^{-3}$	$0.797\,07 \cdot 10^{-5}$	$0.520\,59 \cdot 10^{-7}$		
5		Stable	$0.797\,01 \cdot 10^{-5}$	$0.516\,81 \cdot 10^{-7}$	$-0.628\,99 \cdot 10^{-10}$	
6			Stable	$0.515\,67 \cdot 10^{-7}$	$-0.994\,76 \cdot 10^{-10}$	$-0.452\,77 \cdot 10^{-11}$
7				$0.515\,65 \cdot 10^{-7}$	$-0.101\,80 \cdot 10^{-9}$	$-0.502\,93 \cdot 10^{-11}$
8				Stable	$-0.101\,87 \cdot 10^{-9}$	$-0.505\,49 \cdot 10^{-11}$
9					Stable	$-0.505\,56 \cdot 10^{-11}$
10						Stable

Table 2. Ground-state energy of the gx^4 anharmonic oscillator. The degree of agreement (%) between the approximate results obtained in this work and the Borel–Padé exact ones (Graffi *et al* 1970) is displayed as a function of g.

g	E_0 (%)	g	E_0 (%)
0.1	99.96	0.6	97.91
0.2	99.79	0.7	97.22
0.3	99.48	0.8	96.51
0.4	99.04	0.9	95.75
0.5	98.50	1.0	94.98

Table 3. First excited state of the gx^4 anharmonic oscillator. The degree of agreement (%) between the approximate results and those obtained with the Hill determinant method (Biswas *et al* 1971) is displayed as a function of g.

g	E_0 (%)	g	E_0 (%)
0.1	99.87	0.6	95.22
0.2	99.38	0.7	93.95
0.3	98.59	0.8	92.65
0.4	97.59	0.9	91.35
0.5	96.45	1.0	90.05

Table 4. Ground-state energy of the gx^6 anharmonic oscillator. The degree of agreement (%) between the approximate results obtained in this work and the Borel–Padé (Graffi *et al* 1970) exact ones is displayed as a function of g.

g	E_0 (%)	g	E_0 (%)
0.1	98.71	0.6	83.09
0.2	95.87	0.7	80.37
0.3	92.55	0.8	74.82
0.4	89.30	0.9	73.54
0.5	86.52	1.0	72.14

equations one is dealing with attains only modest proportions and poses an extremely simple computational problem. We do not show more examples, for other values of j and n, for the sake of brevity. They have been investigated, however, and support the conclusions drawn above.

We present in this paper numerical results for $V(x) = gx^n$ with $n = 4$ in tables 1–3, and with $n = 6$ in table 4. The degree of agreement between our approximate results and those arising from exact treatments is rather good, both for the GS energies and for those corresponding to the first excited state.

The results show that our method may be useful to provide approximate values for the energies in cases in which the numerical effort required with other approaches becomes prohibitive (n large). It should be pointed out, in this respect, that the numerical effort involved in the cases of large values of n is not appreciably greater than for $n = 4$ or $n = 6$.

A variational approach frequently employed is that of expanding the trial function in terms of the eigenstates of the unperturbed Hamiltonian

$$|\Phi(\text{trial})\rangle = \sum_{i=1}^{M} c_i |\phi_i\rangle \tag{3.1}$$

where the M states $|\phi_i\rangle$ *do not* span the corresponding Hilbert space. Variation with respect to the c_i leads to an eigenvalue problem involving an $M \times M$ diagonalisation of the corresponding Hamiltonian. It may be of interest to compare results of our procedure with the variational ones obtained with the method just described. As an example, let us consider the GS energy for the perturbation gx^4. We have performed the corresponding diagonalisations for $M = 4$, 6, 12 for $g = 0.1$. The agreement with the *exact* GS energy (%) is as follows: for $M = 4$, 99.94%; for $M = 6$, 99.99% and for $M = 12$†, 100% (up to nine digits). On the other hand, our approach coincides with the exact one up to 99.96% (and involves, as in all examples given in this paper, truncation at $N = 3$; i.e. a 3×3 linear system). The method of the present work is not, of course, as good as the one which uses the trial wavefunction (3.1), but it is not too far off, either.

The main advantage of the method proposed here, lies in its computational simplicity, as it is able to replace the nonlinear problem posed by the ordinary approach by a *linear* one, albeit sacrificing some precision.

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Appendix. On the calculation of expectation values

In order to evaluate the expectation values (2.9) we shall utilise the identity (remember the definition (2.8))

$$e_2^{i\hat{F}_j} \hat{H} e_2^{i\hat{F}_j} = \hat{H} + i\{\hat{H}, \hat{F}_j\} - \tfrac{1}{2}\{\{\hat{h}, \hat{F}_j\}, \hat{F}_j\} \equiv \hat{Q}_j \tag{A1}$$

and try to express $\hat{Q}_j$ in terms of our basic quantities $h_j^{(k)}$. The result has a rather

† Of course, we are considering the first M eigenvectors of the unperturbed Hamiltonian.

formidable appearance, and a few preliminary definitions will prove to be of help. In the first place, it is convenient to have a common notation for both creation and destruction operators, and to this end we shall employ greek superscripts, i.e. λ, μ ($\lambda, \mu =$ '+' or '−') and write the corresponding operator as a^{λ}, a^{μ}. Next we introduce a special symbol for the commutator between the nth power of the operator $\hat{B}$ (equation (2.13)) and the kth power of the creation (or destruction) operator a^{λ}

$$\Gamma^{(n)}_{\lambda k} \equiv \{\hat{B}^n, (\hat{a}^{\lambda})^k\}$$
$$= \sum_{r=0}^{k-1} \{(\hat{a}^{\lambda})^r \hat{B}^n (\hat{a}^{\lambda})^{k-r} - (\hat{a}^{\lambda})^{r+1} \hat{B}^n (\hat{a}^{\lambda})^{k-r-1}\}. \tag{A2}$$

The commutator of $\Gamma^{(n)}_{\lambda k}$ with the rth power of a^{μ} is

$$\Gamma^{(n,r)}_{\lambda,k,\mu} \equiv \{\Gamma^{(n)}_{\lambda k}, (a^{\mu})^r\} = \sum_{t=0}^{r-1} (\hat{a}^{\mu})^t \Gamma^{(n,1)}_{\lambda k} (\hat{a}^{\mu})^{r-t-1}. \tag{A3}$$

We shall also need the following commutators

$$x^{(j)}_{\lambda\mu\rho} \equiv \{a^{\lambda} a^{\mu}, (a^{\rho})^j\}$$
$$= 2j\rho\{a^{\lambda}(a^{\rho})^{j-1}(1-\delta_{\mu\rho}) + (a^{\rho})^{j-1} a^{\mu}(1-\delta_{\lambda\rho})\} \tag{A4}$$

and

$$Y^{(j,k)}_{\lambda\mu\rho\omega} \equiv \{x^{(j)}_{\lambda\mu\rho}, (a^{\omega})^j\}$$
$$= \sum_{t=0}^{k-1} \{(a^{\omega})^t x^{(j)}_{\lambda\mu\rho} (a^{\omega})^{k-1} - (a^{\omega})^{t+1} x^{(j)}_{\lambda\mu\rho} (a^{\omega})^{k-t-1}\}. \tag{A5}$$

Setting $\gamma = g/2^{2n}$ the previous definitions enable us to write for $\hat{Q}_p$ the following expression

$$\hat{Q}_p = H - \sum_{j-1}^{\infty} h_j^{(p)} \{x^{(2j)}_{+--+} - x^{(2j)}_{+--} + \gamma(\Gamma^{(n)}_{+,2j} - \Gamma^{(n)}_{-,2j})\}$$
$$+ \tfrac{1}{2} \sum_{j,k=1}^{\infty} h_j^{(p)} h_k^{(p)} \{Y^{(2j,2k)}_{+---+} + Y^{(2j,2k)}_{+----} - Y^{(2j,2k)}_{+--+-} - Y^{(2j,2k)}_{+---+}$$
$$+ \gamma(\Gamma^{(n,2k)}_{+,2j,+} + \Gamma^{(n,2k)}_{-,2j,-} - \Gamma^{(n,2k)}_{+,2j,-} - \Gamma^{(n,2k)}_{-,2j,+})\}. \tag{A6}$$

In order to obtain the expectation value (2.9) one needs only to evaluate the quantity $\langle p|\hat{Q}_p|p\rangle$ which, according to (A6) and the preceding definitions, ultimately involves just the action of the creation (destruction) operator a^{μ} upon the unperturbed harmonic oscillator state $|p\rangle$. We give below the expectation values that are required in order to evaluate the GS energy ($p = 0$).

$$\langle p=0|x^{(2)}_{\lambda\mu\rho}|p=0\rangle = 8\rho\delta_{\lambda\mu} \tag{A7}$$

$$\langle p=0|\Gamma^{(n)}_{\lambda k}|p=0\rangle = 2^{k/2}(k!)^{1/2}\{\delta_{\lambda+} b^{(n)}_{0k} - \delta_{\lambda-} b^{(n)}_{k0}\}. \tag{A8}$$

$$\langle p=0|Y^{(j,k)}_{\lambda\mu\rho\omega}|p=0\rangle = 2^{(k+2)/2}(k!)^{1/2}\rho j\{2^{3/2}\delta_{j=1}\delta_{jk}\delta_{\rho\omega}\delta_{\lambda\mu}(\delta_{\lambda-}\delta_{\rho+} - \delta_{\rho-}\delta_{\lambda+})$$
$$+ 2^{j/2}(j!)^{1/2}\delta_{jk}\delta_{\lambda+}\delta_{\mu-}(\delta_{\lambda\omega}\delta_{\mu\rho} - \delta_{\mu\omega}\delta_{\lambda\rho})$$
$$+ 2^{(j+2)/2}(j!)^{1/2}\delta_{jk}\delta_{\lambda-}\delta_{\mu+}(\delta_{\lambda\rho}\delta_{\mu\omega} - \delta_{\lambda\omega}\delta_{\mu\rho})$$
$$+ 2^{j/2}\{(j-1)(j-1)!\}^{1/2}\delta_{j-1,k+1}\delta_{j\geq 2}\delta_{\lambda\mu}\delta_{\mu\omega}(\delta_{\lambda+}\delta_{\rho-} - \delta_{\lambda-}\delta_{\rho+}) \tag{A9}$$

and

$$\langle p=0|\Gamma^{(n,r)}_{\lambda k\mu}|p=0\rangle = 2^{(k+2)/2}(r!)^{1/2}[[(k+r)!/r!]^{1/2}\delta_{\lambda\mu}(\delta_{\lambda+}b^{(n)}_{0,k+r} + \delta_{\lambda-}b^{(n)}_{k+r,0}) + (\delta_{\lambda+}\delta_{\mu-} + \delta_{\mu+}\delta_{\lambda-}) \times\{-(k!)^{1/2}b^{(n)}_{k,r} + [r!/(r-k)!]^{1/2}\delta_{r\geqslant k}b^{(n)}_{0,r-k}\}]. \tag{A10}$$

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