Perturbative calculation of energy levels for coupled oscillators using the inner product technique

M R M Witwit

Department of Applied Mathematics, University of Hull, HU6 7RX, UK

Abstract : The energy levels of the Schrödinger equation are calculated for several forms of potentials in two-dimensional space using the inner product technique for several eigenstates and over a wide range of values of the perturbation parameters The obtained numerical results are compared with those previously reported by other methods

Keywords : Coupled-oscillators, inner product, numerical results.

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1. Introduction

The study of systems of coupled oscillators is important and has wide applications; for instance, in the field of molecular physics, this model has been applied to intramolecular vibrational energy transfer [1–3], vibrational spectroscopy of polyatomic molecules, intramolecular [4,5], and unimolecular reaction [6], etc.

The inner product technique of eigenvalue calculation investigated by Blankenbecker *et al* [7] and applied to one- and two-dimensional problems. Killingbeck and Jones [8] used a renormalized version of inner product theory to calculate energy eigenvalues for two-dimensional oscillator.

The aim of this paper is to calculate the energy levels of the Henon-Heiles potential, and to modify the inner product technique to treat potentials with mixed parity. We consider here the generalization of the Henon-Heiles system, which can be expressed as

$$V(x,y) = x^2 + y^2 + \lambda \left[x^I y^J + \mu x^L y^K \right].$$

(1)

The potential (1) has the general form, and with different values of the parameters (I,J,L,K,μ), the potential (1) takes different types, for example at $(I = 1, J = 2, \mu = -\frac{1}{3},$ $L = 3, K = 0)$ it reduces to the Henon-Heiles potential. We should mention here, that for ease of comparison with results available in the literature, the potential will be taken as

$$V(x,y) = \frac{1}{2}\omega_x^2 x^2 + \frac{1}{2}\omega_y^2 y^2 + \lambda \left[xy^2 + \mu x^3\right]. \tag{2}$$

The energy levels of the Henon-Heiles potential (2) has been calculated by semiclassical techniques as well as by quantum mechanical techniques; for instance, various authors [9–12] have made numerical studies of the Henon-Heiles potential. The eigenvalues and wavefunctions for the potential based on the adiabatic approximation theory have also been calculated [13]. The hypervirial perturbation theory with adiabatic approximation has been used to calculate the energy levels for various state numbers [14]. Also the perturbative semiclassical methods have been used to calculate the energy values for the same potential for various eigenstates [15]. Recently the WKB approximation, which is the so-called semiclassical method, has been used to treat the same potential [16].

The Henon-Heiles potential has no strictly bound quantum mechanical states due to tunnelling; though for small excitations, the error in assuming discrete eigenvalues is small. The quantal energy spectrum of a nonintegrable Hamiltonian is expected to exhibit two types of behaviour. At low energies the energy levels belong to a regular spectrum, and at higher energies it is predicted that energy levels exist belonging to an irregular spectrum. The energy levels of an irregular spectrum are more sensitive to a slowly changing or fixed perturbation than those of the regular spectrum.

To overcome the divergence problem we use a renormalization parameter α and write the potential (1) in renormalized form as

$$V'(x,y) = \beta^2\left[x^2 + y^2\right] + \left[V(x,y) - \lambda\alpha\left(x^2 + y^2\right)\right], \tag{3}$$

where

$$\beta^2 = 1 + \lambda\alpha. \tag{4}$$

The ground energy level for potential (1) is calculated for different values of (λ,I,J,L,K,μ). and the results are shown in Table 1. Also the ground and the first three excited states are calculated for potential (2) for different values of the perturbation parameters.

In rectangular coordinates, the Schrödinger equation for the potential $V(x,y)$ can be written as

$$-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(x,y) \ \Psi_{n_1,n_1}(x,y) = E\Psi_{n_1,n_1}(x,y). \tag{5}$$

The energy E_{n_x,n_y} and wavefunction corresponding to the Schrödinger equation (5) for potential (1) when the perturbation parameter $\lambda = 0$ can be expressed as

$$E_{n_x,n_y} = 2n_x + 2n_y + 2, \qquad n_x,n_y = 0, 1, 2...., \tag{6}$$

$$\Psi_{n_x,n_y}(x,y) = \left[\pi\ 2^{nx+ny} n_x! n_y\right]^{-1/2} H_{n_x}(x) \exp\left| \qquad \left|H_{n_y}(y) \exp\right| -\frac{\cdot}{\cdot} \tag{7}$$

where $H_{n_x}(x)$ and $H_{n_y}(y)$ are Hermite polynomials.

2. The recurrence relation for the two dimensional-system using the inner product technique

The inner product technique is a perturbative technique which gained certain popularity to handle numerical calculations of eigenvalue problems in multidimensional systems for various types of potentials.

The inner product technique has been applied to two-dimensional oscillators with even parity of perturbation [8,17]. In this section, we intend to point out the flexibility of the inner product perturbation theory to handle mixed parity perturbations.

The strategy applied to solve the Schrödinger eq. (5) to obtain the corresponding eigenvalue, begins with the use of the following reference wavefunction :

$$\phi(x,y) = \left(x^{nx} y^{ny}\right) \exp\left[-\frac{\beta}{2}\left(x^2 + y^2\right)\right], \tag{8}$$

where β is a real positive variable and n_x and n_y are non-negative integers (state numbers). The reference function $\phi(x,y)$ becomes a correct unperturbed state wavefunction only for the special cases $\beta = 1$ and (n_x, $n_y = 0$, 1), but otherwise the general calculations involve various overlap integrals between it and the accurate wavefunction $\Psi(x,y)$. It might be conjectured that the optimum choice of β corresponds to some situation of maximum overlap of ϕ with Ψ; however, β was simply varied empirically to obtain the best results. The next step to be taken is to introduce the inner product in the form

$$R(M,N) = \langle\phi|x^M y^N|\Psi\rangle \tag{9}$$

which plays a major role in this technique, where the $R(M,N)$ are sometimes called moments. The final step is to work out the quantity

$$ER(M,N) = \langle\Psi|H x^M y^N|\phi\rangle, \tag{10}$$

obtained by taking the inner product of the Schrödinger eq. (5) with the product $x^N y^N|\phi\rangle$, and then inserting the perturbation expansions

$$R(M,N) = \sum_K R(M,N,K)\lambda^K, \tag{11}$$

$$E = \sum_L E(L)\lambda^L. \tag{12}$$

into relation (10), we obtain the following recurrence relation with three-dimensional arrays, after some algebra

$$\sum_{L=0}^{K=50} E(L)R(M,N,K-L) = R(M+I,N+J,K-1) + \mu R(M+L,J+P,K-1) - \alpha$$

$$[R(M+2,N,K-1) + R(M,N+2,K-1)] + 2\beta[M+N+n_x+n_y+1]$$

$$R(M,N,K) - [M^2+2Mn_x-M]R(M-2,N,K) - [N^2+2Nn_y-N]$$

$$R(M,N-2,K). \tag{13}$$

The unperturbed energy can be expressed as

$$E(0) = 2\beta[n_x+n_y+1]. \tag{14}$$

The recurrence relation (13) is then used as follows : If the energy sum up to $E(Q)\lambda^Q$ is required, then the indices have the ranges set out below

$$K = 0, 1, 2, \ldots\ldots, Q$$

$$\text{(fixed } K) \; N = 0, 1, 2, \ldots\ldots, Q$$

$$\text{(fixed } K, N) \, M = 0, 1, 2, \ldots\ldots, Q$$

the indices are scanned in the order given above and the relation (13) is used to work out $R(M,N,K)$ in term of lower order elements which are already known. $E(K)$ is found from the eq. (13) for the special case $M = n_x$, $N = n_y$, because in this case the relation (13) is used differently and the sum on the left hand side becomes $E(K)$, because of the intermediate normalization convention $R(n_x, n_y) = 1$ which we impose on the algorithm. This gives the value of the energy coefficient $E(K)$ in terms of already calculated elements of the three-dimensional arrays $R(M,N,K)$. The sum of the energy perturbation series can then be calculated term by term, and α is varied to give the best possible convergence of the perturbation series. The computation was carried out to double-precision accuracy by using VME system with Fortran (77) program. On the other hand, the algorithm outlined above can be implemented on microcomputer [8].

In the present paper, we have found a further application for the energy eigenvalues by calculating the expectation values without using wavefunctions. To find expectation values of type $< (x^{2N}y^{2N}) >$ for the potential

$$V(x,y) = x^2 + y^2 + \lambda x^2 y^2. \tag{15}$$

We need to have the eigenfunction $\Psi(x,y)$ for all x and y if we wish to apply the definition

$$\left\langle x^{2N}y^{2N} \right\rangle = \int \Psi^2(x,y) \, x^{2N} y^{2N} \, dx \, dy. \tag{16}$$

To find $\Psi(x,y)$ for arbitrary x, y and for any state number (n_x, $n_y = 0$, 1, 2,..), is not easy. However, Killingbeck [18] has applied a very simple perturbative numerical algorithm for the calculation of an expectation value, based on the formula

$$\left\langle x^{2N}y^{2N}\right\rangle = \mathrm{Lt}_{\varepsilon\to 0}\ \frac{1}{2\varepsilon}\left[E\left(H + \varepsilon x^{2N}y^{2N}\right) - E\left(H - \varepsilon x^{2N}y^{2N}\right)\right]. \qquad (17)$$

This algorithm demonstrates that expectation values can be determined by an approach based on eigenvalue calculations, without the explicit use of wavefunctions. The way in which we can calculate is as follows; we do two calculations, to get two E values, with $\mp\,\varepsilon x^{2N}y^{2N}$ included in the potential

$$E_+ = x^2 + y^2 + \lambda x^2 y^2 + \varepsilon x^{2N}y^{2N} \quad \text{and} \qquad (18)$$

$$E_- = x^2 + y^2 + \lambda x^2 y^2 - \varepsilon x^{2N}y^{2N} \qquad (19)$$

where ε is a very small number, typically ($10^{-7} \le \varepsilon \le 10^{-3}$). The value of $\left\langle x^{2N}y^{2N}\right\rangle$ is then given by

$$\left\langle x^{2N}y^{2N}\right\rangle = \frac{1}{2\varepsilon}\left[E_+ - E_-\right], \qquad (20)$$

for example at $2N = 2$, $\lambda = 0.5$ and $\varepsilon = 10^{-7}$ for eigenstate $n_x = n_y = 0$, eq. (20) becomes

$$\left\langle x^2 y^2\right\rangle = \left|\frac{10^-}{2}\right.\ [2.10821379884 - 2.10821376055] = 0.19145000029. \qquad (21)$$

3. Results and discussion

The numerical results for a two-dimensional system are presented in Table 1, for the ground state E_{00} with different values of perturbation parameters; it is clear that the inner product

Table 1. Energy values for the ground-state for the potential (1), for several sets of perturbation parameters.

λ	I 1	J 2	L 3	K 0	μ $-\frac{1}{3}$	I 1	J 2	L 3	K 0	μ $\frac{1}{3}$	I 2	J 2	L 1	K 1	μ 1
0.001			1.9999999444444317					1.9999996944442650					2.0002498439138079		
0.005			1.9999986111031538					1.9999923609989839					2.0012461140999907		
0.01			1.9999944443171231					1.9999694426502501					2.0024845365616810		
0.02			1.999977775740322					1.9998777490604472					2.0049387732394514		
0.03			1.99994998968273					1.9997248545321512					2.0073636095761402		
0.04			1.99991107849175					1.9995106509779684					2.0097598943891263		
0.05			1.99986103143719					1.999234986534003					2.0121284301189 83		
0.06			1.99979983469471					1.99889766501212					2.014469976669919		
0.07			1.99972747132432					1.99849844518677					2.016785254817740		

Table 2. (*Contd.*)

ω_x^2	ω_y^2	μ	λ	n_x	n_y	E_{n_x, n_y}
				0	0	1.2034048952926
				1	0	2.6260612389250
2.0	1.0	0.15	–0.1	0	1	2.1874957318595
				1	1	3.5672929910501
				0	0	1.2241791322612
				1	0	2.4476784531188
1.5	1.5	–0.15	0.1	0	1	2.4447092929989
				1	1	3.6671666346361
				0	0	1.4023329575697
				1	0	2.6257575055191
1.5	2.5	–0.15	0.15	0	1	2.9783453992141
				1	1	4.2024677843936
				0	0	0.9985114296570
				1	0	1.9958178856053
1.0	1.0	–0.1	0.1	0	1	1.9881289674396
				1	1	2.9811862589588

approximation [14], semiclassical [15] and hypervirial methods [13] for several sets of perturbation parameters (λ, ω_x^2, ω_y^2, μ). It is seen that the inner product results are excellent relative to the previous ones.

Table 3. Comparison energy values for Henon-Heiles potential with variation in perturbation parameters λ. $\omega_x^2 = 0.49$, $\omega_y^2 = 1.69$, $\lambda = -\mu$. The empty spaces mean the results are not available.

$-\lambda$	n_x, n_y	Present results	BQ	AA	SC	HR
0.01		0.99997659863626				
0.02		0.99998995929848				
0.03		0.99975622899927				
0.04		0.99953288293574				
0.05		0.99921417130018				
0.06		0.99878298845122	0.9988	0.9988	0.9987	0.9988
0.08		0.99750503091855	0.9975	0.9975	0.9975	0.9975
0.10		0.99551888097989	0.9955	0.9956	0.9955	0.9956
0.12		0.99259494493192	0.9926	0.9927	0.9927	0.9927
0.14	0,0	0.988426091755	0.9884	0.9887	0.9889	0.9885
0.15		0.985744249175				
0.16		0.98256799465	0.9826	0.9833	0.9836	0.9827
0.17		0.978879628				

Table 3. (*Contd.*)

$-\lambda$	n_x, n_y	Present results	BQ	AA	SC	HR
0.18		0.9742855	0.9743	0.9761	0.9764	0.9745
0.20		0.9616	0.9621	0.9668	0.9667	0.9625
0.01		1.69995555128649				
0.02		1.69979746999234				
0.03		1.69948173066612				
0.04		1.69895486257244				
0.05		1.69815352711693				
0.06		1.69700382620682	1.6970	1.6971	1.6970	1.6971
0.08		1.69330381519851	1.6933	1.6934	1.6933	1.6934
0.10		1.68699427768	1.6870	1.6873	1.6870	1.6872
0.12	1,0	1.6768856678	1.6769	1.6777	1.6770	1.6772
0.14		1.66120482	1.6612	1.6634	1.6617	1.6616
0.15		1.65041381				
0.16		1.6369055	1.6370	1.6430	1.6382	1.6376
0.17		1.61968				
0.18		1.59655	1.5980	1.6149	1.6010	1.5983
0.01		2.29983980109581				
0.02		2.29933791454876				
0.03		2.29846052411376				
0.04		2.29717064908641				
0.05		2.29542873627763				
0.06		2.29318930861531	2.2932	2.2932	2.2932	2.2932
0.08		2.28701021758891	2.2870	2.2871	2.2870	2.2871
0.10		2.27813159395040	2.2781	2.2783	2.2782	2.2783
0.12	0,1	2.265844300562	2.2658	2.2663	2.2661	2.2661
0.14		2.249041496882	2.2490	2.2502	2.2496	2.2494
0.15		2.23838283				
0.16		2.2257015	2.2257	2.2288	2.2268	2.2263
0.17		2.221026				
0.18		2.1906				
0.01		2.99977678225502				
0.02		2.99904122607814				
0.03		2.99768585988190				
0.04		2.99559052822714				
0.05		2.99262029135626				
0.06		2.98862233945227				
0.08		2.97681366046227				
0.10		2.95835268513667				

Table 3. (*Contd.*)

$-\lambda$	n_x, n_y	Present results	BQ	AA	SC	HR
0.12	1,1	2.9305035186199				
0.14		2.88843544175				
0.15		2.859086				
0.16		2.82045				
0.17		2.7615				
0.18		2.67				
0.20		2.55				

We should note that (as pointed out by a referee) there are several tricks for accelerating the rate of convergence of the perturbation series such as Padé approximants and Euler's transformations can be a powerful tool for alternating series. Euler's transformation can be applied not only to convergent series, in some cases it will produce accurate answers from the first few terms of a series that is formally divergent. It is widely used in the summation of asymptotic series, defined by

$$\int_0^\infty e^{-t} [1 + \lambda t]^{-1} \, dt = \sum (-1)^n \, n! \, \lambda^n. \tag{22}$$

In present work Aitken's transformation was used in order to improve the convergence of the calculations. This is a simple formula for extrapolating the partial sums of a series whose convergence is approximately geometric. If $E(I-1)$, $E(I)$, $E(I+1)$ are three successive partial sums, then an improved estimate is

$$E_I = \left[E(I-1)E(I+1) - E(I)E(I) \right]^2 \left[E(I+1) - 2E(I) + E(I-1) \right]^{-1}, \tag{23}$$

it seems to play a role in improving the accuracy of our results to extra digits.

Killingbeck [19] tested the Padé approximants, Euler's transformation and Aitken's transformation on perturbation series for two-dimensional oscillators to improve the convergence of the perturbation series, the test was implemented on microcomputer.

It is interesting to note that for these types of perturbation the contribution to the perturbation energy series comes from the even terms only, because the energy of a perturbed oscillator with an odd perturbation are even functions of the perturbation parameter λ.

Our confidence in the accuracy of our results comes from the checks, the agreement between our results and those produced by the Hill determinant approach. Also two separate computations for some eigenstates with slightly increasing or decreasing the value of α, yielded eigenvalue agreeing to all digits.

Acknowledgment

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