

Energy levels of a two-dimensional anharmonic oscillator: Hill determinant approach

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Abstract. The energy levels of the Schrödinger equation for the potential $x^2 + y^2 + \lambda[a_{xx}x^4 + 2a_{xy}x^2y^2 + a_{yy}y^4]$ are calculated using Hill determinant approach for several eigenstates and over a wide range of values of perturbation parameters. The obtained numerical results agree with those previously reported by other methods.

Keywords. Schrödinger equations; Hill determinant; numerical results.

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1. Introduction

Harmonic oscillator models have played an important role in the evolution of a number of areas of physics ranging from vibrations of crystal lattices to black body radiation to elasticity to acoustic, to molecular dynamics, etc.

This paper aims to calculate the energy levels of the two-dimensional oscillator which is expressed by the potential

$$V(x, y) = x^2 + y^2 + \lambda[a_{xx}x^4 + 2a_{xy}x^2y^2 + a_{yy}y^4]. \quad (1)$$

The two-dimensional anharmonic oscillator $V(x, y)$ has received a lot of attention recently as it is related to several interesting physical problems. Many techniques have been used to obtain the energy eigenvalues [1–8].

In this paper, some extended numerical calculations are, presented, using the Hill determinant approach (iterative technique) to calculate the energy levels of the Schrödinger equation for the potential (1) over a wide range of values of the perturbation parameters and for various eigenstates. The convergence of the energy depends upon the choice of an adjustable parameter β . However the convergence rate is relatively good, with better choice of β as will see later.

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

$$\left[-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(x, y) \right] \Psi_{n_x, n_y}(x, y) = E \Psi_{n_x, n_y}(x, y). \quad (2)$$

The energy E_{n_x, n_y} and wavefunction $\Psi_{n_x, n_y}(x, y)$ corresponding to the Schrödinger equation (2) when the perturbation parameter $\lambda = 0$ can be expressed as:

$$E_{n_x, n_y} = (2n_x + 1) + (2n_y + 1) \equiv 2n + 2 \quad n_x, n_y = 0, 1, 2, \dots \quad (3)$$

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$$\Psi_{n_x, n_y}(x, y) = \phi_{n_x}(x)\phi_{n_y}(y), \quad (4)$$

$$\phi_{n_x}(x) = \left[\frac{1}{2^{n_x} n_x!} (\alpha/\pi)^{\frac{1}{2}} \right]^{\frac{1}{2}} H_{n_x}(\sqrt{\alpha}x) \exp -(\alpha/2)x^2. \quad (5)$$

As indicated earlier [7], eq (2) has a circular symmetry when the relationship $a_{xx} = a_{yy} = a_{xy} = 1$ holds for the potential (2). The energy levels are then most appropriately characterized by the quantum numbers (n_r, M) rather than (n_x, n_y) . The radial part of the eigenvalue equation (2) can be expressed as:

$$\left[-\frac{d^2}{dr^2} + \left[M^2 - \frac{1}{4} \right] r^{-2} + r^2 + \lambda r^4 \right] \Psi(r) = E\Psi(r). \quad (6)$$

The unperturbative energy in polar coordinates can be expressed as:

$$E_{n_r, M} = 4n_r + 2|M| + 2 \equiv E_{n_x, n_y} \quad (7)$$

where $n_r = 0, 1, 2, 3, \dots$ and $M = 0, \mp 1, \mp 2, \dots$ are the orbital quantum number and the magnetic quantum number.

In each state the energy levels depend on the pair quantum numbers (n_x, n_y) . The degeneracy degree of n th level is equal to the number of ways in which n can be divided into the sum of two positive integral (or zero) numbers; which is $n + 1$.

In (2) we have supposed that, to each eigenvalue E_{n_x, n_y} there corresponds just one eigenfunction $\Psi_{n_x, n_y}(x, y)$. In the degenerate case several eigenfunctions correspond to the same eigenvalue. We notice that, as a result of the perturbation, an originally degenerate energy level ceases in general to be degenerate, because the perturbation removes the degeneracy. For example the states (1, 1; even-0, 2; even-2, 0; odd) start off to degenerate at $\lambda = 0$, but split up into three separate levels respectively as λ increases.

2. Hill determinant approach and its implementation to the two-dimensional oscillator and its recurrence relations

The Hill determinant approach is a non-perturbative technique and can handle numerical calculations of the eigenvalue problem in one-dimensional case for various types of potentials [10, 11, 12].

The polynomial potential given by (1) is non-separable in cartesian coordinates, but shows a high symmetry. Due to this symmetry it is possible to cut down the amount of computation needed in the program. The more general anisotropic case can also be treated by our technique.

We stress that the Hill determinant approach has been found comparable to the inner product method when applied to the same perturbation in multidimensional systems.

To find the recurrence relations which allow us to calculate the eigenvalues, we introduce the following wavefunction:

$$\Psi_{n_x, n_y}(x, y) = \exp \left[-\frac{\beta}{2}(x^2 + y^2) \right] \sum_{L, I} F(L, I)(x^L y^I). \quad (8)$$

By substituting $\Psi_{n_x, n_y}(x, y)$ in (2) and after some algebra, we get the following

recurrence relation,

$$F(L, I) = W(L, I)[2\beta(L + I + 1) - E]^{-1}, \quad (9)$$

where

$$W(L, I) = (L + 2)(L + 1)F(L + 2, I) + (I + 2)(I + 1)F(L, I + 2) + (\beta^2 - 1) \\ [F(L - 2, I) + F(L, I - 2)] \\ - \lambda[a_{xx}F(L - 4, I) + a_{yy}F(L, I - 4) + 2a_{xy}F(L - 2, I - 2)]. \quad (10)$$

For calculations, we set the initial coefficient $F(L_0, I_0) = 1$. All the $S(L, I)$ with $(L, I) \neq (L_0, I_0)$ are treated according to (9) for some trial values of β and E . From experience it is seen that the best initial energy to start the calculation should be a little higher than the required eigenvalue [13]. The value of β increases as the perturbation parameter λ increases. At this stage, naturally, the question that arises is whether β can give the best convergence eigenvalue. In the present calculations, the value of β which gave the best converged eigenvalue was taken. Table 1 shows the rate of convergence by this technique for some eigenstates for $\lambda = 0.1, 10, 100, 10^5$ in the special case, wherein the potential has circular symmetry. It is known from experience, that the rate of the convergence decreases as values of the perturbation parameter λ and eigenstate number (n_x, n_y) increase.

The standard technique for evaluation of the energy is based on (9), that for the special case $L = L_0, I = I_0$, the coefficient on the left-hand side becomes $F(L_0, I_0) = 1$, and this initial condition is imposed on the algorithm. After this adjustment a revised E estimate is calculated using the assignment statements

$$E_e = 2\beta(L_0 + I_0 + 1) - W(L_0, I_0). \quad (11)$$

$$E = RE_e + (1 - R)E. \quad (12)$$

The value of the relaxation parameter R can be decreased or increased to help in improving and stabilizing a convergence of the eigenvalue to a reasonable accuracy. The parity index P_{xy} (for interchange coordinates $x \leftrightarrow y$) is used for the potential $V(x, y)$, in the case of symmetry interaction which means $a_{IJ} = a_{JI}$. The relation between the coefficients hold (for interchange $x \leftrightarrow y$).

$$F(L, I) = P_{xy}F(I, L). \quad (13)$$

For even eigenstates $P_{xy} = 1$ and for odd eigenstates $P_{xy} = -1$ and β is varied to give the best possible convergence of the estimated energy.

3. Results and discussion

The Hill determinant approach has been applied in this paper to the Schrödinger equation with a perturbed potential in a two-dimensional system. It is found very effective to treat symmetry perturbation i.e. $a_{IJ} = a_{JI}$ and unsymmetry perturbation i.e. $a_{IJ} \neq a_{JI}$ for several eigenstates and various values of perturbation parameters.

The adjustable parameter β plays an important role in the convergence aspects of the present calculations. The β values for the dimensional oscillator $V(x, y)$ calculation are in the range $1.3 \leq \beta \leq 350$. The general consideration that governs our choice is that, as λ increases, β also increases, for example $\beta = 1.3$ at $\lambda = 0.01$ and $\beta = 350$ at $\lambda = 10^6$.

Table 1. Convergence for some eigenvalues for (n_x, n_y, n_z, π) of the two dimensional oscillator for the case $a_{xx} = a_{yy} = a_{zz} = 1$, for $\lambda = 0.1, 10, 100, 10^5$ with various values of the adjustable parameter β . The empty spaces mean the corresponding eigenvalues cannot be obtained with these values of β .

λ	(0,0,+)	β	(1,0; \mp)	β	(1,1,+)	β
0.1	2-16	0.5		1		1
		1	4-4776003	1.5	6-9083321	1.6
	2-1685972	1.4	4-47760036076	1.7	6-90833211231871	2.0
	2-1685972112693	1.8	4-47760036076821	2.0	6-90833211231871	2.2
	2-168597211269291	2.5	4-47760036076821	2.5	6-90833211231871	2.5
10	5-3493	3		4		5
		6	12-138224	7	19-936	7
	5-349352819406	8	12-1382247388	8	19-936900374	8
	5-34935281940641	9	12-13822473889884	9	19-9369003740113	9
	5-34935281940641	10	12-13822473889884	10	19-9369003740113	10
100	11-023	8		8		10
		12	25-27998	14	41-76874	15
	11-0235979	15	25-2799851433	17	41-76874434397	18
	11-0235979287809	20	25-27998514334519	20	41-7687443439749	20
	11-0235979287809	24	25-27998514334519	24	41-7687443439749	24
10 ⁵	108-85135	80		90		100
		140	250-402	140	414-4377	150
	108-8513595772	180	250-4021140684	180	414-4377597604	180
	108-851359577201	200	250-402114068453	200	414-437759760461	200
	108-851359577201	220	250-402114068453	220	414-437759760461	220

Table 2. Energy values of $(n_x, n_y; \pi)$, for the potential $V(x, y)$ for several sets of perturbation parameters. The parity label $\pi = +, -$; even, odd for the $x \leftrightarrow y$ interchange symmetry.

λ	$a_{xx} = a_{yy} = 0, a_{xy} = \frac{1}{2}$			
	(0, 0; +)	(1, 0; \pm)	(1, 1; +)	(2, 0; -)
0-1	2-02413832141573	4-0708639128944	6-2082907985657	6-0716400174184
0-2	2-04679571883258	4-1350822342067	6-3912911417583	6-1377408133565
0-3	2-068242130731	4-1942935736199	6-564773059808	6-1995318631918
0-4	2-088667659069	4-2495313630102	6-7081422885770	6-2578183515335
0-5	2-108213779698	4-301504505315	6-8490530489122	6-313168654731
0-6	2-126989929539	4-35072736225	6-9811280772305	6-36600479493
0-7	2-1450832429	4-3975886228	7-1057672375444	6-4166518870
0-8	2-1625646859	4-4423912545	7-2240314806597	6-465367562
0-9	2-1794931153	4-485377268	7-3367489236663	6-512360604
1-0	2-195918086	4-526743874	7-444581361569	6-557803326
2-0	2-3395662	4-87770957	8-3394493229	6-9506339
3-0	2-4583769	5-1579605	9-034854244	7-271682
4-0	2-5616266	5-396806	9-6175878	7-549157
5-0	2-6539097	5-60757	10-1256931	7-79644
6-0	2-7379188	5-79769	10-5798578	8-0212
7-0	2-8153967	5-97184	10-0992791	8-2283
8-0	2-8875504	6-13341	11-372950	8-4214
9-0	2-955257	6-28596	11-726290	8-6019
10-0	3-019178	6-42591	12-057188	8-773
15-0	3-29685	7-03842	13-469681	9-515
20-0	3-52692	7-54125	14-616918	10-131
50-0	4-47652	9-60194	19-21721	12-685
100	5-46097	12-2666	23-86291	15-349
1000	11-23243	24-2562	50-39571	31-13
5000	19-03854	41-2135	85-85665	52-61
10000	23-94599	51-6251	108-0969	66-13
10 ⁵	51-4718	110-5191	232-6638	142-2

λ	$a_{xx} = a_{yy} = 1, a_{xy} = -1$ (0, 0; +)	$a_{xx} = \frac{1}{2}, a_{yy} = \frac{1}{4}, a_{xy} = \frac{1}{8}$ (1, 0; -)	$a_{xx} = \frac{1}{2}, a_{yy} = \frac{1}{4}, a_{xy} = \frac{1}{8}$ (1, 1; +)
0.01	2.00985521060372	4.0220907755723	6.033322273821
0.1	2.08866765907315	4.2014184255855	6.302730175585
0.5	2.339566211	4.776661317376	7.170817128601
1	2.56162658	5.28444637458	7.9385946295
10	4.21175722	8.99050466	13.54179268
100	8.36832652	18.139463	27.355525
1000	17.68691	38.4951	58.0717
2000	22.2399	48.4255	73.0545
10000	37.945	82.6619	124.7086

λ	$a_{xx} = 1, a_{yy} = \frac{1}{2}, a_{xy} = \frac{1}{4}$ (0, 0; +)	$a_{xx} = \frac{1}{3}, a_{yy} = \frac{1}{4}, a_{xy} = \frac{1}{2}$ (0, 0; +)	$a_{xx} = \frac{1}{3}, a_{yy} = \frac{1}{4}, a_{xy} = \frac{1}{2}$ (1, 0; -)
0.01	2.01231228718489	4.0438677204024	4.021621108365
1	2.6863516426	6.02495513951	5.281706465822
5	3.8255941189	8.9905464633	7.47632663472
10	4.619200437	10.991656058	9.01371371691
50	7.50300538	18.13946345	14.6138003405
100	9.3555061	22.69326466	18.2150199295
500	15.809344	38.4950971	30.767112789
1000	19.87269	48.425489	38.671655693
10000	42.6818	104.112662	83.04905
10 ⁵	91.8949	224.20318	178.7999

$a_{xx} = \frac{1}{3}, a_{yy} = \frac{1}{6}, a_{xy} = \frac{1}{3}$		$a_{xx} = 0, a_{yy} = 1, a_{xy} = \frac{1}{2}$	
λ	(0, 1; +)	(1, 0; -)	(0, 0; +)
0-01	4-0116729015606	4-016594932356	2-00982882574815
0-1	4-1106369197386	4-154229422204	2-08694982082748
0-5	4-466738393841	4-622448523457	2-32310658866
1	4-81001774999	5-053036645166	2-52658354
10	7-59082621315	8-335444773	4-00772
100	14-8799478	16-63230785	7-7615
1000	31-3501683	35-2005676	16-26
5000	53-387759	59-9954	27-67
10000	67-2109	75-5418	34-83
100000	144-648	162-612	74-9
$a_{xx} = \frac{1}{3}, a_{yy} = \frac{1}{4}, a_{xy} = \frac{1}{2}$		$a_{xx} = a_{yy} = \frac{1}{3}, a_{xy} = \frac{1}{4}$	
λ	(1, 1; +)	(1, 1; +)	(0, 2; +)
0-01	6-0436934891649	6-0241668378937	6-043135666616
1	8-3665961639843	7-5602656974176	8-38684555658
5	12-1540605363882	10-4238563537005	12-2283227870
10	14-75829350949	12-471386219668	14-8663230227
50	24-149078364	20-0155548073	24-3660855
100	30-158605748	24-893689976	30-4406285
500	51-0558236	41-9417026	51-555132
1000	64-201194	52-690847	64-834505
10000	137-95683	113-0797	139-3334
100000	297-0515	243-418	300-0232
		$(2, 0; -)$	
			6-038232473314
			8-164167323602
			11-733936775982
			14-207348368038
			23-1626619844
			28-9045928065
			48-8897072
			61-4667308
			132-05022
			284-3189

$a_{xx} = a_{yy} = a_{xy} = 1$		$a_{xx} = a_{yy} = 1, a_{xy} = 0$	
λ	(0, 0; +)	(0, 1; \mp)	(1, 1; +) = (2, 0; -)
0.01	2-0195708085219	4-0581733885884	6-115306125265
1	2-952050091966	6-46290599986	10-390627295503
5	4-3810888395	9-87059482807	16-146296004255
10	5-3493528194	12-13822473884	19-936900374011
50	8-814283232	20-1770296484	33-304412267221
100	11-023597928	25-2798514335	41-768744343975
500	18-69290316	42-9558103393	71-054463932988
1000	23-51338918	54-054857958	89-943343403375
10000	50-54804495	116-267380968	192-420561201906
100000	108-85135957	250-402114065	414-437759760460
10 ⁶	234-48942203	539-433981018	892-823487959

$a_{xx} = a_{yy} = 1, a_{xy} = 0$		$a_{xx} = 1, a_{yy} = \frac{1}{2}, a_{xy} = 1$	
λ	(0, 0; +)	(0, 1; \mp)	(0, 1; +)
0.01	2-0147473441627	4-0438989765947	4-040310310588
1	2-7847032830606	6-0411643457423	5-929093989647
5	4-0366812987306	9-0318198351823	8-8068361776
10	4-898348144236	11-0481775269262	10-7552685288
50	8-007985536555	18-245699764189	17-7255829568
100	9-998835090275	22-829610261090	22-1694645877
500	16-923285258162	38-733147884922	35-5949254503
1000	21-279577422656	48-72662217071	41-9482797882
10000	45-723217740545	104-76492582355	52-7836179925
100000	98-450895516845	225-61007058467	113-5233045707
10 ⁶	212-07965847	486-01614822	244-4877262122

The results are in good agreement with available literature. For accurate results, the best values of β , have been chosen, which were obtained by testing many parameter values until the best convergence was obtained.

Some important consequences of our investigation are as follows:

1. The Hill determinant approach can be used to calculate several eigenstates with excellent accuracy for the two-dimensional oscillator for several perturbation parameters. Table 2 covers a wide range of λ values ($10^{-2} \leq \lambda \leq 10^6$) and various cases wherein the potential has interchange symmetry. The λ value obtained by us is twice the λ value obtained by Nasit and Demiralp [1] and Hioe *et al* [3] and their Hamiltonian differs by a factor 1/2.

Several external checks were devised to verify the correctness of the energy values. For example using the inner product technique, we obtained agreement between some of the present results and those obtained by inner product [7]. For the two special cases $a_{xx} = a_{yy} = a_{xy} = 1$ and $a_{xx} = a_{yy} = 1, a_{xy} = 0$, the potential (1) has circular symmetry, and reduces to the two independent oscillators respectively. We have checked the energies obtained by the present technique against results obtained by the hypervirial method [7].

2. For symmetric perturbation i.e. $a_{JJ} = a_{JI}$, it is seen from our calculations that the energy levels characterized by eigenstates (n_x, n_y) , with n_x and n_y having different parity, i.e. (odd, even) or (even, odd) remain doubly degenerated and unsplit as λ is varied from zero value. This means that the perturbation does not break the degeneracy of the perturbed system. The energy levels which show such behaviour in our calculations are (E_{10}, E_{01}) . Unsymmetry perturbation i.e. $a_{JJ} \neq a_{JI}$ shows interesting splitting effects as a_{JJ} and a_{JI} vary. In this case the degeneracy is broken by the perturbation and this behaviour is clear from our calculations in table 2.

Also there is a crossing between the energy levels for the two eigenstates E_{11}^+ and E_{20}^- at $a_{xx} = a_{yy} = a_{xy} = 1$; (circular symmetry), but when this symmetry is removed, the doubly degenerate levels split into different levels, and this confirmed by our results in table 2.

3. The phenomenon of bogus convergence is avoided by computing the energy eigenvalues for different values of the adjustable parameter β . To select the correct converge energy we require stability of the results with respect to the small variation of β at a given value of the perturbation parameter λ .

We have also used Aitken's transformation [14] to improve the convergence of the calculations and it has helped in improving our results.

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