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Calculation of highly excited eigenstates of chaotic quantum systems

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Abstract. Computational methods for the calculation of a large number of eigenstates of coupled oscillator system are developed and discussed. These calculations have enabled us to identify and investigate properties of an infinite set of states sharply localized in configuration space in this system. Some of the results and their significance are discussed. Extensions to three-dimensional systems are also briefly considered.

Keywords. Quantum chaos; wave functions; excited states.

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1. Introduction

The classical dynamics of generic time independent Hamiltonian systems with two or more degrees of freedom exhibits chaos, i.e., its phase space dynamics shows extreme sensitivity to initial conditions. Quantum systems for which the underlying classical dynamics is chaotic are an active area of research and atomic and molecular systems provide numerous examples of such quantum systems. One of the simplest of chaotic quantum systems is a one electron atom in an external magnetic field. For Rydberg states of the atom, however, the external field strength can become comparable with the attractive electrostatic field felt by the electron and this results in chaotic classical dynamics for the electron. The spectra of Rydberg states of such systems have been measured as a function of the external field strength [1, 2]. Experiments have also been performed on many electron atoms in high external magnetic fields and involve detection of Rydberg atoms after laser excitation [3] and recently some new experiments using many-electron atoms have been suggested to study quantum chaos in such systems [4]. On the theoretical side the Hamiltonian for the hydrogen atom in an external magnetic field can be transformed using semi-parabolic coordinates to that for two nonlinearly coupled harmonic oscillators [1]. Another problem which has been extensively studied is that of two coupled quartic oscillators [5, 6, 7]. In both these problems the accurate eigenenergies and eigenfunctions of highly excited states are required to be calculated in order to elucidate the effect of classical chaos in quantum systems. The eigenvalues and eigenfunctions are obtained by diagonalizing the Hamiltonian matrix in a suitable complete set of basis states. The choice of basis states is dictated by physical considerations and by

computational convenience. In practice, an optimal choice between these two has to be made. In this paper we shall discuss strategies for an optimal choice with reference to the problem we have extensively dealt with, namely, the coupled quartic oscillator problem. We believe that the strategy we propose is applicable to a wide class of matrix eigenvalue problems. We also give some examples of the result we have obtained.

2. Coupled quartic oscillators

In this section we briefly sketch our model. Our model is defined by the Hamiltonian,

$$H(p_x, p_y, x, y; \alpha) = p_x^2 + p_y^2 + x^4 + y^4 + \alpha x^2 y^2, \tag{1}$$

where α is a parameter and we have taken $\hbar = h/2\pi = 1$ throughout this paper. The classical dynamics of this Hamiltonian has been extensively studied [8, 5] and a glance at eq. (1) shows that for $\alpha = 0, 2, 6$ the equation is separable and the dynamics is regular. It has been previously shown that the following transformation,

$$\alpha' = \frac{(12 - 2\alpha)}{(2 + \alpha)} \tag{2}$$

exists for the parametric interval $[0, 2]$ onto $[6, 2]$ and the interval $[-2, 0]$ onto $[\infty, 6]$. A point to note about this Hamiltonian is that, apart from scaling, the classical motion is independent of energy. As $\alpha \to -2$ the classical motion is increasingly chaotic, and as per the transformation this is equivalent to large values of α'. For $\alpha = -2$ the classical motion becomes unbounded. We had also shown that in this limit the Hamiltonian defined by eq. (1) can be transformed into

$$H(\xi, \eta) = p_\xi^2 + p_\eta^2 + 2\,\xi^2 \eta^2, \tag{3}$$

where $\xi = (x - y)/\sqrt{2}$ and $\eta = (x + y)/\sqrt{2}$. The classical dynamics of this system is globally chaotic and studies on its classical, semiclassical and quantum properties have been reported [9]. The calculation of eigenvalues and eigenfunctions for this particular system are extremely difficult because of severe problems in the convergence of the matrix diagonalization procedure and only few tens of eigenstates above the ground state have been reported from a diagonalization of a Hamiltonian matrix of dimensionality of several thousands.

The quantum eigenvalues and eigenfunctions for this coupled quartic oscillator system are obtained by numerically solving the Schrödinger equation,

$$H(x, y; \alpha)\Psi_n^\alpha = E_n^\alpha \Psi_n^\alpha. \tag{4}$$

The classical scaling property of the Hamiltonian implies as usual the connection between spectra at different values of the Planck constant. In particular for the above Hamiltonian we get,

$$E(\hbar; \alpha) = C^4 E(\hbar/C^3; \alpha), \tag{5}$$

where C is any constant. Thus scaling allows us to equate going higher up in the spectrum with getting closer to the classical limit. In addition, the property of duality in the parameter space implies the relationship between spectra at identical values of the Planck

constant but at different values of the coupling constant, those connected by the eq. (2). We also have

$$\frac{E(\hbar;\alpha)}{(2+\alpha)^{1/6}} = \frac{E(\hbar;\alpha')}{(2+\alpha')^{1/6}}. \tag{6}$$

Thus when we study the coupled quantum oscillator at $\alpha = 64.6667$, it is the same as studying it at $\alpha = -1.76$; however the convergence of the number of eigenvalues for a given matrix dimensionality is significantly better for the positive α domain.

Notice that the above Hamiltonian possesses a C_{4v} point group symmetry, with irreducible representations labeled, A_1, A_2, B_1, B_2 and E. The Hamiltonian matrix in any desired irreducible representation is set up by expanding the eigenfunction in terms of appropriately symmeterized two dimensional basis states,

$$\Psi_n^{\alpha}(x,y) = \sum_{j=0}^{\infty} a_{nj}(\alpha)\psi_j(x,y), \tag{7}$$

where, for the states belonging to the A_1 irreducible representation,

$$\psi_j(x,y) = \mathcal{N}(n,m)\{\phi_n(x)\phi_m(y) + \phi_m(x)\phi_n(y)\}, \tag{8}$$

where $\phi_n(x)$ are the eigenfunctions of the one-dimensional quartic oscillator and the index j refers to a *unique* pair of *even* indicies $\{n,m\}$ and $\mathcal{N}(n,m)$ is a normalization factor,

$$\mathcal{N}(n,m) = \frac{1}{\sqrt{(2+2\delta_{n,m})}}. \tag{9}$$

Notice that as per eq. (7), we will have to sum up infinite terms, in principle, to construct the required eigenstate. However, in practice the number of basis states is truncated leading to what is called the convergence problem in the computed eigenvalues.

Before we conclude this section, we make a brief remark on role of certain classical periodic orbits and their influence on the quantum spectrum. Of the dense set of periodic orbits that exist in a chaotic system, it is known that the least unstable periodic orbits affect the quantum spectrum in a profound way. The channel periodic orbit of the coupled quartic oscillator defined by the initial condition $(x, y = 0, p_x, p_y = 0)$ has short time-period and has interesting stability properties. This orbit plays a vital role in the semi-classical and quantum regimes of the oscillator. In the coordinate representation this periodic orbit simply coincides with the x and y axes, which lie along the channels of the potential. The stability of this periodic orbit oscillates as a function of the parameter α. It can be shown that for this periodic orbit, pitchfork bifurcation accompanied by the stability changes occur at values of the parameter given by $\alpha = n(n+1)$, where $n = 1, 2, 3, \ldots$ [10, 11]. We note that $\alpha = 90$ is one such point of pitchfork bifurcation.

2.1 *One dimensional eigenfunctions and matrix elements*

The literature provides few methods, that can be numerically implemented, for solving the one-dimensional Schrödinger equation to obtain the eigenvalues and the eigenfunctions $\phi_n(x)$. One of the well-studied methods used to solve such one-dimensional

Schrödinger equations is the Hill determinant method [13]. In this method, a convenient wave function ansatz is assumed as the basis states and substituted in the Schrödinger equation leading to recurrence relation for the coefficients of the assumed basis states. The condition for non-trivial solutions for the coefficients leads to a determinant whose roots are identified with the eigenvalues. But this method has been shown to be useful to obtain the spectra for certain potentials [14] and unreliable in certain other cases [15]. Moreover, it is not a reliable method for computing highly excited states of the system. Computing eigenfunctions through this method is not straighforward and requires unprecedented accuracy for the eigenenergy to obtain accurate eigenfunctions. In our work the one-dimensional Schrödinger equation is transformed in to a Milne equation [16] and is solved by a generalized phase-amplitude method proposed by Larsen [17]. Thus it is possible to determine accurately the eigenvalues and eigenfunctions for very high quantum numbers.

3. Banded Hamiltonian matrix

Once the two-dimensional basis states $\psi_j(x, y)$ for the desired symmetry are constructed, the next step is to construct the Hamiltonian matrix $\langle\psi_j(x, y)|H|\psi_{j'}(x, y)\rangle$. This requires a large number of integrals of the form

$$\int_{-\infty}^{\infty} \mathrm{d}x\phi_m(x)x^2\phi_n(x) \tag{10}$$

corresponding to the coupling terms in the potential of the Hamiltonian in eq. (1). These are again numerically performed. For the Hamiltonian matrix of order N, the number of such integrals required will be $N(N+1)/2$. In all our calculations, we have typically employed 200 one-dimensional even parity quartic oscillator eigenfunctions to construct Hamiltonian matrices of order about 20000.

Thus both the one dimensional eigenfunctions for the quartic oscillator and the required matrix elements are obtained to a high accuracy numerically. For the A_1 irreducible representation all the matrix elements of the type $\langle n|x^2|n'\rangle$, where both n and n' are even integers, are required. It is well-known that if the states n and n' are harmonic oscillator states then the matrix element is zero for $|n - n'| > 2$. This is so because the eigenfunctions are defined in terms of orthogonal polynomials. In case of polynomials which are not orthogonal or for eigenfunctions obtained numerically there is no such strict cut-off. This cut-off is essential as it gives rise to a banded Hamiltonian matrix for the two dimensional problem. A banded real symmetric matrix, compared to the full real symmetric matrix, takes less storage space on the computer and the CPU time for diagonalization. One of the reasons for the use of harmonic oscillator eigenfunctions is that it leads to banded Hamiltonian matrix. The other reason being, of course, that the matrix element can be explicitly written down and numerical integration can be avoided altogether.

Though in principle any complete orthogonal set of basis states is sufficient to solve the problem, in practice an efficient numerical diagonalization depends crucially on the choice of physically appropriate basis states. In our work, we used the eigenfunctions of the unperturbed problem, namely the $\alpha = 0$ case of the Hamiltonian in eq. (1), rather than using harmonic oscillator eigenfunctions as basis states. Though employing harmonic

oscillator eigenfunctions as basis states are advantageous from the computational point of view, they are not suitable for computing very highly excited states. Firstly, the energy ϵ of the harmonic oscillator is $\epsilon_n \sim n$, where n is the principal quantum number. But, in the case of the quartic oscillator, $\epsilon_n \sim n^{4/3}$. Clearly, for any given n, the energy of the quartic oscillator is higher than the corresponding one for the harmonic oscillator. Thus, for higher values of n, there is a large separation between the energies of harmonic and quartic oscillator. Thus, to build up a two-dimensional eigenstate with the given energy, more number of harmonic oscillator states will be needed. Computation of a large number of converged eigenvalues and eigenfunctions using lesser number of basis states is possible with quartic oscillator eigenfunctions. Such a construction of one-dimensional basis functions is optimal for the calculation of a maximum number of converged eigenvalues and eigenfunctions for a given matrix dimensionality, for the coupling constant α in the range $[6, \infty]$ rather than in the range $[0, -2]$. It is easy to see that in the negative α domain the potential is rotated by 45° with respect to the positive α potential. We have earlier discussed the solution of this one dimensional Schrödinger equation by converting to an equivalent nonlinear second order differential equation. This nonlinear differential equation is solved numerically to obtain eigenvalues and eigenfunctions to machine precision [18].

Even though, quartic oscillator does not allow for exact banding of the Hamiltonian matrix, it is still possible to obtain a banded matrix, to a very good approximation. It is done as follows. In figure 1, we show $|M(n,n')|$ and $\log|M(n,n')|$ plotted against $n' = n + j$ and $j = 0, 2, 4, \ldots, 10$, for three different fixed values of n. This figure shows that the matrix elements fall off exponentially as a function of n'.

Based on the numerical values of the matrix elements, we found that,

$$|\langle\phi_n(x)|x^2|\phi_{n'}(x)\rangle| \approx 10^{-10} \approx 0, \quad n' > (n \pm \mu). \tag{11}$$

By an emperical study of the matrix elements, we fix the value of μ for the problem under consideration. For $\mu \geq 10$, the above condition was satisfied. This condition was imposed on the one-dimensional matrix elements while computing the full Hamiltonian matrix for the coupled quartic oscillator. At this point two salient features need to be noted. From the symmetrized form of the basis states used in eq. (8) we note that the matrix elements for the two-dimensional quartic oscillator actually involves product of the matrix elements given in eq. (10) and hence the numerical banding will be much more effective. Secondly, the magnitude of the matrix elements depends only on the difference $|(n' - n)|$ and not on the magnitude of the individual quantum numbers and so the banding criteria will remain true for all the values of n and n'. In the case of Hamiltonian in eq. (1), we constructed a Hamiltonian matrix of order 12880 and by imposing the above condition the bandwidth, the number of super or sub-diagonals with non-zero entries, was found to be 790. This procedure leads to considerable saving in CPU time and RAM space required for running the programs. For instance, to diagonalize a dense real-symmetric matrix of order about 3000 in IBM RS6000/580 RISC processor, it takes about 4 hours of CPU time. However, diagonalizing banded matrix of order 6000 with a bandwidth of 540 also takes the same amount of time. Thus there is a considerable speed-up and since we can employ bigger matrix sizes we get more number of converged eigenvalues.

All the eigenvalues obtained in the course of this work have an accuracy better than 10^{-6}. We note that the accuracy or the convergence of the eigenvalues is not affected by

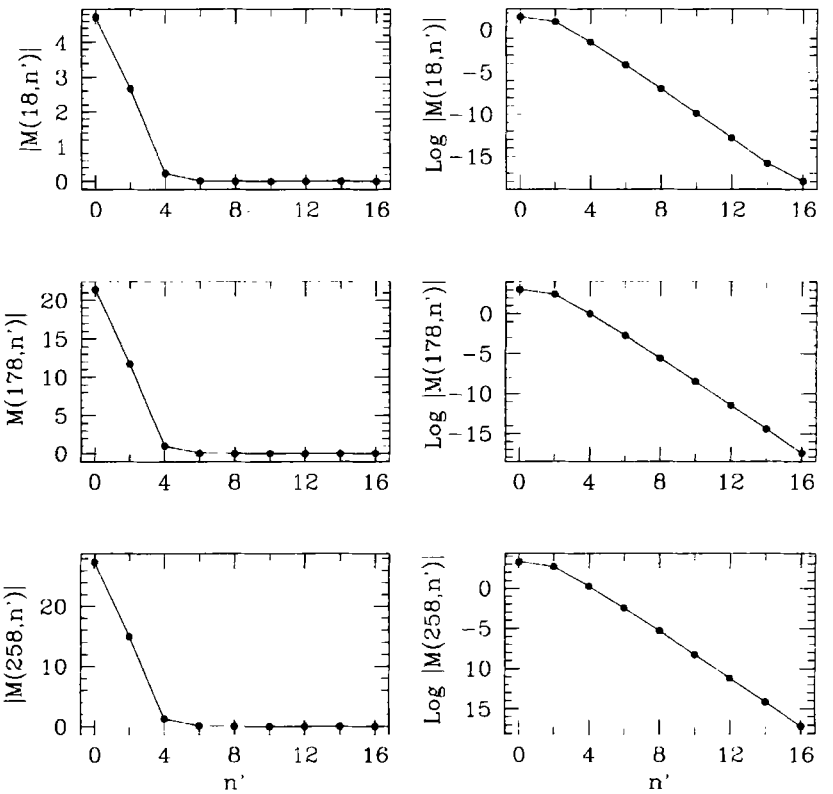

Figure 1. The exponential fall of the matrix elements of x^2 in the one-dimensional quartic oscillator basis. The plots are the matrix elements $|M(n,n')|$ and the logarithm of the matrix elements.

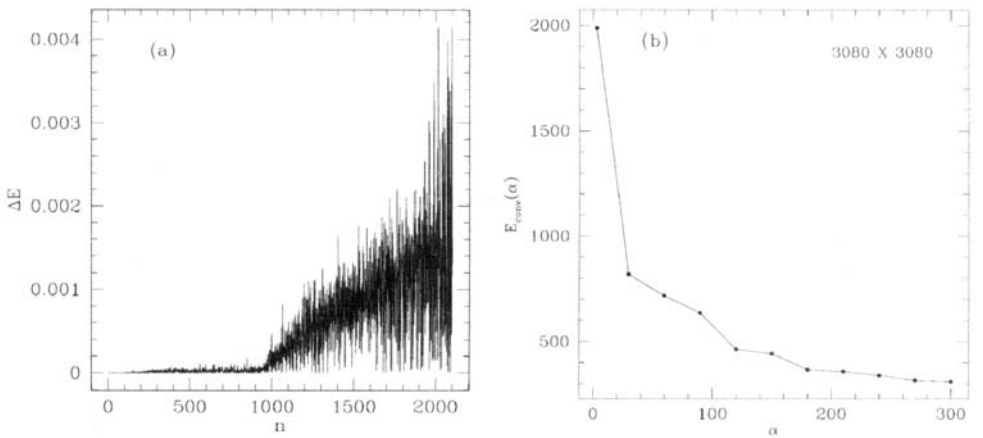

Figure 2. **(a)** The quantity (ΔE) is plotted for first 2000 eigenvalues. The information lost due to approximate banding is insignificant. **(b)** The number of eigenvalues converged E_{conv} as a function of the chaos parameter α. The order of the matrix is fixed at 3080.

the above numerical banding we have performed. In figure 2(a) we show the difference between first 2100 eigenvalues (ΔE) obtained from a diagonalization of a full Hamiltonian matrix of order 6105 and from the corresponding numerically banded matrix of order 6105 and with a bandwidth of 540. If E_f and E_b represent the eigenvalues from the full matrix and eigenvalues from the banded matrix respectively, then $\Delta E = |E_f - E_b|$. The number of converged eigenvalues, about 900 in this case, is also unaffected by the banding procedure. The figure shows that even at the worst, the eigenvalues of the Hamiltonian matrix differ only by about 10^{-3}, even though they may not have converged to the energy eigenvalue of the system being considered.

It is important to note that the data about the number of converged eigenvalues is specific to parametric regimes we worked with, namely $\alpha = 64$ to 96. It is not true in general for any arbitrary value of the parameter. We performed the following exercise to get a general picture about the eigenvalue convergence. In general, the number of converged eigenvalues depends also on the parameter of the system, apart from the size of the Hamiltonian matrix. We recall that the parameter α is indicative of the degree of classical chaos in the system. For the coupled quartic oscillator, for a fixed size of the Hamiltonian matrix, as the chaos parameter α is increased beyond 6, the convergence continuously gets poorer. In figure 2(b) we show the plot of the number of converged eigenvalues against the parameter α. We checked the convergence by diagonalizing Hamiltonian matrices of orders 3080 and 4000 for various values of α. The convergence criteria was that the difference in the eigenvalues computed from the matrices to two different orders mentioned above should not differ by more than 10^{-5}, which is the effective accuracy of the eigenvalues. From the available data, it appears that the convergence goes down as a power-law for the quartic oscillator system. Also note that as α increases beyond integrable parametric values, there is a sharp initial fall in convergence.

The diagonalization of the Hamiltonian matrix is carried out using standard routines from EISPACK and LAPACK [19]. The modus operandi is to tridiagonalize the given matrix first and then obtain the eigenvalues by the well-known bisection method. The eigenvectors are then computed by an inverse iteration process. Since these numerical methods and the computer codes are well documented [20] we will not discuss them here. By this procedure, we obtained about 2600 eigenvalues and eigenfunctions, converged up to 6 decimal places, for the coupled quartic oscillator by diagonalizing Hamiltonian matrices of order 15000.

4. Results

In this section, we will outline some of the results obtained using the numerical procedure we have followed. We have extensively studied the quantum mechanics of the Hamiltonian in eq. (1) whose phase space exhibits a mixture of both regular and chaotic dynamics. It is by now well known that such generic Hamiltonian systems exhibit quantum localization effects, i.e the non-spreading of the quantum wave functions in the entire classically accessible configuration space. Heller [21] has given theoretical arguments to show that the probability density $|\Psi_n(x, y)|^2$ tends to concentrate in the vicinity of the classical least unstable periodic orbits. Such localized enhanced probability density structures are called scars. This variety is called the scarring localization, to distinguish it from the other types

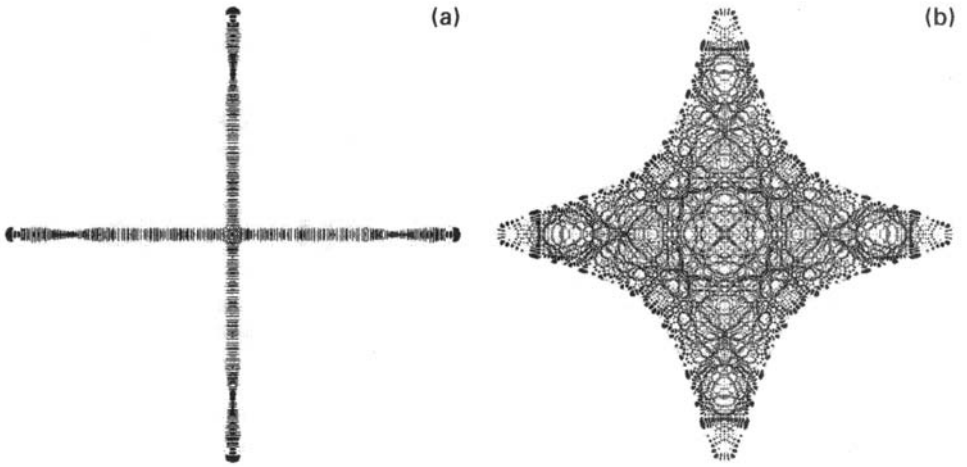

Figure 3. Eigenstates of coupled quartic oscillator: (**a**) A localized state, 1972nd state. (**b**) A typical eigenstate, 1973rd state (both at $\alpha = 90.0$). Note that the grey scale for both the images is the same.

of localization. In fact, the term 'localization' is used in various contexts in the study of quantum systems in different branches of physics. In the particular context of the coupled quartic oscillators we will reserve this term to denote eigenstates scarred by the channel periodic orbit. In the coordinate representation this periodic orbit simply coincides with the x and y axes, which lie along the channels of the potential. In figure 3, we have plotted the $|\Psi_n(x, y)|^2$ as an image plot for two eigenstates consecutive in energy. These are probability density plots with darker regions representing higher intensity and pure white corresponds to zero intensity. The boundary of the typical eigenstate shown corresponds to the boundary of the classically accessible region. As the image shows, the localized state has very less spread in the configuration space.

The difference between a typical state and a localized state is clearly brought out in figure 3. The results we present below pertain to localized states of the kind shown above.

These localized states are remarkable since they form a denumerably infinite series in the spectrum; that is they occur at regular intervals in the spectrum and this interval between the successive localized states keeps increasing as we explore the highly excited regions of the spectrum. For instance, in the region of state numbers 400–500, there are about 15 states between successive localized states whereas high up in the spectral region of 2000th state, there are about 30 states between successive localized states. It must be emphasized that the ability to calculate the accurate eigenenergies and the eigenfunctions for a large number of excited states enabled us to identify this infinite set of localized states in the spectrum of coupled quartic oscillator. Using an information entropy measure, we proposed a numerical method to identify these localized states [12].

Furthermore, we were able to investigate the properties of these localized states mainly because the procedure we followed allowed us to accurately compute the quantum eigenfunctions. Our numerical results show that the channel localized states in the basis-state space are dominated by a few peaks whose fall-off is exponential in nature in the quantum number of the motion perpendicular to the direction of the channel. This is the first

observation of exponential localization in a smooth Hamiltonian system. It may be recalled that the eigenfunctions of the quantum kicked rotor were shown to be exponentially localized in the momentum space. Further we have provided numerical evidence to the effect that the degree of localization, as measured by the information entropy, is related to the stability of the channel periodic orbit. We found that the information entropy of the channel localized state also displays oscillations and is strongly correlated with the stability oscillations of the channel orbit [22]. At the points of pitchfork bifurcations of the channel orbit, like $\alpha = 90$, we found the localization to be sharper and this result was viewed in the light of Berry's scar theory [23]. For more detailed evidence for this behaviour of the eigenfunctions in the unperturbed basis, we refer to [22, 26]. This aspect, namely the effect of a purely classical quantity like the stability of the channel orbit on the localized quantum wave functions has been theoretically predicted by the scar theories of Berry and Bogomolny [23, 24]. Quantitative verification of these theories is not straightforward since they are not directly applicable to an individual wave function in coordinate representation. The evidence for our efficient and accurate numerical procedure comes from our results, in particular, the unmistakable correlation between the stability of the channel orbit and localized states.

5. Three-dimensional systems

The interest in three-dimensional chaotic quantum systems has just begun in the last few years and some of the first results have started appearing in the literature. Both classically and quantum mechanically, the three-dimensional systems are more challenging and reveal a much richer dynamical structure than what can be seen in two-dimensional systems. For instance, classically, the three-dimensional systems exhibit phenomena called Arnold diffusion, which is absent in the two-dimensional systems [25]. The Poincaré section is four dimensional and hence difficult to visualize. One of the challenging problems is to study the signatures of classical Arnold diffusion, if any, in the three-dimensional quantum systems. Thus, while even the classical behaviour of three degree of freedom systems have not yet been exhaustively studied, the quantum mechanics of such systems is still an unexplored area. This is so mainly because of the computational difficulties involved in solving the eigenvalue problem for the highly excited states. In this context, we expect that our approximate banding procedure outlined above will help in overcoming the computational barrier.

We studied the eigenvalue spectrum of the three-dimensional homogeneous Hamiltonian given by [26]

$$H_{3d}(x, y, z; p_x, p_y, p_z; \alpha) = p_x^2 + p_y^2 + p_z^2 + x^4 + y^4 + z^4 + \alpha(x^2y^2 + y^2z^2 + z^2x^2), \tag{12}$$

where n_1, n_2 and n_3 are even integers. To compute the stationary states, we expand the eigenfunction of this system in the basis of the corresponding unperturbed Hamiltonian, namely the $\alpha = 0$ case of eq. (12). The symmetrized form of the basis state is given by

$$\begin{aligned}\psi_j(x, y, z) =& \phi_{n_1}(x)\phi_{n_2}(y)\phi_{n_3}(z) + \phi_{n_1}(y)\phi_{n_2}(x)\phi_{n_3}(z) + \phi_{n_1}(y)\phi_{n_2}(z)\phi_{n_3}(x) \\ &+ \phi_{n_1}(x)\phi_{n_2}(z)\phi_{n_3}(y) + \phi_{n_1}(z)\phi_{n_2}(y)\phi_{n_3}(x) + \phi_{n_1}(z)\phi_{n_2}(x)\phi_{n_3}(y).\end{aligned}$$

Using 30 one-dimensional quartic oscillator basis states, we constructed Hamiltonian matrices of order 7500 and obtained about 800 converged eigenvalues for values of the parameters ranging from $\alpha = 1$ to $\alpha = 60$. Though numerical banding worked well in the case of the two-dimensional quartic oscillator system, it is not very efficient for the three-dimensional quartic oscillator for the following reason; the coupling part of the potential $x^2y^2 + y^2z^2 + x^2z^2$ has three terms, each one coupling only two of the three independent modes. Hence, if we use a basis state of the form in eq. (13) there is atleast one Kronecker delta function in each of them leading to sparse Hamiltonian matrix. We observed that nearly 60% of the matrix elements are exact zeros. On the other hand, presence of three terms in the potential and three quantum numbers (n_1, n_2, n_3) means that the possibility of all the three coupling terms adding to produce a number close to zero is less pronounced. The matrix element would become vanishingly small only if the difference between any pair of quantum numbers is at least, say, larger than 10. Since this condition is difficult to satisfy for all the three coupling terms simultaneously, the numerical banding is not very effective, but can still be done. Hence, this situation presents itself as a sparse and banded matrix eigenvalue problem. The clue to computing highly excited states in systems of this type lies in taking advantage of the sparsity and bandedness of the Hamiltonian matrix simultaneously. We are now adopting Lanczos algorithm for sparse matrices to compute the quantum spectrum of this system. The results will be presented elsewhere.

6. Conclusion

We have presented some techniques to compute the highly excited states of certain coupled two-dimensional nonlinear oscillators. Basically we adopt the basis set diagonalization, though we have shown how the Hamiltonian matrix can be tuned so that we obtain a large number of converged eigenvalues for a given matrix dimensionality. The method presented above is quite general and can be applied in similar situations, which commonly arise while studying the quantum mechanics of various systems in physics and chemistry. We have presented results from our study of the two-dimensional coupled quartic oscillator, particularly the eigenfunctions of highly excited states with state numbers reaching 2000 counted sequentially from the ground state. It must again be emphasized that the results on the eigenfunctions of this system presented in this paper could be obtained mainly because of the efficient implementation of the numerical technique presented above. Since it is likely that saturation may be reached, sooner or later, in the computer processor speed it is imperative to explore better algorithms and efficient means to implement them.

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