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# Survival probabilities of complex Gaussian wavepackets in chaotic and regular systems by the Lanczos recursion method\*

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**Abstract.** The survival probability  $P(t) = |\langle \phi_0 | \phi(t) \rangle|^2$  for an initial complex Gaussian wavepacket  $\phi_0$  is calculated here for the first time by the Lanczos recursion method combined with the QL algorithm *without* computing the eigenfunctions of the Hamiltonian. Consequently, for an  $N \times N$  Hamiltonian matrix the correct dynamical behaviour of the system is obtained by carrying out  $nN^2$  numerical operations rather than  $N^3$ , where  $n$  is the number of Lanczos recursions.

We show that when  $\phi_0$  is located in the regular region of the classical phase space the ratio  $n/N$  is smaller than in the case when it is located in the chaotic regime. This ratio is reduced as the values of  $t$  become smaller.

## 1. Introduction

The time evolution of a wavepacket for time independent model Hamiltonians can be studied by two different approaches.

By taking the direct approach, the time dependent Schrödinger equation is solved for a specific given time  $t$ . There are, of course, many methods for wavepacket propagation. For example, two computational methods which are successfully and widely used in the study of different physical problems are Heller's approach (1981) where the initially Gaussian wavepacket follows the classical dynamics of its centre, and Kosloff's method (Bisseling *et al* 1987) where the exact time dependent solution is obtained by expanding the evolution operator  $e^{iHt/\hbar}$  in a Chebychev polynomial series. Recently, Park and Light (1986) developed another quantum time evolution method for wavepackets on the basis of the Lanczos algorithm. In their method  $n$ , independent Lanczos recursive vectors provide the desired coefficients in the series expansion of the time evaluated wavepacket. The time dependent solution of the Schrödinger equation is accurate over time interval  $0 < t < \tau$  for given  $n$  Lanczos recursive vectors. For short time calculation  $n$  is much smaller than the dimension of the original Hamiltonian matrix. Therefore, this method allows us to study the dynamics of very large systems when the optimal  $\tau$  is a function of the desired accuracy and of the available computational facilities.

The second approach to obtain the time dependent solution of the Schrödinger equation is to calculate the variational eigenfunctions of the time independent Hamiltonian,  $|E_\alpha\rangle$  and then to project  $\phi_0$  on the variational eigenfunctions; i.e. to calculate  $\langle \phi_0 | E_\alpha \rangle$ . This variational method is limited to small systems which can be represented

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by a relatively small Hamiltonian matrix  $N < 1000$ , since the computational time required to calculate the eigenvectors of  $\mathbf{H}$  increases as  $N^3$ .

A promising procedure which reduces the computational time was used by Cederbaum, Freed, Wyatt and their co-workers (Haller *et al* 1980, 1985, Moro *et al* 1980, 1981, Nauts and Wyatt 1983, Wyatt and Scott 1986). This procedure is based on the Lanczos recursion method (Lanczos 1950). By the Lanczos algorithm the  $N \times N$  Hamiltonian matrix is transformed to an  $n \times n$  tridiagonal matrix,  $\mathbf{T}$ .

The Lanczos algorithm has been used in molecular dynamics not only to get the eigenvalues of very large matrices but also to calculate other molecular properties. Moro and Freed (1980, 1981) used the Lanczos algorithm in calculating the frequency dependence of the spectral density, Cederbaum and co-workers in the study of vibronic coupling problems (Haller *et al* 1980, 1985), Berman and Domke (1984) in the evaluation of the optical potential for electron-molecule scattering, Friesner *et al* (1987) in the study of multiphoton excitations Wyatt (1985) in the study of the flux autocorrelation functions and reaction rate constants, Bard and Friesner (to be published) in the simulation of electrode processes, Marshall and Hutchinson (1987) in the study of intramolecular energy transfer in propargyl alcohol, and recently Kolin *et al* (1988) in the calculation of the coupling strength between a resonance state and different scattering channels of HD from a flat Ag(111) surface.

When the first Lanczos recursive vector is taken as  $\langle \phi_0 | \chi_i \rangle$ ;  $i = 1, \dots, N$  ( $\{\chi_i\}$  are the basis functions which were used to construct the Hamiltonian matrix), the first row of the eigenvector matrix of  $\mathbf{T}$  provides the coefficients  $\langle \phi_0 | E_\alpha \rangle$  in the series expansion of  $\phi(t)$ . The first row eigenvector coefficients are calculated during the diagonalization procedure when the QL algorithm is used. In passing, note that the combination of the Lanczos algorithm with the QL algorithm is not new. It has been used before by Haller *et al* (1985) and also by Wyatt and Scott (1986).

In order to get the time dependent properties of the studied system *all* possible transition amplitudes  $\langle \phi_i | E_\alpha \rangle \langle E_\alpha | \phi_j \rangle$  should be calculated. However, either with the residue algebra (Moiseyev *et al* 1986) or with the efficient block-Lanczos algorithm most recently developed by Meyer and Pal (1989), the CPU time is reduced by a factor of  $\sim N$ . Therefore, for large systems which are represented by very large Hamiltonian matrices, the Lanczos recursive method together with the QL algorithm is suitable, in particular, for calculating properties which depend on the *squares* of the eigenvector matrix  $|\langle \phi_0 | E_\alpha \rangle|^2$ , such as the survival probability  $P(t)$ . In this sense the method is less general than the direct methods mentioned above. However, it is applicable to problems with more than two degrees of freedom, and only three out of the  $n$  computed recursive vectors are stored.

In this paper we apply the Lanczos recursion method combined with the QL algorithm to stochastic systems.

Our purposes are as follows.

(1) To test the efficiency of the method for an initial complex wavepacket which is a 'natural' choice, for example, in the study of classical against quantum dynamics.

(2) To provide a simple formula from which one can get an upper bound to the number of Lanczos recursions,  $n$ , which are required to get  $P(t)$  with a given accuracy over a time interval  $0 < t < \tau$ .

(3) To study the role of symmetry mixing solutions in the mechanism which leads to quasiperiodic and stochastic behaviour of  $P(t)$ .

This method has a practical value in the study of the dynamics of very large systems (represented by an  $N \times N$  Hamiltonian matrix) since it requires  $nN^2$  numerical

operations rather than  $N^3$  in the calculation of  $P(t)$  with a given accuracy. Moreover, the numerical results presented in section 3 illustrate the fact that  $n \ll N$  when  $\phi_0$  is located in the regular region of the classical phase space rather than in the chaotic regime and also, as  $t$  becomes shorter.

In section 2 we show analytically that  $P(t)$  can be obtained with a given accuracy after applying less than  $n$  Lanczos recursion steps, over a time interval  $\tau$  which is greater than  $n\mu_n^{-1/n}/e$ .  $\mu_n$  is the  $n$ th moment of the Hamiltonian which can be obtained during the Lanczos recursion procedures. For nonlinear stochastic systems (such as the non-integrable Henon-Heiles system and the integrable second harmonic generation Hamiltonian)  $n$  is proportional to  $\tau$ . Indeed, the numerical results presented in section 3 confirm this suspicion.

The numerical results presented in section 4 indicate that the role of mixing different symmetry solutions in the mechanism which lead to quasiperiodic or stochastic behaviour of  $P(t)$  is strongly dependent on the location of initial wavepacket in the classical phase space.

## 2. Dynamics of a complex initial wavepacket by the Lanczos recursion method combined with the QL algorithm

Within the framework of the finite basis set approximation the Hamiltonian is constructed of  $N$  basis functions  $\{\chi_i\}$ . In the first step of the calculation the  $N \times N$  Hamiltonian matrix is recursively converted into an  $n \times n$  tridiagonal symmetric matrix  $T$ , where

$$T_{i,i} = \alpha_i \quad T_{i+1,i} = T_{i,i+1} = \beta_i. \quad (1)$$

The recursive vectors which provide the transformation matrix  $\mathbf{U}_1 = (U_1, U_2, \dots, U_n)$  for which  $\mathbf{T} = \mathbf{U}'\mathbf{H}\mathbf{U}$  are obtained by the Lanczos algorithm. For a general complex initial state the Lanczos recursions are carried out:

$$U_{n+1} = \rho_{n+1}/\beta \quad (2)$$

where

$$\rho_{n+1} = (\mathbf{H} - \alpha_n \mathbf{1})U_n - \beta_{n-1}U_{n-1} \quad \alpha_n = U_n'^* \mathbf{H} U_n \quad U_n'^* U_n = \delta_{n,n'} \quad (3)$$

and therefore

$$\beta_n = (\rho_{n+1}'^* \rho_{n+1})^{1/2}. \quad (4)$$

In the second step of the calculations the QL algorithm is used to get the eigenvalues of  $\mathbf{T}$ . In the QL algorithm the tridiagonal matrix  $\mathbf{T}$  is taken into a diagonal form by carrying out a similarity transformation

$$\mathbf{S}_k^{-1} \mathbf{T} \mathbf{S}_k = \mathbf{L}_k \mathbf{Q}_k \quad \text{as } k \rightarrow \infty$$

where

$$\mathbf{S}_k = \mathbf{Q}_1 \dots \mathbf{Q}_k \quad (5)$$

and  $\mathbf{L}_k$  is a lower triangular matrix. As pointed out by Haller *et al* (1985) and also by Wyatt and Scott (1986), when the eigenvalues  $\{E_\alpha\}$  are calculated simultaneously one can obtain the first row eigenvector matrix of  $\mathbf{T}$ ,  $C_{1\alpha} = U_1' C_\alpha$ , by operating on the right of each transformation as it is generated

$$e_1' \mathbf{S}_k = (1, 0, \dots) \mathbf{Q}_1 \mathbf{Q}_2 \dots \mathbf{Q}_k. \quad (6)$$

Note that  $C_\alpha$  are the linear variational coefficients (which are not(!) calculated) of the exact eigenfunction  $|E_\alpha\rangle$ ,

$$|E_\alpha\rangle = \sum_i C_{i\alpha} |\chi_i\rangle. \tag{7}$$

Therefore, if  $U_1$  is the projection of  $\phi_0$  on the basis functions  $U_1 = \{|\phi_0|\chi_i\rangle; i = 1, \dots, N\}$  then the desired coefficients are given by

$$\langle \phi_0 | E_\alpha \rangle = U_1^\dagger C_\alpha = C_{1\alpha} \tag{8}$$

and the time dependent survival probability is given by

$$P(t) = \sum_{\alpha, \alpha'} |C_{1\alpha}|^2 |C_{1\alpha'}|^2 \cos[(E_\alpha - E_{\alpha'})t/\hbar]. \tag{9}$$

As discussed by Park and Light (1986) there is a strong correlation between the time interval  $\tau$  for which the dynamics can be obtained for a given accuracy and the number of Lanczos recursions which are carried out during the numerical computations. A closed analytical equation from which one can estimate the number of Lanczos recursions which are required to get the 'correct' dynamics over a time interval  $\tau$  can be obtained. The time evaluated wavepacket can be expanded in a power series of the Hamiltonian  $\hat{H}$ , that is,

$$\phi(t) = e^{-i\hat{H}t/\hbar} \phi_0 = \sum_{n=0}^{\infty} \frac{(-it/\hbar)^n}{n!} \hat{H}^n \phi_0 \tag{10}$$

where  $\{\hat{H}^n \phi_0\}$  are the non-orthogonal Krylov states that after Schmidt orthogonalization provide the  $n$  Lanczos recursive states. By making use of the Stirling's formula (for  $n > n'$ )

$$\ln(n!) \sim (n) \ln(n) - n \tag{11}$$

one can get from (10) that the survival probability  $P(t)$  is given by

$$P(t) = \left| \sum_{n=0}^{n'} \frac{1}{n!} \left(-\frac{it}{\hbar}\right)^n \mu_n + \sum_{n=n'}^{\infty} (-i)^n T_n \right|^2 \tag{12}$$

where

$$T_n = \frac{e^{\mu_n^{1/n}}}{\hbar n} t \tag{13}$$

and  $\mu_n$  is the  $n$ th moment of the Hamiltonian

$$\mu_n = \langle \phi_0 | \hat{H}^n | \phi_0 \rangle. \tag{14}$$

For a given time  $t < \tau$  convergence of the power series in (12) is guaranteed after  $n$  Lanczos recursions if

$$T_n < 1. \tag{15}$$

Therefore, after  $n$  Lanczos recursions  $P(t)$  within a given accuracy can be obtained over a time interval  $\tau$  when (for  $\hbar = 1$ )

$$n \ll e^{\mu_n^{1/n}} \tau. \tag{16}$$

The moments of the Hamiltonian,  $\{\mu_n\}$ , can be obtained *during* the Lanczos recursive procedure (Schek and Wyatt 1985). The calculations of high-order moments are expected to be numerically unstable. In the case where  $\mu_n$  varies slowly with  $n$ , then  $\tau \propto n$ , and the interval  $\tau$  for which  $P(t)$  is obtained within a given accuracy is linearly dependent on the number of Lanczos recursions which were carried out during the numerical computation.

### 3. The survival probability for chaotic and regular systems by the Lanczos algorithm

In the comparison of quantum and classical behaviour of chaotic and regular systems, a natural choice is to follow the evolution of wavepacket initially given as

$$\phi_0(x, y) = (\pi\hbar)^{-1/2} \exp\left[-\frac{(x-x_0)^2}{2\hbar} + \frac{i\dot{x}_0x}{\hbar} - \frac{(y-y_0)^2}{2\hbar} + \frac{i\dot{y}_0y}{\hbar}\right] \quad (17)$$

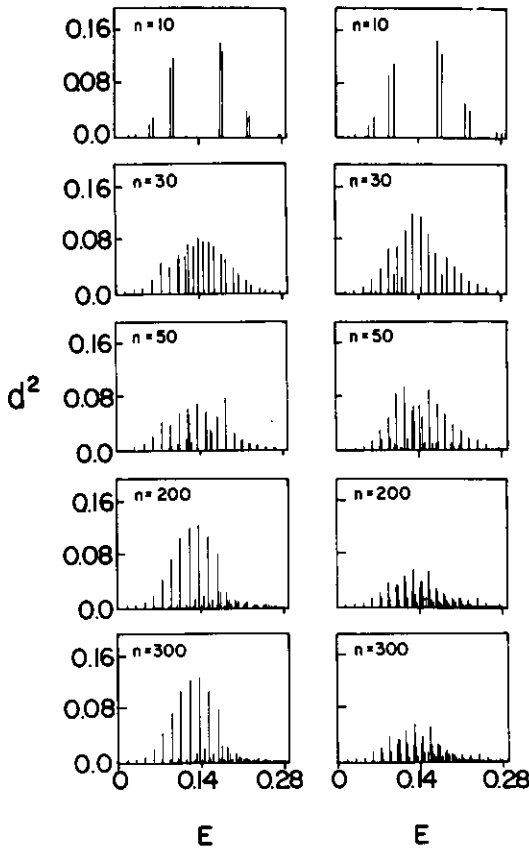
when  $x_0$ ,  $y_0$  and  $\dot{x}_0$ ,  $\dot{y}_0$  are constants which define a point in the classical phase space. A wavepacket placed in the regular region will disperse slowly in time, whereas a wavepacket located in the chaotic region will disperse *much* more rapidly (Moiseyev and Peres 1983) and in a relatively short period of time the system will not 'remember' its initial condition (Moiseyev 1983). In such a case the dynamics of the system can be studied by statistical approaches such as RRM. The explanation of the difference in the rate of spreading of wavepackets is based on the fact that the quantum energy spectrum of a classically regular system consists of families of equally spaced levels, but there is *no* such regularity for a classical chaotic system (Moiseyev and Peres 1983). Indeed, numerical calculations for the Henon-Heiles system show that the levels for which  $|\langle\phi_0|E_\alpha\rangle|^2 \neq 0$  are approximately equally spaced for the wavepacket  $\phi_0$  which is initially placed in the regular region (Moiseyev and Peres 1983). As the semiclassical limit of  $\hbar \rightarrow 0$  is approached, more states,  $|E_\alpha\rangle$  are involved in the dynamics and the Hamiltonian should be represented by a larger matrix. Large Hamiltonian matrices can be used when  $|\langle\phi_0|E_\alpha\rangle|^2$  is calculated *without* explicitly constructing eigenvalues by the Lanczos recursion method combined with the QL algorithm. Moreover, we show here that if  $\phi_0$  is placed in the regular region, the dynamics (i.e. calculating  $|\langle\phi_0|E_\alpha\rangle|^2$  of an  $N \times N$  Hamiltonian matrix) is obtained by the diagonalization of a smaller  $n \times n$  tridiagonal matrix ( $n \ll N$ ). The results presented in figure 1 show the population of the various energy levels for two wavepackets which have the *same* energy

$$\langle\phi_0^I|\hat{H}|\phi_0^I\rangle = \langle\phi_0^{II}|\hat{H}|\phi_0^{II}\rangle \quad (18)$$

the same width, centred on classical orbits which have about the *same* periodicity  $\tau$ , but placed in *different* regions of the classical phase space.  $\phi_0^I$  is centred on a stable periodic orbit and  $\phi_0^{II}$  on an unstable periodic orbit (the values of the initial parameters are given in a previous work of Moiseyev and Peres (1983) and in figure 1). The converged results which were obtained by calculating only the first row of the eigenvector matrix of a tridiagonal symmetric matrix (i.e.  $N^2$  numerical operations) are identical to the results which were obtained by Moiseyev and Peres when the entire eigenvector matrix of the Henon-Heiles Hamiltonian matrix was calculated (i.e.  $N^3$  numerical operations). (The  $N = 400$  basis functions are products of harmonic oscillator eigenfunctions in the  $x$  and  $y$  directions.) From the results presented in figure 1 one can see that:

(a) For a  $400 \times 400$  Hamiltonian matrix the converged population probabilities were obtained after  $n = 200$  recursions when the initial wavepacket  $\phi_0$  is placed in the regular region, and after  $n = 300$  recursions when  $\phi_0$  is located in the chaotic region. Therefore,  $P(t)$  is obtained by carrying out half of the numerical operations, which are required when the standard diagonalization procedures are used.

(b) Using 10-15 recursions, similar population probabilities were obtained for the two different initial wavepackets,  $\phi_0^I$  and  $\phi_0^{II}$  (in figure 1 we represent only the results for 10 recursions). This result seems to be consistent with the numerical evidence that for a short time,  $\sim 6$  time units, the spreading rates of the two different initial



**Figure 1.** Populations of various energy levels of the Henon-Heiles system,  $d^2$ , for two coherent wavepackets,  $\phi_0^I$  and  $\phi_0^{II}$  (which have the same energy,  $E = \frac{1}{8}$ ; same width,  $\hbar = 0.015$ ; centred on classical orbits which have about the same periodicity,  $\tau \approx 6$ ) for different numbers of the Lanczos recursions  $n$ . The population probabilities on the LHS are for  $\phi_0^I$  which is centred at  $x_0 = y_0, y_0 = 0.302\ 668\ 17$  and those on the RHS are obtained for  $\phi_0^{II}$  which is centred at  $x_0 = y_0 = 0$  and  $y_0 = -0.185\ 405\ 087$ .

wavepackets are very similar (Moiseyev and Peres 1983). Therefore, following the discussion in section 2, for chaotic systems  $n \approx \tau e$  and  $n$  is expected to be equal to  $6e$  (about 16). This is in agreement with the numerical evidence that up to  $n \approx 15$  recursions similar population probabilities were obtained for the two wavepackets  $\phi^I$  and  $\phi^{II}$ .

The dynamics of the nonlinear, integrable (in classical mechanics) and *exactly soluble* (in quantum mechanics) systems which are described by the Hamiltonians

$$\hat{H} = \hat{a}^\dagger \hat{a} + \hat{b}^\dagger \hat{b} + \lambda [(\hat{a}^\dagger)^k \hat{b} + \hat{b}^\dagger \hat{a}^k] \quad k = 1, 2, 3 \tag{19}$$

was previously studied (Moiseyev 1983). By using the counter rotational approximation the Henon-Heiles Hamiltonian is reduced to the special case of  $l = 2$  (known as the second harmonic generation Hamiltonian) where

$$\lambda = \frac{1}{2} \sqrt{\frac{1}{2} \hbar}. \tag{20}$$

The survival probabilities for the initial wavepacket (with  $\hbar = 0.015$ ) as a function of the Lanczos recursion number  $n$  are given in figure 2. These results indicate that the

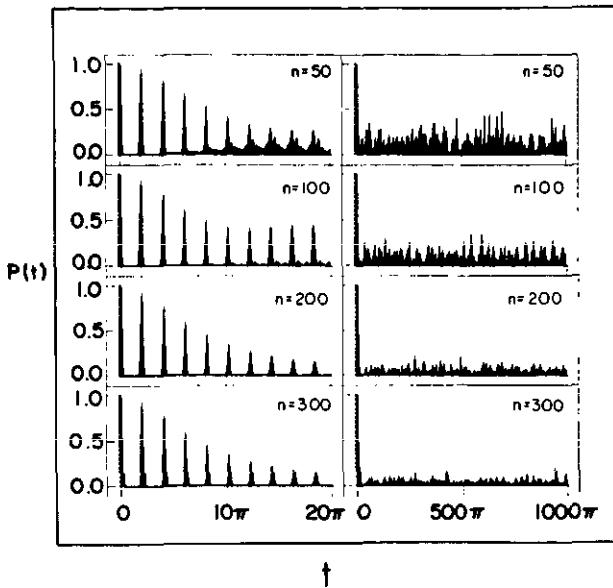


Figure 2. Survival probabilities  $P(t) = |\langle \phi_0^1 | \phi(t) \rangle|^2$  for the second harmonic generation Hamiltonian given in (26), for different numbers of the Lanczos recursions  $n$ .

number of recursions required for convergence of the survival probabilities increases with time:

(a) For  $t \leq 4\pi$ , converged results are obtained after 50 recursions (i.e. diagonalization of a tridiagonal matrix with the number of non-zero matrix elements which is smaller by a factor of 1000(!) from the number of the non-zero matrix elements in the original  $400 \times 400$  Hamiltonian matrix). This result illustrates the practical value of the combined Lanczos and QL algorithms in the study of very large systems.

(b) For  $t \leq 20\pi$ , only 200 recursions are required to get an accurate survival probability, and for  $t = 1000\pi$ , more than 400(!) recursions are needed.

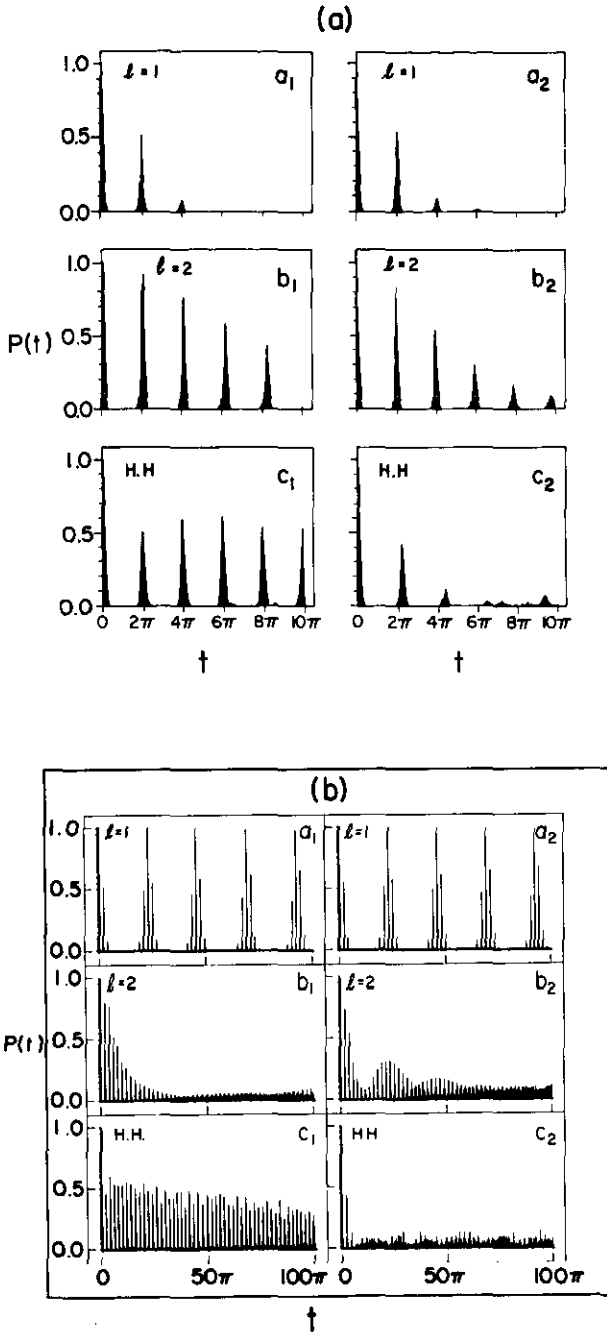
(c) After 50 recursions  $P(t)$  is converged (to the accuracy given in figure 2) for  $0 < t < 6\pi$ . After 100 Lanczos recursions a converged result for  $P(t)$  is obtained for  $0 < t < 10\pi$ , and after 200 recursions for  $0 < t < 20\pi$ .

Thus, the time interval for which  $P(t)$  can be obtained to a given accuracy depends linearly on the number of Lanczos recursions, as was proposed for stochastic systems in section 2.

#### 4. Quasiperiodic and stochastic behaviour of $P(t)$

The dependence of the rate of decay of the survival  $P(t)$  on the initial state and on the particular Hamiltonian studied was extensively discussed in the literature (see for example, Brumer and Shapiro 1980, 1982, Davis *et al* 1980, Hutchinson and Wyatt 1980, 1981, Weisman and Jortner 1981, 1982, Heller and Stechel 1982, Pechukas 1982). The difference of the quantum dynamics in the regular and chaotic regimes is not necessarily expressed by the slow or quick decaying of  $P(t)$ . As pointed out by Peres (1982), even a system of two *uncoupled* harmonic oscillators with incommensurate periods will have infinitely long recurrence time. As a matter of fact *any* behaviour of





**Figure 3.** The time dependent survival probabilities for three different model Hamiltonians:  $l=1$  stands for two linearly coupled harmonic oscillators (see (19)),  $l=2$  stands for the second harmonic generation Hamiltonian and H.H. for the Henon-Heiles system  $H = 1/2(P_x^2 + P_y^2 + x^2 + y^2) + x^2y - 1/3y^3$  with  $\hbar = 0.015$ . The results of  $P(t)$  which are presented in  $a_1, b_1, c_1$  were obtained for the initial wavepacket  $\phi_0^I$  and figures  $a_2, b_2, c_2$  for the initial wavepacket  $\phi_0^{II}$ . (a) Short-time behaviour. (b) Long-time behaviour.

$P(t)$  can be reproduced, to a given accuracy, by selecting a proper specially designed initial wavepacket for *one-dimensional* harmonic oscillator with small enough frequency. However, the initial wavepacket cannot be randomly selected and is determined by the experiment or by specific theoretical requirements. For example, in the comparison of classical against chaotic dynamics we should require that  $\phi_0$  will 'shrink' to a point in the classical phase space as  $\hbar \rightarrow 0$ . In figure 3 the survival probabilities  $P(t)$  are presented for two different initial wavepackets which are given by (17) and for different model Hamiltonians. Figure 3(a) shows the short-time behaviour of  $P(t)$ . Rapid decay of  $P(t)$  is obtained even for the second harmonic generation and the linear coupling harmonic oscillator Hamiltonians. As one can see from the long time behaviour of  $P(t)$  presented in figure 3(b), periodic behaviour of  $P(t)$  is obtained for the linearly coupled two harmonic oscillators but not for the second harmonic generation Hamiltonian. The recurrence time  $\tau$  is about equal to  $\pi/\lambda = 2\pi\sqrt{2/\hbar}$  and therefore, in the classical limit of  $\hbar \rightarrow 0$ ,  $\tau \rightarrow \infty$  even in the separable case of the linearly coupled two harmonic oscillators. Consequently, the surprising result is not the fast decay of  $P(t)$  but the quasiperiodic behaviour obtained for the Henon-Heiles system at high energy, where most of the regions in the classical phase space are chaotic. The quasiperiodic behaviour of  $P(t)$  was obtained for small values of  $\hbar$  when  $\phi_0$  is placed in the classical regular regime.

It is obvious that if  $P_1(t)$  and  $P_2(t)$  are the survival probabilities obtained for two different symmetry adapted eigenfunctions, then the mixing of the two symmetry solutions makes  $P(t)$  to be a linear combination of  $P_1(t)$  and  $P_2(t)$ . One may expect, however, that in the general case  $P_1(t)$  and  $P_2(t)$  should not necessarily show exactly the same time-dependent periodic behaviour and therefore  $P(t)$  will *not* have a periodic or quasiperiodic behaviour (although  $P_1(t)$  and  $P_2(t)$  do have a periodic or

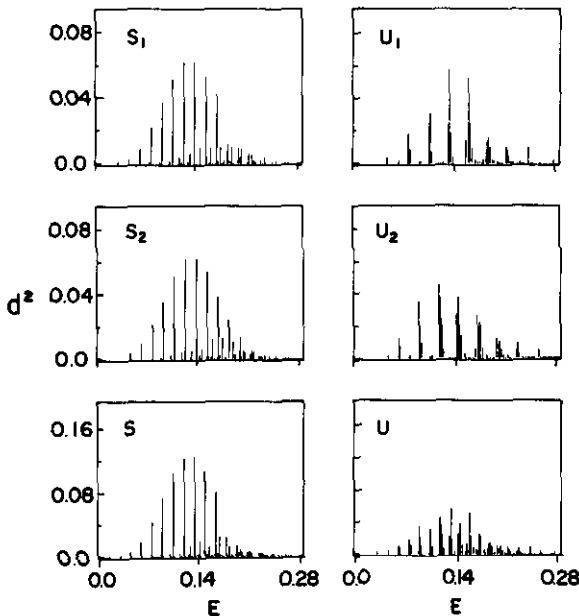


Figure 4. Populations of the various energy levels of the Henon-Heiles system when only odd (denoted by 1), even (denoted by 2) or both symmetry solutions are used to construct  $\phi_0^I$  (denoted by S) and  $\phi_0^{II}$  (denoted by U).

quasiperiodic behaviour). As we show here  $P(t)$  should have a time periodic or quasiperiodic behaviour *only* when the initial wavepacket is placed in the regular regime of the classical phase space. From the results presented in figure 4 one can see:

(a) When  $\phi_0$  is placed on a classical stable periodic orbit (denoted by S), the dominant population probabilities,  $|\langle \phi_0 | E_\alpha \rangle|^2$ , are equally-spaced. Moreover the results obtained for even (S2) or odd (S1) symmetry adapted eigenfunctions  $|E_\alpha\rangle$  are identical. Therefore, the mixing of different symmetry adapted solutions, S, increases the *regular* behaviour of  $|\langle \phi_0 | E_\alpha \rangle|^2$  against  $E_\alpha$ , and  $P(t)$  will show a quasiperiodic behaviour.

(b) When  $\phi_0$  is placed on an unstable periodic orbit (i.e.  $\phi_0$  is located in the classical chaotic regime denoted here by U for unstable), different results are obtained when  $\phi_0$  is projected on even,  $U_2$ , or odd,  $U_1$ , symmetry adapted eigenfunctions. Therefore the mixing of the different symmetry adapted solutions, U, increases the *irregular* behaviour of  $|\langle \phi_0 | E_\alpha \rangle|^2$  against  $E_\alpha$  and  $P(t)$  will show a stochastic behaviour.

## 5. Concluding remarks

The Lanczos recursion method combined with the QL algorithm as used by Haller *et al* (1985) and described in some more detail by Wyatt and Scott (1986) enable us to calculate the survival probability for a given initial wavepacket from the first row of the eigenvector matrix of a tridiagonal Hamiltonian matrix. The Lanczos and the QL algorithms were used to calculate population probabilities and survival probabilities,  $P(t)$ , for initial *complex* Gaussian wavepackets. The dimension of the tridiagonal matrix for which  $P(t)$  is calculated within a given accuracy over a time interval  $0 < t \leq \tau$  is smaller as  $\tau$  becomes shorter and is affected by the location of  $\phi_0$  in the classical phase space.

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