Classical Chaos and Quantum Mechanical Solvability in Inverse Problem

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Abstract We present a classically chaotic model in two-dimension whose Hamiltonian is $C_3$-symmetric and is bounded from below. In its quantal version, the ground state wave function and the energy eigenvalues of the Hamiltonian for low quantum numbers are exactly known. Excited energy levels with higher quantum numbers are calculated by numerically solving simple algebraic equations. The energy spectrum does not depend on the model parameter which is relevant to the $O(2)$-breaking. Schrödinger equation for the excited states is reduced to a set of recursion differential equations. The energy eigenstates are easily constructed by solving this recursion equation. The level statistics is Poissonian and the level-crossings are observed. We finally note the occurrence of the spontaneous symmetry breaking in the $O(2)$-symmetric model.

Keywords: Hénon-Heiles potential, Quantum chaos, Inverse problem

1. Introduction

The Hénon–Heiles (HH) potential, which was first presented to analyse astrophysical stability problem of galaxy, has arrested much attention in the field of deterministic chaos because of its conceptual simplicity (Hénon and Heiles 1964). It is a one-body potential of two degrees of freedom that is autonomous and non-singular, and has $C_3$ symmetry of the point group. Geometrically, the HH potential has a hollow surrounded by convex foots of walls, a similarity to the Sinai’s billiards, in which exponential separation of the classical paths is known to take place through repeated elastic collisions with fixed spheres (Sinai 1970). Non-integrability, the necessary condition for chaos, is realized by the $O(2)$ breaking. Surely, the HH model has excited interests on chaos in conservative systems with a non-trivial potential.

On the other hand, whether the system inherits some chaotic nature after quantization has been an intriguing question because the Heisenberg’s uncertainty inhibits precise determination of orbits in phase space. Phenomenologically, there are several criteria for ‘quantum chaos’ (Weissman and Jortner 1981): avoided crossing of energy levels, avoided contour crossing in wave function, irregulari-
ties in spatial and temporal behaviour of wave function, etc. Of course, whether a quantum system with these features is worth to be said chaotic is questionable. For instance, some authors claim that quantum chaos does not exist in such a quantized classically chaotic system as the Arnold’s cat map because of the absence of enough complexity in physical quantities in the classical limit (Ford et al. 1991; Ford and Mantica 1992. However, see Belot and Earman 1997). More pertinent problem to be addressed is therefore by what generic quantal features the classically chaotic quantum systems are discriminated from the classically integrable quantum systems. This may be what Berry aimed by advocating quantum chaology (Berry 1989a). The problem addressed in this way can be extended to the quantum field theory, since we know even a well-known renormalizable quantum field theory exhibits chaos in classical dynamics (Takahashi 2010).

In the context of chaos, it is natural to give an attention to randomness in any sense observed in the quantal system. According to the random matrix theory, the randomness of the Hamiltonian is specifically manifested by the Wigner distribution of the energy levels (Wigner 1951, Mehta 2004). Such a classically chaotic system as the kicked rotator is in fact known to leads via quantization, to a system with a (pseudo) random Hamiltonian (Fishman et al. 1982, Grempel and Prange 1984). Another important question then naturally arises: whether the classical chaos always implies quantal Wigner distribution, which is remaining unsolved.

Several authors sought signatures of chaos in the quantized system of the HH-type by diagonalizing the Hamiltonian in terms of a large set of the wave functions of the unperturbed harmonic oscillator (Pomphrey 1974, Noid et al. 1980, Weissman and Jortner 1981, Pullen and Edmonds 1981a, Park 2001). In the HH-like model, Cremers and Mielke (1999) employed the ‘flow equation’ that makes the Hamiltonian diagonal by continuous unitary transformation. Pomphrey (1974), Noid et al. (1980), Pullen and Edmonds (1981a) and Park (2001) have observed the avoided level crossings that give rise to the Wigner distribution for the level spacings and are usually regarded as the sign of quantum chaos due to the non-integrability and/or the sensitivity on the coupling of the underlying dynamics (Wigner 1951, Pechukas 1983, Yukawa 1985, Gaspard 1990).

Nevertheless, something worrisome has been left aside: the original HH potential and many HH-type potentials do not have the global minimum and there remains an insecurity about the meaning of eigenvalue or eigenfunction, especially near the escape energy. This casts a doubt for the meaning of the level statistics. To the author’s knowledge, no bounded and tractable $C^3$ symmetric potential models have been known so far.

A physically well-defined model calculation was performed by Pullen and Edmond (1981b). They
utilized a bounded $C_4$ symmetric potential that displays chaos in classical mechanics. In its quantum mechanical version, they observed level repulsions. Their result seemed to provide an example of a quantal criterion for the classical chaos.

Studying continuous potential models is important in relation to molecular or atomic physics but not an easy task, as long as chaos is concerned. The traditionally employed diagonalization method needs a very large number of base functions to approach the true eigenfunctions of the Hamiltonian, even if symmetries are taken into account. In addition, a large mixture of the base functions generally obscures the meaning of the quantum numbers associated to the constructed eigenfunction.

In the circumstance described above, for the pursuit of ‘quantum chaos’ in the potential problem, it will be worthwhile to proceed on an inverse route. Namely, adopting a certain function with required properties as a candidate of a wave function, we may find a Hamiltonian that yields the presumed function as an exact eigenfunction of that Hamiltonian. Its energy eigenvalue may also be known exactly. Remaining (excited) energy levels will then be found by solving a set of treatable equations. The associated eigenstates will be constructed as an infinite series of angular momentum states that are calculated recursively.

The core ingredient of the calculation method presented in this paper is a perturbative expansion in some combinations of model parameters and is distinct from the semiclassical approximation that has so far widely used to bring about steady developments in the field of quantum chaos. One of them is due to Berry and Tabor (1977) who showed that, in the regular systems, the generic distribution of the level spacing is Poissonian. On the other hand, there seems to be a widely pervaded expectation, but with no proof, that the quantum level spacings for the classically chaotic system should obey the Wigner distribution. Quite interestingly, our model, solvable for the energy spectrum, will show an opposite property: classically the system exhibits chaos, and after quantization, its energy spectrum obeys the Poisson distribution.

In this paper, we proceed the way similar to solving the inverse problems: we first assume the form of the wave function with a required symmetry property for a spin-zero particle trapped in a potential and then construct a two-dimensional Hamiltonian that is bounded from below, $C_4$-invariant and exhibits classical chaos. We elaborate the method of solving the Schrödinger equation and inspect the properties of the solutions by paying attention to the energy spectrum and the pattern of the wave function with low quantum numbers.
2. Bounded $C_{3v}$-symmetric model

The Schrödinger equation for a particle moving under the influence of the potential $V$ in two-dimensional (the coordinate is $q = (q_1, q_2)$) is given by

$$i\frac{\partial}{\partial t} \Phi = H\Phi = E\Phi,$$  \hspace{1cm} (2.1a)

$$H = -\frac{1}{2}\left(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2}\right) + V(q)$$  \hspace{1cm} (2.1b)

$$= \Pi^2 + V(\varphi^*, \varphi),$$

$$\varphi = \frac{1}{\sqrt{2}}(q_1 + iq_2), \quad \Pi = \frac{1}{\sqrt{2}}(p_1 - ip_2).$$ \hspace{1cm} (2.1c)

where $H$ and $E$ are the Hamiltonian and its eigenvalue, $\Pi = -i \frac{\partial}{\partial \varphi}$ and $\Pi^* = -i \frac{\partial}{\partial \varphi^*}$ are the momentum operators conjugate to the newly introduced spatial coordinate variables $\varphi$ and $\varphi^*$, respectively. The asterisk denotes the hermitian conjugate. The quantization condition reads (we choose the natural unit $\hbar = 1$)

$$[\Pi, \varphi] = [\Pi^*, \varphi^*] = -i. \hspace{1cm} (2.2)$$

$V(q) \equiv V(\varphi^*, \varphi)$ is the one-body potential. The potential of the classical HH model takes the form (Hénon and Heiles 1964)

$$V_{\text{HH}}(\varphi^*, \varphi) = \varphi^* \varphi - \left(\sqrt{2}/p_i\right) \varphi^* \varphi + (-\varphi)^p, \hspace{1cm} (2.3)$$

with $p = 3$. In this case, the second term on the r.h.s. of (2.3) is proportional to $3q_1^2q_2 - q_2^3$. The point group symmetry $C_{3v}$ that involves the reflection $R$ with respect to $q_2$ axis, i.e., the interchange $\varphi \leftrightarrow -\varphi^*$ are obvious. On the other hand, $O(2) \sim U(1)$ invariance under the global phase change of $\varphi$ is broken. Irrespective of this breaking, we shall see later that the ‘angular momentum quantum number’ is useful to label the wave functions.

For the wave function, we substitute the function of the form

$$\Phi = Ae^{i(\varphi^*, \varphi)}, \hspace{1cm} (2.4)$$

to the eigenvalue equation $H\Phi = E\Phi$, where $A$ is the normalization constant. We obtain

$$(-\partial_1 \partial \varphi^* - \partial_2 \partial \varphi + V) \Phi = E\Phi. \hspace{1cm} (2.5)$$

(Here and hereafter, abbreviations $\partial = \partial / \partial \varphi, \partial^* = \partial / \partial \varphi^*$ are used.) This implies that if the potential is of the form
then the function (2.4) is a solution of the eigenvalue equation (2.5) with the energy eigenvalue $E_0$. We would like to find $V$ that is derived from a function $f(\varphi^*, \varphi)$ through (2.6) and resembles $V_{\text{HH}}$ as much as possible. In other words, $V$ should be $C_3$-invariant, be bounded from below, be a polynomial in $\varphi$ and $\varphi^*$ with as low a power as possible. This procedure resembles solving the well-known inverse problems that aim to find the cause from the effect and are employed in a wide range of research fields (For a review, see, e.g., Groetsch 1999, Samarskii and Vabishchevich 2007). For our purpose, however, we will not need any of the detailed knowledge of the highly technical and complicated the methods. Once $V$ is found, we will directly solve (2.5) to find the excited states by a simple approximation method.

We adopt the following form for $f$ as the simplest one

$$f(\varphi^*, \varphi) = a(\varphi^* \varphi) - \frac{b}{p} \frac{1}{p^p} (\varphi^p + (-\varphi)^p),$$  \hspace{1cm} (2.7a)  

$$a(x) \equiv a_1 x + \frac{2a_2}{p+1} x^{(p+1)/2}, \hspace{0.5cm} a_2 < 0,$$ \hspace{1cm} (2.7b)

where $p$ is a positive integer in order for the wave function to be single-valued. There are three parameters $a_1, a_2$ and $b$ that are supposed to be real in this paper. This implies $f$ is also real. We write the corresponding wave function (2.4) as $\Phi_0$. For the normalizability of $\Phi_0$, $a_2$ must be negative. With this choice for the form of $f$, $\Phi_0$ consists of infinite number of states with the angular momenta equal to integer multiples of $p$.

From (2.6) and (2.7), the potential takes on the form

$$V = E_0 + a_1 + \frac{p+1}{2} \frac{1}{a_2} (\varphi^* \varphi)^{(p-1)/2} + a_2^2 \varphi^* \varphi + 2a_1 a_2 (\varphi^* \varphi)^{(p+1)/2} + b^2 (\varphi^* \varphi)^{p-1}$$

$$- b (a_1 + a_2 (\varphi^* \varphi)^{(p-1)/2}) i^p (\varphi^p + (-\varphi)^p) + a_2^2 (\varphi^* \varphi)^p.$$

(2.8)

$V$ is bounded from below for arbitrary $p>0$. We readily see that $V$ with $p=3$ is the preferable one to construct an HH-type potential. We restrict ourselves to this case hereafter. All of $a_1, a_2$ and $b$ contribute to the breaking of $U(1)$, which is recovered by setting $b=0$. For $p=3$, the number of the types of ‘interactions’ is four, while the number of the independent control parameters is three. The effect of this restriction on the number of the control parameters may manifest itself as a special pattern of the energy spectrum. We will come back to this point later. For convenience, we require $V$ to vanish at the origin. This implies $E_0 = -a_1$. In the most part of this paper, the parameters are fixed as $a_1 = a_2 = -1, b = 1$. 

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Note that, while the wave function $\Phi_0$ depends on all the three parameters, the energy $E_0$ is independent of $a_2$ and $b$. This is also understood by examining the identities:

$$\frac{\partial E}{\partial a_1} = \int (\varphi^* \partial f + \varphi \partial f) \Phi^* \Phi df \varphi d\varphi^*, \quad \text{(2.9a)}$$

$$\frac{\partial E}{\partial a_2} = \int (\varphi^* \partial f + \varphi \partial f + 2) \varphi^* \varphi \Phi^* \Phi df \varphi d\varphi^*, \quad \text{(2.9b)}$$

$$\frac{\partial E}{\partial b} = i \int (\varphi^* \partial f - \varphi^* \partial f) \Phi^* \Phi df \varphi d\varphi^*. \quad \text{(2.9c)}$$

These are derived from the Hellmann–Feynman theorem together with (2.6) and (2.7). Inserting the form (2.4) for the wave function into (2.9b) and (2.9c) and noting $\partial / \partial \Phi^* \Phi_0 = (\Phi^* \Phi_0)^2$, etc, we see that the r.h.s. of (2.9b) and (2.9c) identically vanish for $\Phi = \Phi_0$, while the r.h.s. of (2.9a) is equal to minus one.

Fundamental properties of the classical dynamics described by the above Hamiltonian are as follows. There exists seven fixed points in the phase space with zero momentum. Their spatial coordinates are O (0, 0), A (0, 0.3088), B (0.7071, 1.2247) and those obtained by rotations $2\pi/3$ and $4\pi/3$ of A and B about the origin in the $q_1$-$q_2$ plane. Their total energies are $E_a=0$, $E_A=-0.0189$ and $E_B=-1$, respectively. Eigenvalues of the Jacobian matrix associated with each of these equilibrium points are $\lambda_a=\pm 1$ (doubly degenerated), $\lambda_A=\pm 1.435$, $\pm 1.188i$ and $\lambda_B=\pm 2.449i$, $\pm 4.243i$, respectively. B is stable, while O (saddle) and A (saddle–centre) are unstable.

There exist regions in the parameter space where classical chaos is observed. The critical energy for the transition from regular to chaotic motion may be $E_c \approx 0$. In Fig. 1 we present an example of the Poincare sections of various classical orbits with $E=0.2$. We readily admit a sea of chaotic motions surrounding islands of regular (i.e., quasiperiodic) motions.

In Fig. 1, we also present the Poincare sections for $a_1=a_2=-1$, $b=0.1$ and $E=0.1$. (The pattern for $E=1$ is quite similar to that for $E=0.1$, which we do not display here.) Being obviously distinct from the result for $b=1$, we see that the pattern of the chaotic orbital motions is sensitive to the parameter $b$.

For a later use, we show an example of the almost periodic orbit in real space in Fig. 2. The energy is chosen as $E=46.862$. (In a two dimensional autonomous system, the orbit that smoothly closes is periodic because of the energy conservation. The orbit in Fig. 2 is ‘almost’ periodic in a sense that finer tunings of the initial condition will improve the orbital pattern toward perfect periodicity.) For the classical orbits in the HH model, Noid and Marcus (1977) have noted two types. One is the ‘precessing’ orbit that keeps $C_3$ symmetry as a whole. The other is the ‘librating’ orbit that breaks
The orbit shown in Fig. 2 corresponds to the former. It is easy to examine by numerical calculations that this orbit is surrounded by dense chaotic orbits.

3. Eigenvalue equation

Now let us go back to quantum mechanics and try to seek energy eigenvalues and eigenfunctions of the system (2.1). We write the wave function with the energy eigenvalue $E$ as

$$
\Phi = e^{i\theta(x)} \phi_0.
$$

(3.1)
Substituting (3.1) into (2.5), we have
\[ \partial^2 Q + \partial_t Q + \partial^2 Q + \partial_t Q + \partial^2 Q + \partial_t Q + \varepsilon = 0, \]
where \( \varepsilon \equiv E - E_0 \) and \( \partial^2 f = (a_1 + a_2 \varphi \varphi')\varphi' + i^2 b \varphi^2 \). \( Q \) may again involve the states of unlimitedly higher angular momenta via the coupling with \( \varphi^n + (-\varphi)^n \)-term in \( V \).

For a later convenience, we introduce functions
\[
c_{jk} = (\varphi^j \varphi^k + (-\varphi^j)(-\varphi^k))/2, \quad s_{jk} = (\varphi^j \varphi^k - (-\varphi^j)(-\varphi^k))/2. \tag{3.3}
\]
These are products of a power of \( |\varphi| \) and trigonometric functions. \( c_{jk} \) and \( s_{jk} \) themselves are eigenfunctions of \( R \) with the eigenvalues \( +1 \) and \( -1 \), respectively. Operation of \( c_{0,p} \) in the potential \( V \) on \( c_{jk} \) and \( s_{jk} \) increases their indices by \( p \), e.g., \( c_{0,p} c_{j,k} = (c_{j+p,k} + c_{j,k+p})/2 \). Together with the \( R \) invariance this suggests that the generic eigenstates involve the terms \( c_{jk} (R = +1) \) or \( s_{jk} (R = -1) \) where \( j \)'s (and \( k \)'s) are all equal modulo \( p \). Furthermore, eigenstates will be doubly degenerated except for \( j = k \) for which \( s_{jk} \) identically vanishes. Hereafter we restrict ourselves to the case of \( R = +1 \).

Our ansatz for the functional form of \( Q \) is
\[
Q(\varphi, \varphi^*) = a(x) + \beta(c_{0,1}/p + \ln Y_{jk}(\varphi^*, \varphi)). \tag{3.4a}
\]
\[
Y_{jk}(\varphi^*, \varphi) = \sum_{j' \geq j, k' \geq k} x^{-j} L_{j,k'}(x)c_{j,k'} \quad x \equiv |\varphi|. \tag{3.4b}
\]
Summation in (3.4b) is done over all integers \( j' (\geq j) \) and \( k' (\geq k) \) such that \( k' = k, j' = j \), modulo \( p \). Extracting a factor \( x^{-j'} \) in front of \( L_{j',k'} \) in (3.4b) implies \( j' \leq k' \) in order for a pole-like singularity...
in \( Y_{j,k} \) not to appear at \( x=0 \). By writing \( Q(\varphi, \varphi) \) in the form (3.4), each of \( \alpha, \beta \) and \( L'_{j,k} \) has been assumed to be a polynomial of \( x \). In particular, \( L'_{j',k} \) should not behave as an exponential function; such a behaviour is expected to have been absorbed into \( \varphi(x) \).

Note that the decomposition of \( Y \) in the form (3.4b) is not unique because of the identity \( c_{j,k} = x^r c_{j-k,r} \) that holds for arbitrary integer \( r \). In other words, the set \( \{x^r c_{j,k}\} \) is overcomplete and there are some arbitrariness in the functional form of \( L'_{j,k} \). We are going to derive a tractable sequence of equations that determine \( \alpha, \beta \) and \( L'_{j,k} \) by making use of this freedom. Since the highest power of \( x \) in \( f \) is two, \( \alpha(x) \) may be at most quadratic in \( x \). \( \beta \) is a function of \( c_{0,p} \) only. Substituting (3.4) into (3.2), multiplying \( Y \) on both sides of the equation and equating the coefficient of \( c_{j,k} \) to zero, we have (see the Appendix, where formulae useful for this procedure are given)

\[
L''_{j,k} + \left( \frac{k'-j'+1}{x} + 2(\alpha' + \alpha') \right)L'_{j,k} + \left( \frac{\alpha' + \alpha'}{x} \right)^2 L_{j,k} = 0,
\]

(3.5a)

\[
\frac{2b + \beta'}{2x} \left( x^p L_{j-k,p} + L'_{j-k,p} + (k + p)x^{p-1} L_{j-k,p} + \frac{j'}{x} L_{j-k,p} \right) h(x) = \varepsilon + \alpha' + \alpha^2 + 2\alpha \alpha' x + \frac{1}{4} \left( p\beta'' + \beta'^2 + 4h\beta' \right) x^2.
\]

(3.5b)

A single (double) prime on functions \( L, \alpha, \beta \) stands for the first (second) derivative of the function in terms of its variable: \( \alpha' = d\alpha(x)/dx, \beta' = d\beta(c_{0,p})/dc_{0,p} \), etc. These equations look like a perturbative expansion of \( L_{j,k} \) in terms of \( b \) and \( \beta \). The advantage of our method is manifested in (3.5): it is the recursion differential equation that enables us to determine higher-mode amplitudes of any step from those just one step before. The price one has to pay is that the differential equation is second-order at each step of calculation. However, the equation is linear. In addition, it is easily checked that the equation has normalizable solutions that is consistent with our assumption only when \( \alpha(x) \) is linear in \( x \), i.e., \( \alpha' = \text{constant} \equiv \alpha_1 \). This makes the problem quite simple.

We first consider the case of minimum indices on the l.h.s. of (3.5a), \( j' = j, k' = k \). In this case, the r.h.s. vanishes, and we have

\[
L''_{j,k} + \left( \frac{l+1}{x} + 2(\alpha_1 + \alpha_1) + 2a_2 x \right)L'_{j,k} + \left[ \frac{\varepsilon + \alpha_1 + \alpha_1(\alpha_1 + \alpha_1)}{x} \right] L_{j,k} + \frac{1}{4}(8a_2 \alpha_1 + p\beta'' + \beta'^2 + 4h\beta') x L_{j,k} = 0,
\]

(3.6)

where \( \ell \equiv k - j \). The equation (3.6) will have various types of solutions depending on the parameters. We will show that, when \( x \) term on the l.h.s. of (3.6) is absent, the solutions can be polyno-
mials as was assumed below (3.4) and reveal particularly interesting properties. Hereafter, we restrict ourselves solely to this case.

\[ xL_{j,k} \text{-term is eliminated by requiring } \beta' = \text{constant} = \beta, \]  

and

\[ \beta_1 = -2b \mp 2 \sqrt{b^2 - 2a_2 \alpha_1}. \]  

(3.7)

Let the degree of the polynomial be \( n \). Then, writing \( L_{n,\ell} \equiv L_{(j,k)} \), we rewrite (3.6) as

\[ L_{n,\ell}'' + \left( \frac{u_0}{x} + u_1 + 2a_2 x \right) L_{n,\ell}' + \left( \frac{v_0}{x} + v_1 \right) L_{n,\ell} = 0, \]  

(3.8a)

\[ u_0 = \ell + 1, \ u_1 = 2(\alpha_1 + \alpha_0), \]  

(3.8b)

\[ v_0 = \varepsilon + \alpha_1 + \ell(\alpha_1 + \alpha_0), \ v_1 = \ell a_2 + \alpha_1^2 + 2a_2 \alpha_1. \]  

(3.8c)

We expand the solution as \( L_{n,\ell}(x) = \sum_{r=0}^{n} \zeta_r^{(n,\ell)} x^r \). Substituting this into (3.8), we have a recursion relation (dropping the suffices \( n \) and \( \ell \))

\[ (2a_2 (r-1) + v_1) \zeta_{r-1} + (u_1 r + v_0) \zeta_r + (r+1)(r+u_0) \zeta_{r+1} = 0. \]  

(3.9)

Note that, for \( b = \beta' = 0 = a_2 \), our system is nothing but the two-dimensional harmonic oscillator and (3.9) implies \( L_{n,\ell}(x) \) to be the Laguerre’s polynomials (See, e.g., Louck and Shaffer 1960).

\( \zeta_r \) must vanish for \( r < 0 \) or \( r > n \). These conditions are assured to be fulfilled by

\[ u_0 \zeta_1 + v_0 \zeta_0 = 0, \]  

(3.10a)

\[ (u_1 n + v_0) \zeta_n + (2a_2 (n-1) + v_1) \zeta_{n-1} = 0, \]  

(3.10b)

\[ (2a_2 n + v_1) \zeta_n = 0. \]  

(3.10c)

Condition (3.10c) leads to \( 2a_2 n + v_1 = 0 \) or

\[ \alpha_1 + \alpha_0 = \pm \sqrt{a_1^2 - a_2 (2n + \ell)} = \pm d(n, \ell). \]  

(3.11)

\( \alpha_1 \) is real since \( a_2 < 0 \).

Remaining parameters \( u_1, v_0 \) and \( v_1 \) are determined from (3.8b) and (3.8c) as

\[ u_1 = \pm 2d(n, \ell), \ v_0 = \varepsilon - \alpha_1 \pm (\ell + 1) d(n, \ell), \ v_1 = -2a_2 n. \]  

(3.12)

Accordingly, the recursion relation (3.9) can be cast into an eigenvalue equation for an \((n+1) \times (n+1)\) matrix

\[ W \zeta = (\varepsilon - \alpha_1) \zeta, \]  

(3.13a)
\[
W = \begin{pmatrix}
\mp(\ell+1)d(n, \ell) & -\ell - 1 & 0 & \cdots & 0 \\
2a_2 n & \mp(\ell+3)d(n, \ell) & -2(\ell+2) & 0 \\
0 & 2a_2(n-1) & \mp(\ell+5)d(n, \ell) & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & -n(\ell+n) \\
0 & 0 & 0 & \cdots & \mp(\ell+2n+1)d(n, \ell)
\end{pmatrix},
\]

where \( \xi = (\xi_0, \xi_1, \cdots, \xi_n)^T \) is an \( n+1 \) component vector. The double signs for the diagonal components of \( W \) are due to the double signs in (3.11). Since \( \epsilon - \alpha_i = E, W \) is nothing but the matrix representation of the system’s Hamiltonian.

Note that \( W \) does not depend on the coupling \( b \). This fact leads to a remarkable outcome of our model that the energy spectrum is also independent of \( b \), provided that the r.h.s. of (3.4b) converges. The whole effect of \( b \) is absorbed into the wave functions. The cause of this result is traced back to the eigenvalue equation (3.2) and the reduction of the number of the control parameters that will be the generic feature of the inverse problem. Our method will also be applicable for \( p \geq 4 \). However, whether this non-dependence on \( b \) really holds, or, equivalently, whether the r.h.s. of (3.4b) always converges under the condition that \( \epsilon \) is determined by the zeroth step equation (3.8), is an open question. Later on, we shall numerically inspect this convergence for \( p = 3 \).

We readily see from (3.13a) and (3.13b) that the positive energy solutions will correspond to the lower sign of the diagonal components of \( W \). This means that we should choose the minus sign for \( \alpha_i + \alpha_i \) in (3.11).

In passing, we note that the parameter \( b \) can be extended to complex number without spoiling the validity of the derivation of (3.9) or (3.13). In particular, the energy spectrum remains real for a complex \( b \). In such a case, the model considered here is regarded as a member of the family of quantum complex potential models (Bender et al. 2001 and references cited therein).

For a given \( n \), the eigenvalue equation is an algebraic equation of degree \( n+1 \), which yields real roots for \( \epsilon \) provided that \( \ell \geq -n \). Among them only the largest real one seems to allow \( L_{\alpha_i} \)’s to share the common feature of the orthogonal polynomial system: the components of \( \xi \) have alternating signs. Furthermore, only in this case the higher modes \( L_{(j',m',k+\alpha,m')} (m \text{ and } m' \text{ are zero or positive integers}) \) determined by (3.5) seem to render the series (3.4b) convergent. We have not proved this convergence but assume hereafter.

We label \( \epsilon \) thus obtained for a given set of \( n \) and \( \ell \) as \( \epsilon_{n,\ell} \). These numbers will be related to the customarily used ‘principal quantum number’ \( N \) and ‘approximate angular momentum quantum number’ \( l \) by \( n = (N + l)/2 \) and \( \ell = (N - l)/2, \ -N \leq \ell \leq N \) (Louck and Shaffer 1960, Noid and Marcus
Although we have two labels to discriminate the states, no actions exist to be related to them as in integrable systems. In fact, although $\ell$ has been defined as the minimum value of $k' - j'$ for the suffix appearing in the expansion (3.4b) of $Y_{j,k}$, our starting wave function $\Phi_0$ already consists of an infinite number of angular momentum states.

The exact expressions of $\varepsilon_{n,0} = E_{n,0} + a_1$ for the three lowest $n$ are easily obtained by directly solving the algebraic equations derived from (3.13). They are given, for $n = 0, 1$ and 2, by

\begin{align*}
\varepsilon_{0,0} &= a_1 + (\ell + 1)d(0, \ell), \\
\varepsilon_{1,0} &= a_1 + (\ell + 2)d(1, \ell) + \sqrt{-3a_2\ell} + a_1^2 - 4a_2, \\
\varepsilon_{2,0} &= a_1 + (\ell + 3)d(2, \ell) + 2\text{Re}\left[-4a_2 + 4\sqrt{a_2^2 - 4}\left((-3a_2\ell + a_1^2 - 7a_2)/3\right)^3\right].
\end{align*}

These solutions for the energies are assured to remain positive in the limit of large $\ell$. The state $\Phi_0$ we constructed at the beginning should have the energy $\varepsilon_{0,0} = 0$ and is identified as the ground state. We may be able to find the explicit form of $\varepsilon_{0,0,0}$, too, by way of Ferrari’s formula.

Unfortunately, it may be impossible to express $\varepsilon_{n,0}$ as an analytic function of $n$ and $\ell$, as is anticipated from the expressions (3.13a–c). Nevertheless, we can guess, from the structure of $W$, $\varepsilon_{n,0}$ to behave as $\ell^{3/2}$ for large $\ell$’s. The large $n$ behaviour (or, more important equi-energy contours in the $n-\ell$ space) is not known. The 66 levels for $0 \leq n \leq 5$ and $0 \leq \ell \leq 10$ are given in Table 1.

Equation (3.13) is equivalent to the Schrödinger equation of a particle hopping from site to site on an open linear lattice of length $n$ with the probability amplitude $\xi_r$ for the particle to be on the $r$th site. In this interpretation, both of the ‘potential’ $W_{rr}$ and the ‘bond strength’ $W_{rr'}$ ($r \neq r'$) are neither periodic as a regular lattice nor random as the Anderson model for a lattice containing impurities (Anderson 1958, Stöckmann 1999 and references cited therein). This view is parallel to the one presented by Fishman et al. for the kicked rotator model (Fishman et al. 1982) for understanding the dynamical localization (Casati et al. 1979). Owing to this aspect of $W$, the amplitude $\xi$ will not spread over

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\ell$</th>
<th>$E_{n,0}$ for $0 \leq n \leq 5$ and $0 \leq \ell \leq 10$.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>0</td>
<td>0.0</td>
<td>1.8</td>
</tr>
<tr>
<td>1</td>
<td>4.7</td>
<td>7.8</td>
</tr>
<tr>
<td>2</td>
<td>11.6</td>
<td>15.6</td>
</tr>
<tr>
<td>3</td>
<td>20.2</td>
<td>24.9</td>
</tr>
<tr>
<td>4</td>
<td>30.1</td>
<td>35.5</td>
</tr>
<tr>
<td>5</td>
<td>41.3</td>
<td>47.2</td>
</tr>
</tbody>
</table>
the lattice nor localize randomly at a number of sites.

4. Energy spectrum and quantum numbers

In order to see the degree of randomness of the system, we draw the distribution of the neighbouring level gap $S$ in Fig. 3. The energy range is $0 < \varepsilon < 400$. Although the number of samples may not be large, they seem consistent with the Poisson distribution usually featured in uncorrelated or integrable systems as Berry and Tabor (1977) have shown within semiclassical theory. Their analysis requires the knowledge of the functional structure of the energy level as a function of actions. Our system is not integrable but the quantum states can be labelled by the well-defined ‘quantum numbers.’ One peculiarity is that there may not be an analytic expression of the energy as a function of the ‘quantum numbers’ as can be guessed from (3.14a)–(3.14c). Probably, the result of the semiclassical analysis is not straightforwardly applied to our system. Rather, our result exhibits the con-

![Fig 3. Distribution of neighbouring level gaps for $0 < \varepsilon_{n,\ell} < 200$ involving 270 levels (left panel) and $200 < \varepsilon_{n,\ell} < 400$ involving 381 levels (right panel). The largest $n$ and $\ell$ are 23 and 53, respectively.](image)

![Fig 4. Parameter dependences of the energy levels in $34 < E_{n,\ell} < 40$ a. Left panel] $a_1$-dependences for $-2 < a_1 < 1$ and $a_2 = 1$. Quantum numbers are $(n, \ell) = (2,5), (3,3), (0,10), (1,4), (1,8)$ and $(2,6)$ from bottom to top at $a_1 = 0.5$. The levels (0,10) and (1,4) crosses at $a_1 = 1$. Right panel] $a_2$-dependences for $-2.5 < a_2 < -0.5$ and $a_1 = 1$. Not all levels are displayed. Quantum numbers are $(n, \ell) = (3,1), (0,8), (1,9), (3,2), (4,0), (2,5), (1,8), (1,9)$ and $(5,1)$ from left to right.](image)
ceptual consistency with the random matrix theory (Wigner 1951, Mehta 2004): the Poisson and Wigner distributions are the direct reflections of the regularity and randomness of the Hamiltonian, respectively. We have seen in the previous section that our system is not random. Thus we arrived at the most significant conclusion that classical chaos does not necessarily mean quantal Wigner distribution.

In Fig. 4, \( a_1 \)- and \( a_2 \)-dependences of some energy levels in \( 34 < n, k < 40 \) are plotted. The sensitivity to \( a_2 \) is very high as compared to \( a_1 \). The absence of inter-level correlation may also be observed from a level-crossing occurring when \( a_i \) is varied. Although we have not surveyed wider parameter region, this is a rather anticipated result. The model parameter \( b \), which is responsible for the classical chaos, does not contribute to the recursion relation (3.9) that determines the energy spectrum of the quantal system.

5. Wave function

The wave function is a superposition of an infinite number of eigenstates of the angular momentum. It is obtained by solving (3.5) step by step from low to high indices. Suppose \( j \neq 0 \). Then the term most singular term at \( x = 0 \) on r.h.s of (3.5a) may be \( -j'/x^2 \). The solution will have a power series expansion as \( x^{-\epsilon} \sum_{i=0}^{\ell'} B_i x^{i} \) with \( \ell' = k' - j' \), which causes the resulting wave function to be unnormalizable. Therefore we set \( j' = j = 0 \). Then writing \( k' = \ell + sp \), dropping the suffix \( j' \) and rewriting \( L_{j', k'} \) as \( L_{n, k + sp} \), the equation to be solved is

\[
L_{n, k + sp} + \left( \frac{x + sp + 1}{x} + 2(\alpha' + \alpha) \right)L_{n, k + sp} + \frac{(\alpha' + \alpha)(\ell + sp) + h}{x} L_{n, k + sp} = -\frac{2h + \beta_1}{2x} L_{n, k + (s-1)p},
\]

This is a linear differential equation with the \( b \)-term now playing the role of the source for \( L_{n, k + sp} \) \( (s \geq 1) \). The general solution is given by a linear combination of a special solution and a solution of a homogeneous equation without the source term. The homogeneous equation has a same form as (3.8a) with \( \ell \) in (3.8a) being replaced by \( \ell + sp \). Since \( \epsilon \) has already been fixed by (3.9) and (3.10), the solutions of the homogeneous equation for (5.1) can not be of a finite power series. Therefore, in order for the wave function to be normalizable, the solution of (5.1) must be determined so as for the special solution to be a finite power series under the presence of the source term. This is done by appropriately choosing the boundary condition.
The wave functions for the excited states (i.e., \( n \geq 1 \) or \( \ell \geq 1 \)), including the time dependent phase factor, take the form

\[
\Phi_{n,\ell}(\varphi^*, \varphi) = A e^{i(\alpha_1 + \beta_1)\omega} \sum_{s=0}^{\infty} \psi_{n,s}^{(s)}(\varphi^*, \varphi),
\]

(5.2a)

\[
\psi_{n,s}^{(s)}(\varphi^*, \varphi) = L_{n,\ell,s,p}(x) c_{n,s} e^{-iE_{n,\ell,s,p}x + i\alpha_n x},
\]

(5.2b)

where \( E_{n,\ell} = \epsilon_{n,\ell} + E_0 \) and \( A \) is the normalization factor. Remember that \( \alpha_1 \) and \( \beta_1 \) are also dependent on \( n \) and \( \ell \). In particular, since \( \alpha_1 \) can be negative and its absolute value can be arbitrarily large, \( \beta_1 \) given by (3.7) is generally a complex number. Each of the real and imaginary part of \( \Phi_{n,\ell} \), having a factor \( \cos (\text{Im} \beta_1 c_{n,s}/p) \) and \( \sin (\text{Im} \beta_1 c_{n,s}/p) \) respectively, can then have an infinite number of nodes in radial direction. The other zeros of \( \Phi_{n,\ell} \) are determined by the terms involving \( L_{n,\ell,s,p} \) in (5.2).

Irregularity in the wave function is expected to feature quantum chaos. However, we have to notice that, irrespective of whether the system is classical or quantal, a mere uncorrelated superposition of base functions yields irregular structure of the compounded function with a Gaussian distribution for the amplitude (O’Connor et al. 1987, McDonald and Kaufman 1979). Concerning the present system, the results of calculations by (5.1) are depicted in Fig. 5 for \( n = 3 \) and \( \ell = 5 \) as contour maps of

![Contour maps](image-url)
the real part of the wave function. We here chose such low quantum numbers since (5.1) involves no approximation and is free from the restriction posed on the semiclassical approximation. The calculations were performed up to the fifth step \( (s=5) \), namely, \( k'=5, 8, 11, 14, 17 \) and \( 20 \). The approximate \( C_5 \) symmetry observed in the 0th step calculation is gradually lost with the step of calculation and an approximate \( C_{3v} \) symmetry eventually emerges. The traces of the \( C_{3v} \) symmetry of the Hamiltonian are always observed in the peripheral region. Exact \( C_n \) symmetries are violated for all \( n \), while \( R \) symmetry remains unbroken. At each step of calculations the wave function reveals an obvious pattern, but the final 3-D structure is complex with somewhat irregular pattern of contour and height distribution.

We notice that the pattern in the maps seems to converge as the calculation proceeds to higher steps. More quantitatively, we plot in Fig. 6 the integrations of the square of the absolute value of each term, \( \int \psi_{n,l}^{(s)} \bar{\psi}_{n,l} \, d\varphi \, d\varphi^* \) with \( n=3 \) and \( l=5 \), in (5.2) from \( s=0 \) to 6. (For convenience, the term with \( s=0 \) has been normalized to unity.) Obviously, the higher step contributions get less significant as \( s \) becomes larger. Remember that our principal arguments are based on the assumption that the expansion (5.2) converges. The behaviour of \( \int \psi_{n,l}^{(s)} \bar{\psi}_{n,l} \, d\varphi \, d\varphi^* \) depicted in Fig. 6 supports the validity of this assumption.

We have seen that, in our model, the energy levels do not depend on the potential parameter \( b \), i.e., \( \partial E_{n,l} / \partial b = 0 \). According to the Hellmann–Feynman theorem, this differentiation is given by the integration on the r.h.s. of (2.9c). We numerically performed this integration by adopting the finite summations up to the \( s \)-th term in (5.2a) as the approximation to the true wave function:

\[
D_{n,l}^{(s)} = \int \psi_{n,l}^{(s)} \bar{\psi}_{n,l} \, d\varphi \, d\varphi^* .
\]

(5.3)

Fig. 6 Circles: \( s \)-dependence of \( \int \psi_{3,3}^{(s)} \bar{\psi}_{3,3} \, d\varphi \, d\varphi^* \). Squares: \( s \)-dependence of \( D_{3,3}^{(s)} \). Pluses: \( s \)-dependence of \( D_{3,3}^{(s)} \).
The Hellmann–Feynman theorem states $\lim_{s \to \infty} D_{n,s}^{(s)} \rightarrow 0$. The result is also shown in Fig. 6 for $(n, \ell) = (3, 5)$ and $(3, 3)$. We see that $D_{n,s}^{(s)}$ rapidly approaches zero with the increase of $s$. This is another support of the assumption of convergence of (5.2).

We have already calculated a classical and periodic orbit with the same energy as the quantum state with $n = 3, \ell = 3$ and the result were shown in Fig. 2. Comparing Fig. 5 with Fig. 2, we see that the region of large amplitude of the wave function resembles the pattern of the region traced by the classical periodic orbit in Fig. 2. This feature reminiscent of the ‘scar’ in the correspondence between classical and quantum mechanics is explained in terms of semiclassical analysis of dephasing and cancelling effect of the paths that can not fulfil the generalized Bohr–Sommerfeld quantization condition. The footings to legitimate understanding of this phenomenon have been provided by Heller (1984), Bogomolny (1988) and Berry (1989b) within the semiclassical theory. (Their works were then followed by a large number of studies on the quantum scars, for which we do not cite references here because they are not directly relevant to our present problem. For scars in a smooth and bounded Hamiltonian system, see, e.g., Santhanam et al. (1997).) The semiclassical approximation is expected to be valid for large quantum numbers. However, regarding the self-cancelling of aperiodic bound motion as a universal quantal phenomenon, the appearance of a precursor of the ‘scar’ even at such small quantum numbers as ones taken here may be rather natural. We deem this as the third check of the validity of our calculation scheme.

6. Spontaneous symmetry breaking

The most striking phenomenon emerges when we take the limit $b \to 0$, in which the Hamiltonian restores the $O(2) - U(1)$ invariance. In this limit, from (3.7) together with (3.11), the symmetry breaking factor in wave function (5.2) survives:

$$\Phi_{\beta_1} (\varphi, \psi) \sim A e^{i\beta_1 \cdot \varphi}.$$

$$\beta_1 = 2 \sqrt{2} |a| \left( |a_1 + \sqrt{a_1^2 + a_2 (2n + \ell)} | \right).$$

The remaining factor generally yields complex azimuthal angle dependences. Owing to $c_{0,3} = c_{0,3}$ on the exponent in (6.1), the symmetry $U(1)$ breaks to $C_3$.

We found this solution by allowing the $U(1)$-breaking factor $\beta' = \beta_1$ in (3.5a) be nonzero even when $b = 0$. In this case, $\beta_1$ is related to the dynamical model parameters as given by (6.1b). We may call this phenomenon the spontaneous symmetry breaking.
More familiar solutions are obtained by requiring $b_1$ be zero and solving (3.6) for arbitrary $j$ and $k$. This is the equation that is derived by separating the variables for the radial and azimuthal degrees of freedom. The arguments proceed in a same way as those given below (3.8) and result in the exactly same eigenvalue equation (3.13). Since the equation is separable, the infinite summation over the angular momentum variable in (5.2b) is not necessary to express the eigenfunctions.

To make the correspondence to the separable case more clear, we write down the eigenvalue equation in terms of the radial and azimuthal coordinates $r$ and $\theta$ as

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} - \frac{\partial^2}{\partial \theta^2} + V(r)\right) \Phi = E\Phi. \quad (6.2)$$

As usual, separating the eigenfunction of the angular momentum, we next write $\Phi = e^{im\theta}R(r)$ to obtain

$$\left(-\frac{d^2}{dr^2} + \frac{d}{rdr} - \frac{m^2}{r^2} - V + E \right) R = 0. \quad (6.3)$$

The energies are labelled by the principal and azimuthal quantum numbers $n$ and $m$. Each level is generally doubly degenerated. The degeneracy two is insufficient to produce the complex azimuthal patterns of the wave functions expected to be observed in the case $b_1 \neq 0$. In order to construct a state with broken symmetry from the solutions of (6.2) and (6.3), we need infinite number of states with distinct $m$'s that are equal modulo $p$ or states with distinct energies that add up to form states which are not the solutions of (6.2).

7. Summary and remarks

We formulated the problem of investigating quantum chaos as an inverse problem. We started with choosing a certain wave function to construct a bounded Hamiltonian with $C_3$ symmetry that shows the classical chaos. We then quantized the system and obtained exact expressions for the algebraic equation that determines the energy levels.

Exact expressions for the levels with small quantum numbers are obtained. Higher levels are calculated numerically. It turned out that the energy spectrum does not depend on the parameter $b$ that governs the breaking of $U(1)$ invariance and is responsible for the emergence of classical chaos.

In spite of chaos exhibited in the classical system, the eigenvalue equation for the quantized system involves no randomness and the level spacing seems to obey Poisson distribution. This is understandable by noting that the energy spectrum does not depend on $b$ and, in the limit $b \rightarrow 0$, the system recovers $U(1)$ and becomes separable.

Our classically chaotic quantum system is marked by the solvability and the Poissonian level distri-
bution, thereby providing a first counter example against the expectation that the level distribution of any classically chaotic system is Poissonian after quantization. These intriguing aspects of our model may be due to the peculiarity of the inverse method employed to construct the simplest class of potential in two dimension.

The iterative method to calculate the wave function of the excited states seems to converge rapidly as long as the model parameters and the low quantum numbers we adopted are concerned. Whether this convergence is assured in the whole parameter space is not known. In particular, the case with $a_1 > 0$ may be problematic because the energy branch (3.14a) does not yield the correct energy $E_0 = -a_1$ for $n = \ell = 0$. We also expect the feature of our model to persist for other $C_3v$ symmetry with $p \geq 4$ provided that the iteration method converges.

**Appendix**

Here, we collect formulae that are used to derive (3.5) in the text. For brevity, we write

$$
\eta_{f'k'} \equiv x^{-f'} L_{f'k'}(x)
$$

(A1)

in (3.4b). Performing differentiations, we have

$$
\partial_0 \partial Y_{j_k} = \sum_{j'_k > j_k > k} \left( \eta_{j_k'k'} + x \eta_{j_k'k'} + (j_k' + k') \eta_{f'k'} + \eta_{f'k'} k' \right) e_{f'k'},
$$

(A.2)

$$
\partial_0 Q = \alpha' + \varphi' \varphi'' + \frac{1}{p} \partial_0 c_{0p} \beta' + \frac{1}{p} \partial c_{0p} \partial_0 c_{0p} \beta'' + \partial_0 Y_{j_k}/Y_{j_k} - \partial Y_{j_k} \partial Y_{j_k}/Y_{j_k}^2,
$$

(A.3)

$$
\partial_0 Q \partial Q = x \alpha'' + \alpha' c_{0p} \beta' + \frac{4}{p} \beta'^2
$$

$$
+ \left( \varphi \partial Y_{j_k} + \varphi' \partial Y_{j_k} \right) \frac{4}{Y_{j_k}} + \left( \partial_0 c_{0p} \partial Y_{j_k} + \partial c_{0p} \partial Y_{j_k} \right) \frac{4}{Y_{j_k}} + \partial_0 Y_{j_k} \partial Y_{j_k},
$$

(A.4)

$$
\partial_0 f Q + \partial f Q = (a_1 + a_2) \left( 2 \alpha' + \beta' c_{0p} + \frac{1}{Y_{j_k}} \left( \varphi \partial + \varphi' \partial \right) Y_{j_k} \right)
$$

$$
+ 2 b \alpha' c_{0p} + \frac{1}{2} b \beta' (\varphi'' \varphi' \varphi^{-1} + \varphi'' \varphi' \varphi^{-1}) + \frac{b}{Y_{j_k}} \left( \varphi'' \partial Y_{j_k} + \varphi' \partial Y_{j_k} \right),
$$

(A.5)

$$
\partial_0 f Q + \partial f Q = (a_1 + a_2) \left( 2 \alpha' + \beta' c_{0p} + \frac{1}{Y_{j_k}} \left( 2 \eta_{f'k'} + \eta_{f'k'} (j_k' + k') \right) e_{f'k'} \right)
$$

$$
+ 2 b \alpha' c_{0p} + b \beta' c_{2p-1} + \frac{b}{Y_{j_k}} \left( 2 \eta_{f'k'} e_{f'k'} c_{0p} + \frac{\eta_{f'k'}}{x} \left( k' c_{f'p+1} + j' c_{f'p+1} \right) \right),
$$

(A.6)
In the above, summations over \( j' (\geq j) \) and \( k' (\geq k) \) are implied. (3.5) is derived by using identities

\[
c_{f+p-k'-1} = \frac{\partial c_{f+k'} \partial}{\partial x}, \quad \phi \phi \phi c_{f+k'} = \phi \phi c_{f+k'} = \phi c_{f+k'}.
\]

(A.7)

together with (A.1)

*This paper had been completed by April 20, 2011 but its publication was delayed due to March 11 earthquake in Japan.

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