Universal relationship between a quantum phase transition and instability points of classical systems

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The direct and universal relationship between the accumulation of exceptional points in the quantum spectrum at a phase transition and the singularity of the classical action at a homoclinic point of the separatrix is investigated. The particular common features are the analytic structure and, related to it, instability and high sensitivity leading generically to the onset of chaos in both cases under perturbation.

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I. INTRODUCTION

The similarities and connections between classical and quantum mechanics have intrigued physicists since the early days of quantum mechanics. The interest was revived about two decades ago when the question about periodic orbits was raised afresh with the progress made in classical chaos. Many investigations have been devoted to the quantum analog of classical chaos; there are textbooks and monographs where important insights have been laid down, for instance in [1–3]. In the present paper a further particular aspect is addressed where quantum and classical behavior have their parallels. It is the singular behavior of the spectrum associated with level repulsion or tunneling, which occurs usually under parameter variation and is encountered especially in situations where chaotic behavior prevails. The singularities considered here are called exceptional points [4]. Whether these singularities always have a classical analog is not obvious. However, in specific cases there appears to be a definite relation between the singular behavior of the quantum spectrum and the singular behavior of the classical action of the associated Hamilton function.

The very nature of a phase transition is always related to a singularity of the energy under the variation of a relevant parameter such as pressure or temperature. A pertinent description, be it classical or quantum mechanical, has to reproduce such behavior. There are, however, so called phase transitions—not in the strict thermodynamic sense—such as in nuclear physics where we deal with finite systems. One major characteristic of such phase transitions is, just as for an infinite system, the change of the mean field often associated with a change of symmetry (symmetry breaking). It is these type of transitions upon which our interest is focused in the present paper.

We argue that the singular behavior of the quantum spectrum is associated with a particular singular behavior of the classical action in typical situations of instability. These classical instabilities are of a universal nature in that the same pattern occurs generically in systems where the onset of chaotic behavior is discernible as soon as a perturbation is switched on. The points of instability are the homoclinic (and heteroclinic) points of a separatrix associated with resonances. We exploit the fact that generically the topological structure near a periodic orbit of a weakly perturbed integrable system is to first order that of a pendulum. In fact, in an integrable system the orbits move on a torus, meaning that the phase space is, under suitable parametrization in action-angle variables, periodic in the angles. A perturbation is then also periodic in the angles and can therefore be written as a Fourier series in the angles, where the individual Fourier terms depend on the actions only; the dominant angle dependence is thus periodic, as there is no angle dependence of the unperturbed system. For sufficiently small perturbations the dependence on the action is dominated by the dependence of the unperturbed Hamiltonian. Near a resonance the motion is essentially characterized by one angle variable with low frequency [5], while the other angle variables vary at a faster rate. They are eliminated by an averaging procedure. This technique is known as the technique of ‘‘removal of resonances’’ [6]. Our starting point is the remaining Hamiltonian near the periodic orbit, which is associated with low frequency and which is that of a pendulum, viz.,

$$H(\Delta J,\Theta)\approx\Delta J^2+b\cos\Theta+\cdots \tag{1}$$

with b being the appropriate coefficient of the Fourier expansion in the slowly varying angle of the perturbing Hamiltonian.

Here H represents the portion of the energy associated with the resonance. Only one periodic orbit remains generically stable under perturbation in the resonance region. As more energy is put into H, the motion vibrates about the periodic orbit. Once sufficient energy is put into H, the trajectories leave the resonance, and are correctly described by the topology of the original integrable system [5]. The separatrix separates these two modes, and our interest is focused upon this characteristic unstable point in phase space.

We contend that the two seemingly different systems—the quantum mechanical phase transition and the homoclinic point of a separatrix—have common features not only under the regular regime, when the separatrix is still intact, but also in their high sensitivity where the onset of chaos manifests itself under a generic perturbation. For illustration a toy model is presented demonstrating how a quantum mechanical phase transition is closely related to the quantum mechanical *and* classical behavior of single particle motion at a point of instability.

In the following section we concentrate upon the generic aspects of these specific classical instabilities and discuss the consequences for the semiclassical spectrum by considering the classical action. Next the essentials of a toy model are reinvestigated and reformulated as a single particle problem with a potential having just the properties addressed in the previous section. A discussion of the onset of chaos is dealt with in Sec. IV and a summary concludes the paper.

II. SEMICLASSICAL TREATMENT OF CLASSICAL INSTABILITIES

We take the discussion of the Introduction as our point of departure and focus our attention upon the instability point of Eq. (1). There the motion is appropriately described by the reduced Hamiltonian

$$h_{\rm cl}=\frac{p^2}{2}-\frac{b}{2}x^2, \quad b>0, \tag{2}$$

around zero energy. Here we have naturally replaced the second order term ΔJ^2 by the kinetic energy $p^2/2$ and $\cos\Theta$ by $x^2/2$. To ensure bounded motion under $h_{\rm cl}$ we consider the interval $-1\leqslant x\leqslant a, a>0$, with elastic reflection at the boundary walls. The dramatic change of the motion of a pendulum from libration to rotation and vice versa is nicely simulated in Eq. (2) by the change from negative to positive energies where the phase space changes from two disconnected regions to a connected region. For the pendulum and, as we show below, for Eq. (2), the period of the periodic orbits has a logarithmic divergence which is reflected in the actions being the key to semiclassical quantization.

Of interest for our purpose is the action

$$J(E)=\oint p\,dx$$

and we obtain for $E<0$ (right hand periodic orbits)

$$J_<(E)=\frac{1}{\sqrt{b}}\left(a^2b\sqrt{1+\frac{2E}{a^2b}}+2E\,\mathrm{arctanh}\sqrt{1+\frac{2E}{a^2b}}\right) \tag{3}$$

and for $E>0$

$$J_>(E)=\frac{1}{\sqrt{b}}\left(b\sqrt{1+\frac{2E}{b}}+a^2b\sqrt{1+\frac{2E}{a^2b}}+2E\ln a\frac{\sqrt{1+2E/a^2b}+1}{\sqrt{1+2E/b}-1}\right). \tag{4}$$

These two functions have a logarithmic singularity at $E=0$. (This is related to the logarithmic divergence at $E=0$ of the period of the periodic orbits.) In fact, the leading term at $E=0$ of the derivative of $J_>(E)$ is $-2(\ln E)/\sqrt{b}$. It is this point of instability related to the metastable equilibrium of a classical particle at $x=0$ that brings about the singular behavior.

When treating the same problem quantum mechanically, one expects a high level density around $E=0$. In fact, looking at the semiclassical spectrum associated with $h_{\rm cl}$ of Eq. (2) it is for by positive energies given by

$$J_>(E_n)=2\pi n\hbar.$$

The same holds for $J_<(E)$ and its left hand orbit analog. The two functions have the same singularity at $E=0$. As a consequence, due to the infinite slope at $E=0$ of $J_>(E)$ and $J_<(E)$, there is a high level density around zero energy. This high level density is characteristic for a quantum phase transition, as it is encountered, for instance, at the transitional points of nuclei [7]. Moreover, for $E<0$, the heap of the potential separating the left from the right hand side invokes tunneling between the quantum levels on the two sides. Tunneling, in turn, is always associated with the occurrence of exceptional points. In short, the quantum spectrum of Eq. (2) has around $E=0$ all the characteristics of a quantum phase transition, that is, (i) a high level density associated with (ii) a high occurrence of exceptional points [8].

We stress the universal aspect of our findings. Resonant behavior of a softly chaotic system near the homoclinic point of a separatrix is locally equivalent to the behavior around zero energy of Eq. (2); the specific singular behavior at $E=0$ is independent of how the potential is modified for $x>0$ or $x<0$, our choice of elastic bounces is simply convenient. The same holds for the quantum behavior around zero energy. Tunneling is always invoked by a finite barrier, in other words, a finite barrier is always associated with a high density of exceptional points. It is therefore expected that the high sensitivity of the classical system under perturbation—recall that the onset of chaos manifests itself immediately at the homoclinic (heteroclinic) points of a separatrix—carries over to a high sensitivity in the transitional region of a quantum phase transition. This sensitivity is due to the presence of the many exceptional points as was demonstrated in [8].

III. THE LIPKIN MODEL

For further demonstration of our general findings we present a particular model. The Lipkin model [9] serves as a prototype model for a phase transition in a quantum mechanical many body system and has been widely used as a paradigm for deformation and/or superconductivity in nuclear physics [7]. Being a soluble model it has all the important properties such as symmetry breaking when sweeping over the transition point. The symmetry breaking can be associated with an appropriate change of a suitable mean field [10].

We briefly recapitulate the gist of the model and then rather concentrate upon the essentials for our specific purpose.

The model assumes two N-fold degenerate levels separated by the energy 1/2 (in suitable units) where the N particles interact by a specific two-body interaction. In terms of the $(N+1)$-dimensional SU(2) generators $J_i, i=x,y,z$, the model is written as

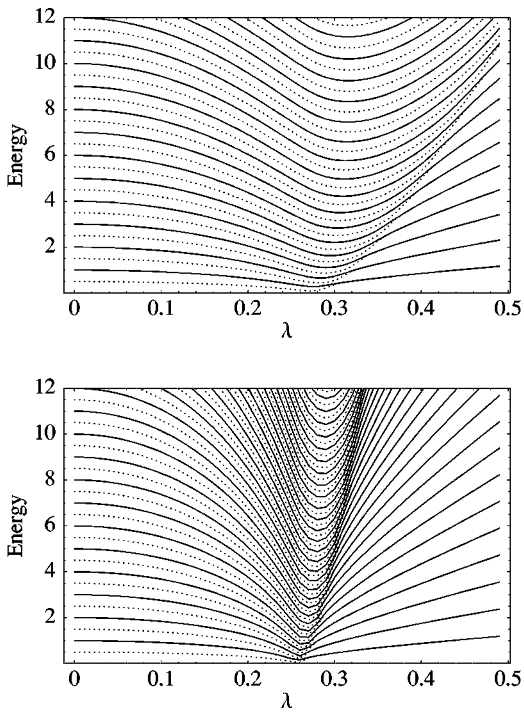

FIG. 1. Spectra of the excited states for $N=100$ (top) and $N=600$ (bottom). The solid (dotted) lines represent the positive (negative) parity states, i.e., the states with an even (odd) number of particle-hole excitations. The units are those of H_0 in Eq. (6) and thus arbitrary.

$$H=H_0-\lambda H_1=J_z-\frac{\lambda}{N}(J_x^2-J_y^2), \tag{5}$$

which, after suitable rescaling, is expressed by the matrices

$$H_0=\frac{k}{2}\delta_{k,k'}, \quad k,k'=0,\ldots,N,$$

$$H_1=\frac{N}{2}\left[1-\left(1-\frac{2k'}{N}\right)^2\right]\delta_{k,k'-1}+\frac{N}{2}\left[1-\left(1-\frac{2k}{N}\right)^2\right]\delta_{k,k'+1}. \tag{6}$$

The model has an internal symmetry, since unperturbed states with an even number of particle-hole excitations do not mix with states of an odd number; the matrices given in Eqs. (6) have been reduced to the even numbers.

In Fig. 1 the excitation spectrum is displayed, setting the ground state level equal to zero for all λ. The figure illustrates the essential aspects of the model, that is, (i) the phase transition[1] at $\lambda\approx 1/4$ and (ii) the type of symmetry breaking for $\lambda>1/4$, in which systematic near-degeneracies occur (not resolvable in the drawing), which can be interpreted as "parity symmetry" breaking when the even and odd numbers of unperturbed ($\lambda=0$) single particle excitations are considered as parity. Note that the transition is the more pronounced the larger the value of N; in particular, at the transitional point the spectrum becomes soft, the more so the larger the particle number N. The spectrum collapses completely for $N\to\infty$. In the vicinity of the transitional point there is a high sensitivity to perturbation [8]. These features can be understood by the high density of exceptional points at the transitional point and their behavior under perturbation [11]. The exceptional points, being square root branch points for finite N, accumulate in the limit $N\to\infty$ at $\lambda=1/4$ and the resulting singularity is then a logarithmic branch point. This was demonstrated in a similar context in [12].

We may view the eigenvalue equation

$$kc_k-\frac{\lambda N}{2}\left[1-\left(1-\frac{2(k+1)}{N}\right)^2\right]c_{k+1}-\frac{\lambda N}{2}\left[1-\left(1-\frac{2k}{N}\right)^2\right]c_{k-1}=Ec_k \tag{7}$$

as the discretized version of a differential equation. Such near-equivalence is the more precise the larger N [13]. Using the near-continuous variable

$$x=\frac{2k}{N}-1$$

we obtain after division by $\lambda N/2$ the differential equation

$$\frac{4}{N^2}\frac{d}{dx}\left((1-x^2)\frac{d}{dx}b(x)\right)+[2(1-x^2)-\kappa(1+x)]b(x)=\frac{2E\kappa}{N}b(x) \tag{8}$$

in the range $|x|\leqslant 1$, where the notation $\kappa=1/\lambda$ is used. With the substitution

$$x=\sin z,$$

$$\psi(z)=\exp\left(-\frac{1}{2}\int^z\tan z'\,dz'\right)b(\sin z),$$

Eq. (8) is transformed into

$$-\tfrac{1}{2}\psi''+\tfrac{1}{2}V(z)\psi=-\tfrac{1}{4}\kappa EN\psi \tag{9}$$

with

$$V(z)=-\frac{\tan^2(z)}{4}-\frac{N^2}{2}\left(\cos^2 z-\frac{\kappa}{2}(1+\sin z)\right) \tag{10}$$

in the range $|z|\leqslant\pi/2$. In deriving Eq. (9) nonsingular terms and terms of lower order than N^2 have been omitted.

The Schrödinger equation Eq. (9) gives, for large values of N, a reliable spectrum of the original problem. The properties of the potential (10) are depicted in Fig. 2. There is a minimum at

[1]It is traditionally called a phase transition also for finite N.

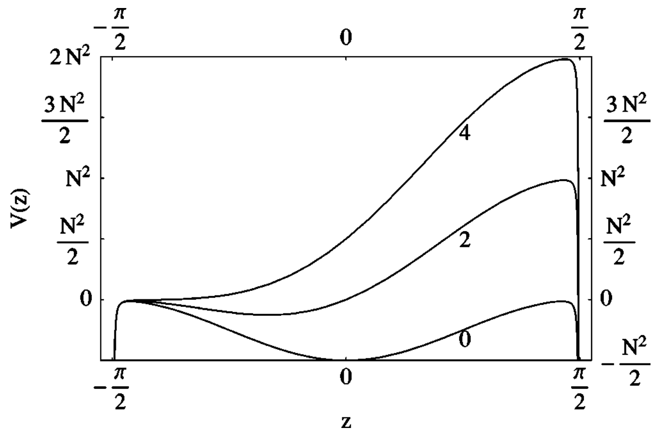

FIG. 2. The single particle potential for various values of κ. Note that the ordinate scales with N^2. As in Fig. 1 the units are arbitrary.

$$z_{\rm min}\approx -\arcsin\frac{\kappa}{4},$$

$$V_{\rm min}\approx -\frac{N^2}{2}\left(1-\frac{\kappa}{4}\right)^2. \tag{11}$$

The minimum becomes flatter when κ increases from zero to 4, where the minimum disappears. There are two pronounced maxima at z values for which $\cos^4 z\approx 1/(2N^2)$, where the potential assumes the values

$$V^{\rm r}_{\rm max}\approx \tfrac{1}{2}N^2\kappa, \tag{12}$$

$$V^{\rm l}_{\rm max}\approx -\left(1-\frac{\kappa}{8}\right)\frac{N}{\sqrt{2}} \tag{13}$$

at the right and left hand maxima, respectively. We use the approximate sign for the relationships as the relations are valid only up to order $1/N^2$. In addition there are second order poles at $z=\pm\pi/2$.

Our attention is focused upon the dependence of the quantum levels on variation of the relative positions, values, and interplay between the minimum and the left hand maximum when $\kappa=1/\lambda$ is varied between zero and infinity. First we note that there is one state denoted by $|\psi_0\rangle$ whose wave function is localized between the left hand singularity of the potential at $z=-\pi/2$ and the left hand maximum at $z=-\arccos(1/\sqrt[4]{2N^2})$. This state has an energy just below $V^{\rm l}_{\rm max}$ and its energy is virtually independent of either κ or N. Next we note that, considering very large values of N, the minimum of the potential is, for $\kappa<\kappa_c=4$, appreciably lower than its maximum. This implies many states being accommodated within the potential mold. These states are pushed out of the mold when κ approaches κ_c. They undergo a level repulsion when they pass the energy associated with $|\psi_0\rangle$. The level repulsions are associated with exceptional points which are square root singularities in the complex κ plane. It is clear from the discussion that a particularly high density of level repulsions and hence exceptional points arises in the vicinity of κ_c; the density of levels within a fixed small window of κ values around κ_c is larger for larger N. For $\kappa<\kappa_c$ the lowest state occurs essentially at $E_0N\kappa/2\approx V_{\rm min}\approx -N^2(1-\kappa/4)^2/2$, i.e., in this range we find $|E_0|/N\sim\lambda$. For $\kappa>\kappa_c=4$ the state of lowest energy is $|\psi_0\rangle$ with an energy that is weakly dependent on κ and N. Remember that $\kappa>\kappa_c=4$ corresponds to the range of interaction strength *before* the phase transition has taken place, while the range $0<\kappa<\kappa_c=4$ corresponds to the region *after* the phase transition has taken place. We recall that in Fig. 1 the ground state energy is set equal to zero before and after the transition point.

In summary, we have demonstrated in the particular case of the Lipkin model how a quantum phase transition is related locally to the behavior of a potential of the type given in Eq. (2) representing generically a classical instability point. For energies around zero Eq. (2) mimics the potential of Fig. 2 for energies around $V^{\rm l}_{\rm max}$. Large values of N^2 in Eq. (10) translate into large values of b in Eq. (2). Variation of κ is emulated by a variation of a.

IV. ONSET OF CHAOS UNDER PERTURBATION

So far we have considered the parallel behavior between the classical instability and the quantum mechanical phase transition under the regular regime (note that $h_{\rm cl}$ is integrable and so is the Lipkin model). Yet the analogy between a transitional point in quantum mechanics and a point of instability of a classical system is upheld also in their respective behaviors under perturbation. It is known [6] that the points of instability—the homoclinic points of a separatrix in phase space—are the points where the onset of chaos manifests itself immediately when a generic perturbation is switched on. It is at these points that the tori associated with the resonances begin to decay first. We understand this from the singularity encountered in the discussion above.

The same holds for the quantum mechanical system at the transitional point. The model considered as an example in the present paper is regular for all values of the interaction strength, i.e., no fluctuations ascribed to quantum chaos occur, including in the transitional region. However, it has been demonstrated [8,11] that even a minute generic perturbation[2] gives rise to the typical fluctuations of the spectrum associated with quantum chaos [14–16]. For large N any small generic perturbation generates a Gaussian orthogonal ensemble (GOE)-type level distribution within the transitional region but leaves the regions outside unaffected. We understand this high sensitivity from the high density of exceptional points at the transition; in particular, it comes as a natural consequence that the sensitivity increases with increasing N.

V. SUMMARY

The close relationship between points of instability—homoclinic points of a separatrix—and the transition point of

[2]The larger N, the smaller the perturbation needed for chaos to occur.

a quantum mechanical phase transition has been shown to be a universal feature and has been demonstrated using a simple model. For the separatrix, there is a typical singular behavior of certain classical quantities (action variable, frequency) and a dramatic change of the type of the motion when switching from inside to outside the separatrix. Under perturbation the onset of chaos manifests itself at these points first. The parallels with the quantum mechanical transition are striking. There is a high density of exceptional points which, in the case of the Lipkin model, becomes a logarithmic branch point in the large N limit. There is likewise a dramatic change of the ground state, i.e., a phase transition, and the transitional region is the most sensitive region to perturbation, leading generically to the typical signature of quantum chaos.

We mention that a semiclassical treatment of tunneling through a potential barrier has been addressed in [17]. The interest was focused in the quoted paper on transition rates and not on the exceptional point connecting two levels, yet the presence of these singularities is quite obvious from the approach. While local aspects of exceptional points are of interest on their own [18], our major point in the present paper is the occurrence of a high density of exceptional points associated with tunneling on a large scale, and the identification of the common origin of these singularities in the classical and quantum mechanical cases.

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