Manifestation of Classical Bifurcation in the Spectrum of the Integrable Quantum Dimer

S. Aubry
Laboratoire Léon Brillouin, CEN Saclay, 91191 Gif-sur-Yvette, France

S. Flach, K. Kladko, and E. Olbrich
Max-Planck-Institute for Physics of Complex Systems, Bayreuther Strasse 40 H.16, D-01187 Dresden, Germany
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We analyze the classical and quantum properties of the integrable dimer problem. The classical version exhibits exactly one bifurcation in phase space, which gives birth to permutational symmetry broken trajectories and a separatrix. The quantum analysis yields all tunneling rates (splittings) in leading order of perturbation. In the semiclassical regime the eigenvalue spectrum obtained by numerically exact diagonalization allows one to conclude about the presence of a separatrix and a bifurcation in the corresponding classical model.

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The problem of correspondence between classical and quantum-mechanical properties of nonlinear systems is currently an object of wide interest [1]. One interesting topic concerns Hamiltonian systems with a given symmetry (e.g., some permutational symmetry), where classical trajectories exist which are not invariant under the corresponding symmetry operation. This topic appears in analyzing selective bond excitation in chemistry and in the quantization of discrete breathers [2].

We consider an integrable system with two degrees of freedom (TDF), whose classical version exhibits exactly one bifurcation (of periodic orbits) and separatrix manifold. This manifold cuts the phase space into three parts—one with invariant trajectories, and two with noninvariant trajectories, where the corresponding symmetry is the permutational one. By varying a single parameter it is possible to "switch" between these phase space parts by crossing the separatrix. It appears natural to expect in the quantum case a drastic change in the splittings of energy levels (which should be zero in the classical limit for the noninvariant phase space parts). However, the splittings are nonzero for any given value of the control parameter. The only way to avoid contradiction between the classical and quantum cases is to assume that the quantum level splittings tend to a steplike function (of, e.g., the level pair number) in the classical limit. The step should occur at the position of the classical separatrix. This problem can be coined also *dynamical tunneling* through a separatrix. There exist studies of the influence of classical chaos on dynamical tunneling [3]. This paper is an extension of previous studies on classical and quantum properties of the dimer system [4–6].

We are able to trace the splittings of the level pairs using *quantum* perturbation methods. We consider the quasiclassical regime and show that the step indeed occurs. Therefore we are able to extract information about the classical separatrix and bifurcation. Further, we show that the quantum density of states (the second integral of motion is fixed) exhibits a sharp maximum at the separatrix energy. By calculating the corresponding classical quantity (with the help of Weyl's formula) we find that this singularity appears due to the integration over a part of the separatrix manifold which includes a hyperbolic isolated orbit.

Let us consider the integrable dimer model with Hamiltonian [4]

$$H = \frac{1}{2}(P_1^2 + P_2^2 + X_1^2 + X_2^2) + \frac{1}{8}[(P_1^2 + X_1^2)^2 + (P_2^2 + X_2^2)^2] + \frac{C}{2}(X_1X_2 + P_1P_2). \quad (1)$$

Here $P_{1,2}, X_{1,2}$ are canonically conjugated momenta and positions of two degrees of freedom. System (1) is integrable, because the classical Poisson bracket of

$$B = P_1^2 + P_2^2 + X_1^2 + X_2^2 \quad (2)$$

with H vanishes. Further (1) is invariant under permutation of indices. In the following we list the classical properties of (1) derived in [4].

With $\Psi = (1/\sqrt{2})(X + iP)$ (1) becomes

$$H = \Psi_1^*\Psi_1 + \Psi_2^*\Psi_2 + \frac{1}{2}[(\Psi_1^*\Psi_1)^2 + (\Psi_2^*\Psi_2)^2] + C(\Psi_1^*\Psi_2 + \Psi_2^*\Psi_1). \quad (3)$$

The equations of motion become $\dot{\Psi}_{1,2} = i\partial H/\partial\Psi_{1,2}^*$.

Isolated periodic orbits (IPO) satisfy the relation $\mathrm{grad}H \parallel \mathrm{grad}B$. Let us parametrize the phase space of (3) with $\Psi_{1,2} = A_{1,2}e^{i\phi_{1,2}}$, $A_{1,2} \geq 0$. It follows $A_{1,2}$ time independent and $\phi_1 = \phi_2 + \Delta$ with $\Delta = 0, \pi$ and $\dot{\phi}_{1,2} = \omega$ time independent. Solving the algebraic equations for the amplitudes of the IPOs we obtain

$$\mathrm{I}: A_{1,2}^2 = \frac{1}{2}B, \ \Delta = 0, \ \omega = 1 + C + \frac{1}{2}B, \quad (4)$$

$$\text{II}: A_{1,2}^2 = \frac{1}{2}B,\ \Delta = \pi,\ \omega = 1 - C + \frac{1}{2}B, \quad (5)$$

$$\text{III}: A_1^2 = \frac{1}{2}B\left(1 \pm \sqrt{1 - 4C^2/B^2}\right),$$

$$\Delta = 0,\ \omega = 1 + B. \quad (6)$$

IPO III corresponds to two elliptic solutions which break the permutational symmetry. IPO III exists for $B \geq B_b$ with $B_b = 2C$ and occurs through a bifurcation from IPO I [4]. The corresponding separatrix manifold is uniquely defined by the energy of IPO I at a given value of $B \geq B_b$. This manifold separates three regions in phase space—two with symmetry broken solutions, each one containing one of the IPOs III, and one with symmetry conserving solutions containing the elliptic IPO II. The separatrix manifold itself contains the hyperbolic IPO I. For $B \leq B_b$ only two IPOs exist—IPO I and II, with both of them being of elliptic character. Remarkably there exist no other IPOs, and the mentioned bifurcation and separatrix manifold are the only ones present in the classical phase space of (1) [4].

To conclude the analysis of the classical part, we calculate the energy properties of the different phase space parts separated by the separatrix manifold. First it is straightforward to show that the IPOs (4)–(6) correspond to maxima, minima, or saddle points of the energy in the allowed energy interval for a given value of B, with no other extrema or saddle points present [4]. It follows

$$E_1 = H(\text{IPO I}) = B + \frac{1}{4}B^2 + CB, \quad (7)$$

$$E_2 = H(\text{IPO II}) = B + \frac{1}{4}B^2 - CB, \quad (8)$$

$$E_3 = H(\text{IPO III}) = B + \frac{1}{2}B^2 + C^2. \quad (9)$$

For $B < B_b$ we have $E_1 > E_2$ (IPO I maximum, IPO II minimum). For $B \geq B_b$ it follows $E_3 > E_1 > E_2$ (IPO III maxima, IPO I saddle, IPO II minimum). If $B < B_b$, then all trajectories are symmetry conserving. If $B \geq B_b$, then trajectories with energies $E_1 < E \leq E_3$ are symmetry breaking, and trajectories with $E_2 \leq E \leq E_1$ are symmetry conserving.

The quantum eigenvalue problem can be properly analyzed in second quantization, which amounts to replacing the complex functions Ψ, Ψ^* in (3) with the boson annihilation and creation operators $a, a^\dagger$ with standard commutation relations [to enforce invariance under exchange $\Psi \Leftrightarrow \Psi^*$ the substitution has to be done after rewriting $\Psi\Psi^* = \frac{1}{2}(\Psi\Psi^* + \Psi^*\Psi)$]:

$$H = \frac{5}{4} + \frac{3}{2}(a_1^\dagger a_1 + a_2^\dagger a_2) + \frac{1}{2}[(a_1^\dagger a_1)^2 + (a_2^\dagger a_2)^2] + C(a_1^\dagger a_2 + a_2^\dagger a_1). \quad (10)$$

Note that $\hbar = 1$ here, so the eigenvalues b of $B = a_1^\dagger a_1 + a_2^\dagger a_2$ are integer numbers. Since B commutes with H, we can diagonalize the Hamiltonian in the basis of eigenfunctions of B. Each value of b spans a subspace of dimension $b + 1$ in the space of eigenfunctions. These eigenfunctions are products of the number states $|n\rangle$ of each degree of freedom and can be characterized by a symbol $|n, m\rangle$, where we have n bosons on site 1 and m bosons on site 2. For a given value b it follows $m = b - n$. So we can actually label each state by just one number n: $|n, b - n\rangle \equiv |n)$. Consequently, the eigenvalue problem at fixed b amounts to diagonalizing the matrix H_{nm} with

$$H_{nm} = \begin{cases} \frac{5}{4} + \frac{3}{2}b + \frac{1}{2}[n^2 + (b-n)^2], & n = m, \\ C\sqrt{n(b+1-n)}, & n = m+1, \\ C\sqrt{(n+1)(b-n)}, & n = m-1, \\ 0, & \text{else}, \end{cases} \quad (11)$$

and $n, m = 0, 1, 2, \ldots, b$. Notice that the matrix H_{nm} is a symmetric band matrix. The additional symmetry $H_{nm} = H_{(b-n),(b-m)}$ is a consequence of the permutational symmetry of H.

For $C = 0$ the matrix H_{nm} is diagonal, with the property that each eigenvalue is doubly degenerated (with exception of the state $|b/2)$ for even values of b). The classical phase space contains only symmetry broken trajectories, with the exception of IPO II and the separatrix with IPO I (in fact, in this limit the separatrix manifold is nothing but a resonant torus containing both IPOs I and II). So with the exception of the separatrix manifold, all tori break permutational symmetry and come in two groups separated by the separatrix. Then quantizing each group will lead to pairs of degenerated eigenvalues—one from each group. There is a clear correspondence to the spectrum of the diagonal ($C = 0$) matrix H_{nm}. The eigenvalues $H_{00} = H_{bb}$ correspond to the quantized IPOs III. With increasing n the eigenvalues $H_{nn} = H_{(b-n),(b-n)}$ correspond to quantized tori further away from the IPO III. Finally the states with $n = b/2$ for even b or $n = (b-1)/2$ for odd b are tori most close to the separatrix. Switching the side diagonals on by increasing C will lead to a splitting of all pairs of eigenvalues. In the case of small values of b these splittings have no correspondence to the classical system properties. However, in the limit of large b we enter the semiclassical regime, and due to the integrability of the system eigenfunctions should correspond to tori in the classical phase space which satisfy the Einstein-Brillouin-Keller quantization rules [1].

Increasing C from zero will lead to a splitting ΔE_n of the eigenvalue doublets of $C = 0$. In other words, we find pairs of eigenvalues, which are related to each other through the symmetry of their eigenvectors and (for small enough C) through the small value of the splitting. Let us calculate the splittings in leading perturbation order. This is done by applying standard perturbation theory to each of the states $|n)$ and $|b - n)$ and calculating the perturbed

eigenvectors until the matrix element of the two perturbed eigenvectors with H does not vanish. Because of the band structure of our matrix the final result has the following form [7]:

$$\Delta E_n = 2 \prod_{i=n}^{b-n-1} H_{i,(i+1)} \prod_{i=n+1}^{b-n-1} (H_{nn} - H_{ii})^{-1}. \quad (12)$$

For even b with $\tilde{n} = n - b/2$ and (11) it follows

$$\Delta E_n = 2C^{2|\tilde{n}|} \frac{(\frac{b}{2} + |\tilde{n}|)!}{(2|\tilde{n}| - 1)!^2 (\frac{b}{2} - |\tilde{n}|)!}. \quad (13)$$

For odd b with $\tilde{n} = n - b/2 + \frac{1}{2}\mathrm{sgn}(n - b/2)$ and (11) we find

$$\Delta E_n = 2C^{2|\tilde{n}|-1} \frac{(\frac{b-1}{2} + |\tilde{n}|)!}{(2|\tilde{n}| - 2)!^2 (\frac{b+1}{2} - |\tilde{n}|)!}. \quad (14)$$

The integer $\tilde{n}$ counts the pairs of equal diagonal elements of (11) from the center of H_{nm} towards the corners [b even: $|\tilde{n}| = 0, 1, 2, \ldots, b/2$ and b odd: $|\tilde{n}| = 1, 2, \ldots, (b + 1)/2$]. Note that for the corner states the obtained expression for the splitting is identical with the results in [5]. Let us define $|\tilde{n}| = \alpha b/2$ with $0 < \alpha < 1$. For fixed α application of Stierling's formula to (13) and (14) yields

$$\Delta E_n \approx \frac{b}{\pi e} \left(\frac{1 + \alpha}{1 - \alpha} \right)^{1/2} \gamma^{\alpha b},$$

$$\gamma = \frac{eC\sqrt{1 - \alpha^2}}{2\alpha(\alpha b - 1)} \left(\frac{1 + \alpha}{1 - \alpha} \right)^{1/(2\alpha)}. \quad (15)$$

For large αb the expression (15) should be close to zero if $\gamma < 1$, and its inverse should be close to zero if $\gamma > 1$. So the perturbation result predicts a steplike change in the splitting values for $\gamma = 1$ in the limit of large αb. The considered asymptotic limit corresponds to the classical limit of (10). Thus we expect that the splittings of the eigenvalue pairs which correspond to symmetry broken classical tori should vanish in this limit. Consequently, the condition $\gamma = 1$ predicts the position of the classical separatrix with respect to the variable α.

Now we calculate the eigenvalue spectrum of (10) numerically (for $b = 20$ this was done in [6]). This was done using standard Fortran routines with double precision. When splittings had to be calculated with values below 10^{-16} we used MATHEMATICA routines, where the precision can be of any value [8]. In Fig. 1 we show the eigenvalues (grouped with respect to their eigenfunctions being symmetric or antisymmetric with respect to permutation) as a function of $\tilde{n}$ for $b = 600$ and $C = 50$. The classical model has symmetry broken trajectories, and a separatrix with energy $E_{\mathrm{sep}} = E_1 = 120\,600$. For the quantum problem we find an inflection point in the eigenvalue spectrum of each subgroup at precisely this energy ($\tilde{n} \approx 150$). Since $\tilde{n}(E)$ is the integrated density of states, its derivative with respect to E gives the density of states $\rho(E)$, which hereby exhibits a peak at the separatrix energy of the classical system

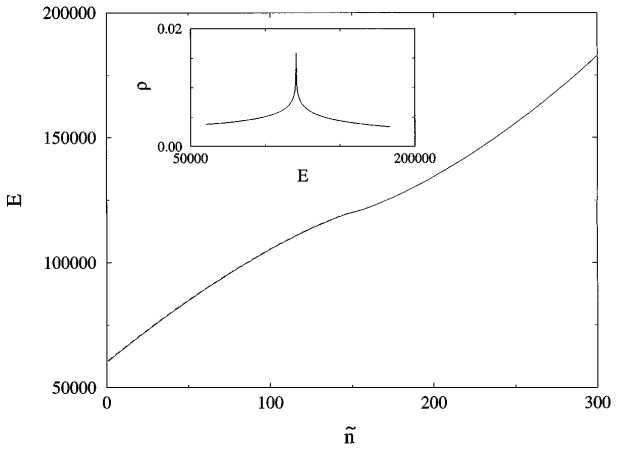

FIG. 1. Eigenvalues of the symmetric eigenstates (solid line) and antisymmetric eigenstates (dashed line) versus quantum number $\tilde{n}$ for $b = 600$ and $C = 50$. Inset: Density of states for the eigenvalue spectrum from above (solid line) versus energy. The dashed line is the classical prediction using Weyl's formula.

(inset in Fig. 1). Using Weyl's formula we can calculate its classical counterpart [1]

$$\rho_{\mathrm{cl}}(E, b) = \int d^2P d^2X \delta(E - H(P, X)) \times \delta(b - B(P, X)). \quad (16)$$

This integral can be rewritten as $\rho_{\mathrm{cl}}(E, b) = \oint 1/(|\nabla H||\nabla B|\sin\Theta) dS$, where the integration is done over the surface of constant H and B and Θ is the angle between the two gradients. The denominator vanishes on IPOs. Expanding the denominator in a Taylor series in the neighborhood of an IPO it follows that for elliptic IPOs no singularity develops (because the torus surface vanishes), whereas for hyperbolic IPOs (i.e., on the separatrix) a logarithmic singularity appears.

By parametrizing the classical phase space using $A_{1,2}$ and $\phi_{1,2}$ the expression (16) can be reduced to a single integral:

$$\rho_{\mathrm{cl}}(E, b) = \frac{1}{\pi} \times \int \frac{dy}{\sqrt{C^2b^2 - 4C^2y^2 - (E - b - b^2/4 - y^2)^2}}. \quad (17)$$

The integration has to be done over all values of y, where the expression under the root is non-negative. This integral shows up with a singularity at the classical separatrix energy. The numerical integration is compared in the inset in Fig. 1 with the quantum density of states. We find excellent agreement. In the inset in Fig. 2 the splittings are shown with respect to $\tilde{n}$. The splittings become anomalously small in the region of

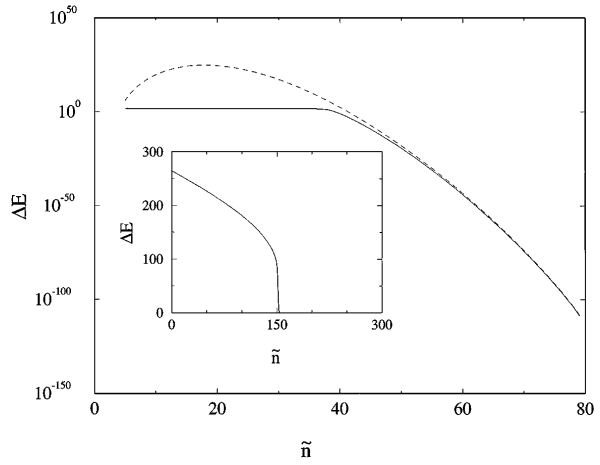

FIG. 2. Eigenvalue splittings versus quantum number $\tilde{n}$ for $b = 150$ and $C = 10$ (calculated with precision 512). Solid line—exact diagonalization, dashed line—perturbation theory result. Note that even for $\tilde{n} \approx 80$ the ratio of both values is of the order of 0.5. Inset: Eigenvalue splittings versus $\tilde{n}$ for $b = 600$ and $C = 50$ (compare Fig. 1) from exact diagonalization. Splittings are of the order of average spacing for $\tilde{n} < 150$ and collapse to zero for $\tilde{n} > 150$.

classical symmetry broken solutions, which is bounded again by the separatrix energy. In Fig. 2 we compare the numerically obtained splittings with the perturbation theory result ($b = 150$, $C = 10$). Even though the true splittings become as small as 10^{-100} compared to the

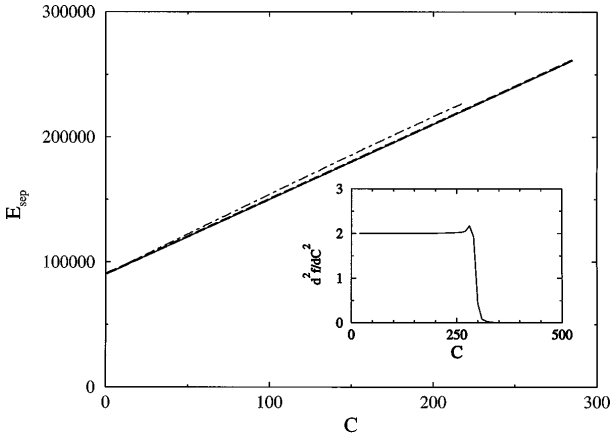

FIG. 3. Separatrix energy versus C for $b = 600$ for the classical system (solid line). The thick long-dashed line is the position of the maximum in the quantum density of states. The thin dash-dotted line is the perturbation theory prediction ($\gamma = 1$). Inset: Second derivative of the C dependence of the maximum eigenvalue of the quantum spectrum for $b = 600$ versus C. The classical prediction is a step function with values 2,0 and step position $C = 300$.

averaged spacings, the perturbation theory reproduces at the best the order of magnitude, but fails by, e.g., 50% in the absolute value. Consequently, we note that higher order terms in the perturbation theory are important even when the true splittings are anomalously small.

Still there is useful information in the perturbation result as shown in (15). In Fig. 3 we show the classical separatrix energy E_1 for different values of C ($b = 600$) and compare it to the peak energy in the quantum density of states *and* to the condition $\gamma = 1$ (which gives us a certain α, which in turn yields a given $\tilde{n}$ and through the numerically obtained quantum eigenvalue spectrum a corresponding energy). First we note the remarkable agreement between the classical curve and the exact quantum counterpart. But even the perturbation theory gives values which deviate by only 6% from the exact result. So while the perturbation theory fails in reproducing the absolute values of the splittings, it still contains the information about a classical separatrix with good precision.

Finally, we can easily trace the classical bifurcation by considering the dependence of the largest eigenvalue of the quantum spectrum as a function of C: $E_{\max} = f(C)$. According to the classical system this function is given by (7) for $C > b/2$ and by (9) for $C < b/2$. Differentiating this function twice with respect to C should thus yield a step function with the step located at $C = b/2$. In the inset of Fig. 3 d^2f/dC^2 is shown for $b = 600$. The step at $C = 300$ is nicely observed.

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