# Classical Resonance Overlapping and Quantum Avoided Crossings

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(Received 24 October 1986)

It is pointed out that for pulsed rotators the classical resonance-overlapping criterion for the onset of chaotic motion implies the existence of avoided crossings among an arbitrarily large number of quantum levels at the classical limit $\hbar$ small, $n\hbar = A$ close to a classical resonance.

PACS numbers: 05.45.+b, 03.65.−w, 05.30.−d

There is currently intense investigation[1] on the so-called "quantum chaos," i.e., the manifestation in quantum mechanics (QM), if any, of the transition from regular to chaotic motion in classical mechanics (CM). A primary candidate for its detection is the stochastic ionization of the H-atom in an intense microwave field,[2,3] because the classical chaotic motions provide the best account so far obtained[4,5] of this phenomenon, which in principle should be best understood in QM.[6–9] A prerequisite for the occurrence of quantum chaos is that the long-time behavior of the system should be sensibly affected. This happens if the spectrum behaves in an irregular way as a function of the coupling constants: in particular, if multiple avoided crossings occur. Therefore the occurrence of this phenomenon has been extensively studied[10–12] in models which classically exhibit the chaotic transition, including the hydrogen photoionization.[13,14] While in CM the transition can be considered well understood through the mechanism of resonance overlapping,[15] which has long been known to yield a simple, but effective, rough estimate of the coupling-constant threshold for its occurrence through the Chirikov criterion,[16] no mechanism has been so far identified in QM which yields at least a similar rough estimate for a global transition in the spectrum, such as multiple avoided crossings, at some critical value of the external parameters.

Here we point out that in semiclassical QM and for the particular case of the pulsed rotators, a coupling-constant threshold for avoided crossings among an arbitrarily large number of quantum levels exists and is the same one predicted by the classical Chirikov criterion. The heart of our argument is precisely to show that the Schrödinger equation can be integrated by the classical algorithm, at least for $\hbar$ small, since it is easier to detect the quantum counterpart of the complexity of the classical motions the closer one works to the classical algorithms developed to describe it.

Consider therefore the pulsed rotator Hamiltonian

$$H_\epsilon(t) = A^2/2 + \epsilon V(\alpha)\cos(\omega t), \tag{1}$$

where $V$ is $2\pi$-periodic in $\alpha$, and $A$ is the conjugate action, or momentum. We prefer to work in the standard time-independent Floquet, or quasienergy, formalism in enlarged phase space: The same motions as (1) are also generated by the two-degree-of-freedom Hamiltonian

$$K_\epsilon = A^2/2 + \omega B + \epsilon V(\alpha,\beta), \tag{2}$$

where also $\beta$ is an angle, and $B$ is the corresponding action. For $\epsilon = 0$ the motions are $\alpha = At$ and $\beta = \omega t$. They are quasiperiodic (and thus regular) with frequencies $A$ and $\omega$, respectively, and can be looked at as free rotations on the two-dimensional torus $\mathbb{T}^2$ labeled by $A$, which can assume all real values, and by $\omega$, which is kept fixed. Any value of $A$ is thus called a torus. If there are integers $(p,q) \neq (0,0)$ such that $Ap + \omega q = 0$, the values $A = A(p,q) = -\omega q/p$ are called resonances, because the rotation frequency is then a rational multiple of the driving one. The resulting motions are therefore periodic. The Kolmogorov-Arnol'd-Moser (KAM) theorem essentially states that, whenever $Ar + \omega s$ does not get too small for any choice of $(r,s) \in \mathbb{Z}^2$ (i.e., if $A$ stays away from resonances) most quasiperiodic motions labeled by $A$ persist for $\epsilon > 0$ small—in particular, most of those lying between two consecutive resonances $A_1$ and $A_2$. However, they are expected to disappear as $\epsilon$ increases beyond a certain value, and the motions to become instead chaotic for such initial conditions.

The Chirikov criterion provides an estimate of the critical $\epsilon$ for the disappearance of all KAM tori between $A_1$ and $A_2$ by the following approximation of $K_\epsilon$. Near any resonance, say $A_1 = A_1(p) = -\omega/p$, we expand the po-

tential in a Fourier series,

$$V(\alpha)\cos\beta=\sum_{r,s=-\infty}^{+\infty}V_{r,s}e^{i(r\alpha+s\beta)}, \tag{3}$$

where $V_{r,s}=V_r(\delta_{s,1}+\delta_{s,-1})$, $V_r$ being the Fourier coefficients of $V(\alpha)$. Then keeping only the primary resonant terms, i.e., extending the sum only to $r=\pm p$ so that $V(\alpha,\beta)=V_p\cos(p\alpha+\beta)$, we perform the linear canonical transformation to $\lambda=(p\alpha-\beta)/2$, $\mu=(p\alpha+\beta)/2$, $L=A/p-B$, and $J=A/p+B$, so that $K_\epsilon$ (written in the new variables) is approximated as follows:

$$K_\epsilon(L,J,\lambda,\mu)\approx K_0(L,J)+\epsilon V_p\cos 2\mu, \tag{4}$$

with $K_0(L,J)=p^2(L+J)/8+\omega(L-J)$. Thus $L$ will stay constant at least to order $\epsilon^2$ (it can indeed be proved[15] that first-order perturbation theory on the "fast" variable $\lambda$, which is simple averaging, amounts to keeping only the resonant Fourier components of $V$). Hence, expanding around $L_1=A_1/p-B_1$ and $J_1=A_1/p+B_1$, where $B_1$ is any constant, and setting $J=J_1+\Delta$, we get the Chirikov quadratic approximation $K_\epsilon\approx$ const $+K_p(\epsilon)$, where $K_p(\epsilon)$ depends only on the "slow" variable $\mu$:

$$K_p(\epsilon)=p^2\Delta^2/8+\epsilon V_p\cos 2\mu \tag{5}$$

(the linear terms vanish because the resonance condition implies $\partial K_0/\partial J_1=0$ at $L=L_1$, $J=J_1$). The approximate Hamiltonian $K_p$ is that of a simple pendulum; its librational motions yield closed orbits in the phase plane $(A,\alpha)$ for any integer value of $2\pi/\omega$, giving rise to the well-known resonance islands. The distance between two consecutive islands is approximated by the distance $\delta A(p)$ between two consecutive resonances, and for $\epsilon$ small enough the islands are separated by the KAM tori. The regular motion will disappear as soon as these KAM tori disappear: This happens when the islands overlap, so that the particle can wander from one island to another, i.e., if the maximum excursion $A^*(\epsilon)$ of $A$ corresponding to the maximum excursion of $\Delta$ along the separatrix of $K_p(\epsilon)$ exceeds $\delta A$. As is well known, one has for the pendulum Hamiltonian $A^*=2p\Delta_{\max}=2(\epsilon V_p)^{1/2}$, so that $A^*/\delta A(p)>1$ if

$$\epsilon>\epsilon_c=\delta A(p)/2V_p^{1/2}, \tag{6}$$

which is the quantitative estimate provided by this resonance-overlapping criterion.

Next, we remark that if (6) holds a short computation shows that there is overlapping also between the corresponding maximum and minimum quasienergies along two consecutive separatrices, given for each integer $p$ by $K_\pm(p)=K_0(A_1(p))\pm\epsilon V_p$; $K_+(p)>K_-(p+1)$ for $\epsilon>\epsilon_c$. Consider the Schrödinger equation for the quasienergy spectrum:

$$S_\epsilon\psi=\left[-\frac{\hbar^2}{2}\frac{\partial^2}{\partial\alpha^2}+\epsilon V(\alpha,\beta)-i\hbar\frac{\partial}{\partial\beta}\right]\psi=E\psi. \tag{7}$$

The eigenvalues of $S_0$ are $E_0=(n\hbar)^2/2+m\hbar\omega$, and can be obtained by Bohr-Sommerfeld quantization of $K_0$ with $E_0(n,m,\hbar)=K_0(n\hbar,m\hbar)$. Look now at the accidentally degenerate levels, defined by all those $n$ and $m$ for which

$$(n+p)^2\hbar^2/2+\omega(m+q)\hbar=(n\hbar)^2/2+\omega m\hbar$$

for some integers $(p,q)\neq(0,0)$. It is easily verified that this relation corresponds to the classical resonance condition $Ap+\omega q=0$ in the classical limit $n\hbar\to A$, $m\hbar\to B$. Hence, the accidentally degenerate levels of $S_0$ can be looked at as coming from the quantization of the resonant actions. This suggests that direct Bohr-Sommerfeld quantization of the Chirikov quadratic approximation, i.e., the formula $E_p(\epsilon)=E_0(p)+E_1(\epsilon)$, with $E_0(p)=K_0(n\hbar,m\hbar)$, $n\hbar=A(p)$, and $E_1(g\hbar,\epsilon)$ implicitly defined by

$$\pm\frac{2}{p}\int_{\chi_-}^{\chi_+}[2(E_1-\epsilon V_p\cos\chi)]^{1/2}d\chi=g\hbar, \tag{8}$$

$$g=1,2,\ldots$$

[$\chi=2\mu$, $\chi_\pm(E_1)$ the classical turning points] should yield a good approximation for the levels that for $\epsilon=0$ are of the above type.

The main point to be understood here is the possibility of identifying and decoupling slow and fast variables in QM near the accidentally degenerate levels. This is precisely what we are going to do, namely, *if* $\hbar\to 0$, $n\hbar\to A$, *and* $Ap+\omega=0$, *then the eigenvalues* $E(n,m,\hbar\epsilon)\equiv E(p)$ *of* $S_\epsilon$ *admit the approximation* $E(p)=E_0+E_1(\epsilon)$ *defined above, up to terms of order* $\epsilon^2$.

The avoided crossings are now a simple consequence of this: The maximum spread in the quantum number $g$ occurs when $E_1$ equals the classical separatrix energy $\epsilon V_p$ of $K_p(\epsilon)$, and correspondingly the maximum and minimum levels in each pack $E(p)$ will be $E_\pm(p)=E_0\pm\epsilon V_p=K_0(A,B)\pm\epsilon V_p$ (with $A,B$ quantized, of course). Therefore when $E_-(p+1)<E_+(p)$, the corresponding packs of levels overlap. This implies overlapping also among all levels emanating from the free ones with actions $n\hbar$ between $A(p)$ and $A(p+1)$, which represent the quantized KAM tori. We remark that these overlappings yield avoided crossings rather than crossings. Apart from the correction of order $\hbar$, the real physical reason seems to be that if $\epsilon$ is larger than the classical threshold the maximum potential of the quantum pendulum near the $p$th resonance is lifted at the minimum potential of the pendulum near the $(p+1)$th one, so that the states in the two wells can start tunneling. This yields a splitting of the order of a barrier penetration, i.e., of order $\exp(-1/\hbar)$. Furthermore, the number of avoided crossings obviously becomes arbitrarily large as $\hbar\to 0$.

Before we give a sketch of the argument (the complete details will appear elsewhere[17]) let us briefly comment upon the limits of validity of the present result. First, it

holds only near the classical limit $\hbar \to 0$, $n\hbar \to A$, where the levels are already very close to each other, and up to a remainder of order $\epsilon^2$, for which a rigorous estimate is not easy to obtain, not to mention convergence. Roughly speaking the problem of the error estimates in the present result is at least as difficult as the corresponding problem in the Chirikov approximation in CM. Accordingly, it is reasonable to expect only a rough estimate of the coupling-constant threshold, valid near the classical limit.

Let us now give a sketch of the argument. To integrate the Hamiltonian (2) we look at the Hamilton-Jacobi equation:

$$\tfrac{1}{2}[\partial W/\partial\alpha]^2+\epsilon V(\alpha)\cos\beta+\omega\,\partial W/\partial\beta=E, \tag{9}$$

for the generating function $W(A,B,\alpha,\beta,\epsilon)$ of the canonical transformation transforming (2) into a function $E(A,B,\epsilon)$ depending only on the actions. Both $W$ and $E$ have to be determined. For $\epsilon=0$, $W_0=A\alpha+B\beta$ generates the identity transformation. Look now for solutions of $S_\epsilon\psi=E\psi$ under the form $\psi=e^{W/i\hbar}$. Then

$$\frac{1}{2}\left(\frac{\partial W}{\partial\alpha}\right)^2+\omega\frac{\partial W}{\partial\beta}+i\frac{\hbar}{2}\frac{\partial^2 W}{\partial\alpha^2}+\epsilon V(\alpha)\cos\beta=E, \tag{10}$$

which reduces to (9) for $\hbar=0$. For $\epsilon=0$ the quantum solution is obviously the classical one at quantized values of the actions, i.e., $W_0=n\hbar\alpha+m\hbar\beta$. Thus we feel free to keep the classical notation in both cases, keeping of course in mind that in QM $A=n\hbar$. We now try to solve (10) recursively through the algorithm of classical perturbation theory assuming the resonance condition $Ap+\omega=0$. We set $E(\epsilon)=E_0+E_1(\epsilon)+E_2(\epsilon)+\ldots$, $W(E,\epsilon)=W_0+W_1(E,\alpha,\beta)+\ldots$ in (10) under the assumption $E_1\ll E_0$, $W_1\ll W_0$, $E_2\ll E_1,\ldots$, justified *a posteriori*. As in the standard derivation of the Chirikov criterion in its simplest form we limit ourselves to first order, i.e., to the determination of $W_1$ and $E_1$. Inserting $E(\epsilon)$ and $W(\epsilon)$ in (10) and expanding we get

$$A\frac{\partial W_1}{\partial\alpha}+\omega\frac{\partial W_1}{\partial\beta}+i\frac{\hbar}{2}\frac{\partial^2 W_1}{\partial\alpha^2}+\frac{1}{2}\left(\frac{\partial W_1}{\partial\alpha}\right)^2+\epsilon V(\alpha)\cos\beta=E_1 \tag{11}$$

since $\partial W_0/\partial\alpha=A$ and $\partial W_0/\partial\beta=B$. To solve (11) look at the Fourier expansion of $W_1$,

$$W_1(E_1,\alpha,\beta)=\sum_{r,s=-\infty}^{+\infty} w_{r,s}^{(1)}e^{ir\alpha+is\beta}, \tag{12}$$

which we divide into the resonant part $S_1$ and nonresonant part $N_1$; $W_1=S_1+N_1$:

$$S_1(E_1,\alpha,\beta)=\sum_{j=-\infty}^{+\infty} w_{pj}^{(1)}e^{i(jp\alpha+j\beta)},$$
$$N_1(E_1,\alpha,\beta)=\sum_{r\neq jp,s} w_{r,s}^{(1)}e^{i(r\alpha+s\beta)}. \tag{13}$$

Accordingly, we split the potential $V(\alpha)$ into its resonant part $V'(\alpha)$ and nonresonant part $V''(\alpha)$. Now the Fourier coefficients of

$$A\,\partial N_1/\partial\alpha+\omega\,\partial N_1/\partial\beta+2^{-1}i\hbar\,\partial^2 N_1/\partial\alpha^2$$

are $i(Ar+\omega s+\hbar r^2/2)w_{r,s}^{(1)}$, $r\neq jp$, and those of

$$A\,\partial S_1/\partial\alpha+\omega\,\partial S_1/\partial\beta+2^{-1}i\hbar\,\partial^2 S_1/\partial\alpha^2$$

are $i\hbar r^2/2$. Modulo a technical condition on $\omega$ and $V_r$ preventing $Ar+\omega s+\hbar r^2/2$, $r=jp$, from becoming too small as $j\to\infty$, we see that in the determination of $N_1$ the quadratic part in (11) can be neglected because the linear terms do not vanish. The Fourier coefficients of $N_1$ will thus be

$$w_{r,s}^{(1)}=-i(Ar+\omega s+\hbar r^2/2)^{-1}V_{r,s},\quad r\neq jp,$$

and the resulting Fourier series is convergent by the above condition. The corresponding first-order quasi-energy correction is zero because $V_{0,0}=0$. $S_1$, however, has to be determined by the quadratic part because the linear terms on the left-hand side of (11) vanish with $\hbar$. Neglecting as in CM all terms with $j\neq\pm1$ in $V'$, we get

$$\frac{1}{2}\left(\frac{\partial S_1}{\partial\alpha}(E_1,\alpha,\beta)\right)^2+i\frac{\hbar}{2}\frac{\partial^2 S_1}{\partial\alpha^2}(E_1,\alpha,\beta)+2\epsilon V_p\cos(p\alpha+\beta)=E_1. \tag{14}$$

Performing now the same canonical transformation used before to decouple slow and fast variables in CM we see that $S_1$ is a function only of $\mu$. With the rescaling of $\mu$, $2\mu=\chi$, and the setting of $R=\exp[ipS_1/\hbar]$, (14) is reduced to the Schrödinger equation for the pendulum,

$$-\tfrac{1}{2}(\hbar p)^2R''(E_1,\chi)+\epsilon V_p\cos(\chi)R(E_1,\chi)=R(E_1,\chi). \tag{15}$$

Since we consider large quantum numbers, the quantized energy correction $E_1$ is given by the WKB formula,

$$\pm\frac{2}{p}\int_{\chi_-}^{\chi_+}[2(E_1-\epsilon V_p\cos\chi)]^{1/2}d\chi=g\hbar, \tag{16}$$
$$g=1,2,\ldots,$$

$\chi_\pm(E_1)$ being the classical turning points. Therefore for all $n\hbar$ close to the classical resonance $A(p)$ the energy levels are to first order $E=E_0(p)+E_1(\epsilon)$, $E_1$ given implicitly by (16), and this concludes the sketch of the argument.

Two of us (S.G. and H.J.S.) acknowledge partial financial support by the National Science Foundation under Grant No. PHY-8502383.

[1]See, e.g., *Chaotic Behavior in Quantum Mechanics*, edited by G. Casati (Plenum, New York, 1984); W. P. Reinhardt, in *The Mathematical Analysis of Physical Systems*, edited by R. Mickens (Van Nostrand, New York, 1984); Proceedings of

the Workshop on Quantum Chaos, Trieste, Italy, 1986, Phys. Scr. (to be published); "Quantum Measurement and Chaos," edited by E. R. Pike (Plenum, New York, to be published).

[2]J. E. Bayfield and P. M. Koch, Phys. Rev. Lett. **33**, 711 (1974).

[3]J. E. Bayfield, C. D. Gardner, and P. M. Koch, Phys. Rev. Lett. **39**, 76 (1977).

[4]R. V. Jensen, Phys. Rev. A **30**, 386 (1984).

[5]K. A. H. van Leeuwen *et al.*, Phys. Rev. Lett. **55**, 2231 (1985).

[6]J. N. Bardsley, B. Sundaram, L. A. Pinnaduwage, and J. E. Bayfield, Phys. Rev. Lett. **56**, 1007 (1986).

[7]G. Casati, B. V. Chirikov, I. Guarneri, and D. L. Shepelyansky, Phys. Rev. Lett. **56**, 2437 (1986); G. Casati, B. V. Chirikov, D. L. Shepelyansky, and I. Guarneri, Phys. Rev. Lett. **57**, 823 (1986).

[8]R. Blümel and U. Smilansky, to be published.

[9]G. Casati, B. V. Chirikov, D. L. Shepelyansky, and I. Guarneri, to be published.

[10]See, e.g., M. V. Berry and R. A. Marcus, in the first work cited in Ref. 1.

[11]T. Uzer, D. W. Noid, and R. A. Marcus, J. Chem. Phys. **79**, 4412 (1983).

[12]T. Uzer and R. A. Marcus, J. Chem. Phys. **81**, 5013 (1984).

[13]G. P. Berman, A. R. Kolowsky, G. M. Zaslavsky, Phys. Lett. **105A** (1984).

[14]R. Blümel and U. Smilansky, to be published.

[15]A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer-Verlag, New York, 1983).

[16]B. V. Chirikov, Phys. Rep. **52**, 263 (1979).

[17]S. Graffi, T. Paul, and H. J. Silverstone, "Resonance Overlapping in Classical Mechanics and Avoided Crossings in Quantum Mechanics," to be published.