Revista Brasileira de Física, Vol. 18, n? 3, 1988

Semiclassical use of Action-Angle Variables in the Presence of Tunnelling

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Recebido em 5 de outubro de 1987

Abstract Semiclassical approximations of quantummechanics are known to be invariant with respect to classical canonical transformations, even though these are not in general isomorphic to unitary transformations in quantum mechanics. However, this rule is not a priori extensive to effects involving tunnelling, since these may be semiclassically small themselves. An important class of canonical transformations brings the system into action-angle variables, which facilitates the study of tunnelling near a classical resonance. We verify computationally that the energy eigenlevels of a resonant system computed in a harmonic oscillator basis are in good agreement with the semiclassical values obtained with the use of action-angle variables.

1. INTRODUCTION

It is well known[1,2] that classical canonical transformation correspond to quantum mechanical transformations which are asymptotically unitary in the limit $\hbar \to 0$. Therefore, in semiclassical problems it is often useful to work with canonical action-angle variables[2,3,4], even though the canonical transformation involved is singular. The problem as to the validity of this procedurearises, however, in cases where there is known to be tunnelling between different parts of classical phase space in the quantized problem. It can then be argued that the semiclassical limit is usually obtained by keeping the lowest terms of a series in powers of $\hbar$, whereas the tunnelling coefficient has an exponentially small dependence on Planck's constant.

The validity of the above criticism becomes less clear when dealing with resonant tunnelling, by which we mean strong tunnelling, such as occurs very close to the barrier top of a double well potential. In this case the deviation of the energy eigenvalues, dwe to tunnelling, from their Bohr-Sommerfeld quantized values, becomes comparable to the level spacing itself. In the limit as $\hbar \to 0$, the n'th level will have an exponentially decreasing tunnelling contribution, but there will always be levels near the barrier top where this effect is large.

This resonant region is of special interest for classical and semiclassical mechanics, in the instance when it arises through the break up of classical invariant tori[2,5]. This is the region where chaotic orbits first appear and it is therefore important to disentangle their effect on the semiclassical spectrum from that of tunnelling.

Through the method of normal forms[2], it becomes possible to study approximations of the resonance which elirninate the chaotic orbits. The normal forms arise in action-angle variables, so it is important to resolve the question as to their valid use in this context. This was presumed in a previous paper[6], which calculated the effect of tunnelling in a resonant normal form. Our purpose here is to show that the same results can be obtained in this simple case by diagonalizing the Hamiltonian matrix in a harmonic oscillator basis.

In section 2 we present the resonant normal form Hamiltonian and explain its general use in the context of classical dynamics. This is quantized both exactly and semiclassically in section 3. Here we will not explicitly use the tunnelling theory previously developed[6], since there it was found that the same results were obtained by diagonalizing a semiclassical matrix. Finally we present and discuss our numerical results in section 4.

2. RESONANT NORMAL FORMS

Consider a conservative autonomous dynamical system with two degrees of freedom and a point of stable equilibrium at the origin. The Hamiltonian can then be expanded in a Taylor series

$$H(\vec{p},\vec{q}) = \omega_1\left(\frac{p_1^2+q_1^2}{2}\right) + \omega_2\left(\frac{p_2^2+q_2^2}{2}\right) + \sum_{\alpha+\beta=3}^{\infty} k_{\vec{\alpha},\vec{\beta}}\, q_1^{\alpha_1}\, q_2^{\alpha_2}\, p_1^{\beta_1}\, p_2^{\beta_2} \quad (1)$$

Through the complex canonical transformation

$$\vec{a} = \frac{1}{\sqrt{2}}\,(\vec{p}+i\vec{q}) \quad , \quad \vec{a}^* = \frac{1}{\sqrt{2}}\,(\vec{p}-i\vec{q}) \quad , \quad (2)$$

we bring this into the form

$$H'(\vec{a},\vec{a}^*) = \omega_1(a_1.a_1^*) + \omega_2(a_2.a_2^*) + \sum_{\vec{\alpha}+\vec{\beta}=3}^{\infty} k'_{\vec{\alpha},\vec{\beta}}\ a_1^{\alpha_1}\ a_2^{\alpha_2}\ a_1^{*\beta_1}\ a_2^{*\beta_2} \qquad (3)$$

According to a theorem by Birkhoff[1,2], it is usually possible to eliminate higher order terms of the series eq. (3), by means of successive canonical transformations, so as to obtain the normal form

$$H(\vec{a},\vec{a}^*) = \omega_1(a_1.a_1^*) + \omega_2(a_2.a_2^*) + b_{4,0}(a_1.a_1^*)^2 + b_{2,2}(a_1.a_1^*)(a_2.a_2^*) + \ldots +$$

$$+ b_{0,2N}(a_2.a_2^*)^N + \sum_{\vec{\alpha}+\vec{\beta}=2N+1}^{\infty} k_{\vec{\alpha},\vec{\beta}}\ a_1^{\alpha_1}\ a_2^{\alpha_2}\ a_1^{*\beta_1}\ a_2^{*\beta_2} \qquad (4)$$

Generally, the remainder of the normal form cannot be eliminated, i.e. the full normal form series does not converge. Also, we must keep further terms in the series if (ω_1/ω_2) is very close to a rational number. If

$$\omega_1/\omega_2 = s/r + h \qquad (5)$$

where s and r are mutually prime integers, we then obtain the *resonant normal* form

$$H(\vec{a},\vec{a}^*) = \omega_1(a_1.a_1^*) + (a_2.a_2^*) + b_{4,0}(a_1.a_1^*)^2 + \ldots + \alpha\left[a_1^r.a_2^{*s} + a_1^{*r}.a_2^s\right] + O(\vec{a}^{r+s+1}) \qquad (6)$$

Going over to action-angle variables, by means of the canonical transformation

$$a_j = \sqrt{I_j}\ \exp(i\phi_j) \quad , \quad a_j^* = \sqrt{I_j}\ \exp(-i\phi_j) \ , \qquad (7)$$

the truncated Hamiltonian takes the form

$$H(\vec{I},\vec{\phi}) = \omega_1 I_1 + \omega_2 I_2 + b_{4,0} I_1^2 + \ldots + \alpha(I_1^r.I_2^s)^{1/2}\cos(r\phi_1 - s\phi_2) \qquad (8)$$

Finally, the linear canonical transformation $(\vec{I},\vec{\phi}) \to (\vec{J},\vec{\theta})$

$$I_1 = rJ_1 \qquad \theta_1 = r\phi_1 - s\phi_2$$
$$I_2 = J_2 - sJ_1 \qquad \theta_2 = \phi_2 \quad , \qquad (9)$$

brings the Hamiltonian into the form

$$H(\vec{J},\vec{\theta}) = \omega_2.(J_2+r\lambda J_1) + r^2 b_{4,0} J_1^2 + \ldots + \alpha(r\, J_1)^{r/2}(J_2-sJ_1)^{s/2}\cos\theta_1 \qquad (10)$$

This approximate Hamiltonian is independent of the angle θ_2. It follows that J_2 is an independent constant of the motion, such that the Poisson bracket $\{H,J_2\} = 0$. So the motion is integrable, i.e. there are no chaotic orbits[2]. These can only appear when we include the higher order terms, which have been neglected in eq. (6). Almost all orbits in phase space are therefore bound to invariant tori. However, not all these tori belong to the same family.

We have studied the typical case where $\omega_2 = 1$ and $\omega_1 = \frac{1}{6} - \lambda$ (in this instance, $b_{4,0} \neq 0$ and the other b_{ij}'s = 0). Fig.1 shows level curves of the Hamiltonian for a fixed value of J_2. The closed curves depicted are the sections of invariant tori. They come in two families: The *rotations* extend from $\theta_1 = 0$ to $\theta_1 = 2\pi$; they are centred on the origin, here extended into the $J_1 = 0$ axis. The *librations* or island tori are centred on stable periodic orbits. The two families of tori are bounded by the *separatrices* or *unstable manifolds* emanating from unstable periodic orbits. The existence of pairs of periodic orbits, arising from the perturbation of a single family of tori, is a consequence of the Poincaré-Birkhoff theorem[1]. The resonant region is that of the island tori.

3. QUANTIZATION

If all the tori in the classically integrable system belonged to a single family, the eigenenergies would be well approxirnated by improved versions of the Bohr-Sommerfeld quantization rules[2]. These are canonically invariant, so they would cover the quantization of all the systems (1) which can be transformed into the hamiltonian eqs. (8) or (10). But the eigenlevels of eq. (10) for a fixed value of J_2, are

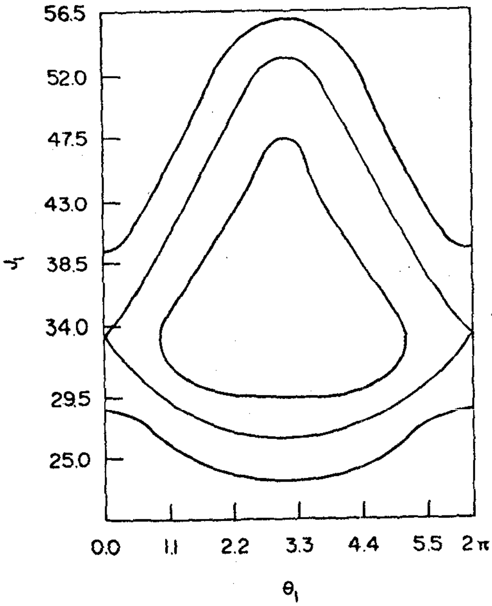

Fig.1 - Level curves of the classical Hamiltonian eq. (10) for the same constants as used for calculating energy levels in table 1.

strongly dependent on tunnelling, according to previous work[6]: there is internal tunnelling of the thin island tori (the motion may skip a turn in the θ_2 windings by jumping across the separatrix) and there is tunnelling between the tori which envelop the resonance.

The results of the tunnelling theory for systems with one degree of freedom, in the aforementioned analysis, were found to be in excellent agreement with those obtained by diagonalizing the semiclassical matrix

$$\langle \ell|\hat{H}|g\rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta_1\ H(\vec{J}_{\frac{\ell+g}{2}},\theta_1)\exp\left[i(\ell-g)\theta_1\right] \quad , \qquad (11)$$

which can be derived from the Wigner-Weyl representation[7]. These are just the matrix elements for a single Isolated block of the full Hamiltonian matrix, which may be considered separately because of classical integrability: for each quantized eigenvalus of J_2, we have a different block. The semiclassical eigenenergies thus obtained are also canonically invariant, i.e. all classical systems with the same normal form will correspond to the same quantized energy levels - provided that it is valid to use action-angle variables in the presence of resonant tunnelling.

It may not be possible to verify completely the validity of the semiclassical matrix (11). Fortunately it is easy to do so in the simple case when the Hamiltonian eq. (3) already has the form eq. (4), without requiring any intermediate transformation. The quantization of eq. (2) can then be interpreted as the definition of the creation and annihilation operators $\hat{\vec{a}}^{+}$ and $\hat{\vec{a}}$ from the standard coordinate and momentum operators:

$$\hat{\vec{a}} = \frac{1}{\sqrt{2}}\,(\hat{\vec{p}}+i\hat{\vec{q}}) \quad , \quad \hat{\vec{a}}^{+} = \frac{1}{\sqrt{2}}\,(\hat{\vec{p}}-i\hat{\vec{q}}) \quad . \tag{12}$$

They obey the commutation relation

$$[\hat{a}_j,\hat{a}_k^{+}] = \hbar\,\delta_{j,k} \quad . \tag{13}$$

The corresponding hamiltonian opetator is then just the polynomial

$$\hat{H} = \omega_1(\hat{a}_1^{+}\hat{a}_1+\frac{\hbar}{2}) + \omega_2(\hat{a}_2^{+}\hat{a}_2+\frac{\hbar}{2}) + b_{4,0}[(\hat{a}_1^{+}\hat{a}_1)^2 + \hbar(\hat{a}_1^{+}.\hat{a}_1) + \frac{\hbar^2}{4}] + \ldots +$$
$$+ \frac{\alpha}{2}\,(\hat{a}_1^{+r}\hat{a}_2^{s} + \hat{a}_1^{r}.\hat{a}_2^{+s}) \tag{14}$$

Using the harmonic oscillator representation $|n_1, n_2>$, such that

$$\hat{a}_1|n_1,n_2> = \sqrt{\hbar\,n_1}\,|n_1-1,n_2> \;,\; \hat{a}_1^{+}|n_1,n_2> = \sqrt{\hbar(n_1+1)}\;|n_1+1,n_2> \tag{15}$$

with similar expressions for n_2, we obtain the Hamiltonian matrix

$$<n_1,n_2|\hat{H}|n_1',n_2'> = [\omega_1\hbar(n_1+\frac{1}{2}) + \omega_2\hbar(n_2+\frac{1}{2})$$
$$+ b_{4,0}\;\hbar^2(n_1^2+n_1+\frac{1}{4}) + \ldots]\;\delta_{n_1,n_1'}.\delta_{n_2,n_2'}$$
$$+ (\frac{\alpha}{2}\,\hbar^{(\frac{r+s}{2})})\,[(n_1+1)\ldots(n_1+r)n_2\ldots(n_2-s+1)]^{1/2}\delta_{n_1,n_1'-r}\,\delta_{n_2,n_2'+s} + \text{h.c.} \tag{16}$$

where h.c. stands for the hermitian conjugate term.

The Hamiltonian is nondiagonal in this representation, which means that it does not commute with either of the oscillators used in the basis. However it can be easily verified that the Hamiltonian does commute with the operator

$$\hat{J}_2 = \frac{1}{r}\,(s\,\hat{a}_1^{+}\hat{a}_1 + r\,\hat{a}_2^{+}\hat{a}_2)\ , \tag{17}$$

corresponding to the classical action J_2 within a small constant. Thus J_2 is an integral of the motion, just as in classical dynarnics. By transforming the base to eigenstates of J_2, we can then reduce the Hamiltonian matrix to a block structure and hence consider the eigenvalues of individual blocks.

To do this we define the operator

$$\hat{J}_1 = (\hat{a}_1^{+}\hat{a}_1)/r\ , \tag{18}$$

also in accordance with eq. (9). Identifying the eigenvalues of $\hat{J}_1$ and $\hat{J}_2$ as $n\hbar$ and $m\hbar$ respectively, we then have the relation between quantum numbers

$$n_1 = rn\ ,\ n_2 = m-sn \tag{19}$$

Thus, defining the states

$$|n,m\rangle = |n_1(n,m),n_2(n,m)\rangle\ , \tag{20}$$

we obtain the hamiltonian matrix

$$\langle n|\hat{H}|n'\rangle_m = \{\hbar\omega_2[\lambda(rn+\tfrac{1}{2}) + \frac{s}{2r} + m + \tfrac{1}{2}] + b_{4,0}\,\hbar^2.[r^2n^2+rn+\tfrac{1}{4}]\}.\,\delta_{n,n'}$$
$$+ \left\{\frac{\alpha\hbar}{2}^{(\frac{s+r}{2})}\right\}\ .\ [(rn+1)\ .\ \ldots\ .\ (rn+r).(m-sn)\ .\ \ldots\ .\ (m-s(n+1)+1)]^{1/2}$$
$$\delta_{n,n'-1} + h.c. \tag{21}$$

for each fixed m. The number n need not be an integer - for eq.(19) to provide all the integers n_1, n has to be a rational number j/r. Let $j = n_0 < r$; then the Hamiltoniam matrix (21) only couples $|n_0/r,m\rangle$ to other states $|N+n_0/r,m>$, where N is an integer. The conditions for n_2 to be an integer now requires that $m = M-sn_0/r$, where M is also an integer.

In any case, for each (fractional) m we obtain a unique block of the Hamiltonian matrix. Each block is tridiagonal and, though infinite, the lower eigenvalues in n can be computed precisely by truncating the block.

The main purpose of this work is to compare the eigenvalues of a block of the exact Hamiltonian matrix (21) with those of the semiclassical Hamiltonian matrix (11). Each element of the latter has to be computed with J_2 and J_1 fixed at half their quantized values:

$$J_1 = \frac{\hbar}{r}\,(n_1+\frac{1}{2}) \quad , \; J_2 = \hbar\left[\frac{s}{r}\,(n_1+\frac{1}{2}) + (n_2+\frac{1}{2})\right] \; . \qquad (22)$$

Again we get a block structure for eq. (11), with each block in the form

$$<n|\hat{H}|n'> = \{\hbar\omega_2\left[\lambda(rn+\frac{1}{2}) + \frac{s}{2r} + m + \frac{1}{2}\right] + b_{4,0}\,\hbar^2(r^2n^2+rn+\frac{1}{4})\}\delta_{n,n'}$$
$$+ \left(\frac{\alpha\hbar^{(\frac{s+r}{2})}}{2}\right) \cdot \left[(m+\frac{s+r}{2r}) - (\frac{n+n'}{2}+\frac{1}{2r})\right]^{s/2} \cdot \left[r(\frac{n+n'}{2}+\frac{1}{2r})\right]^{r/2} \cdot \delta_{n,n'-1} + \text{h.c.}$$
$$(23)$$

Thus the approximate semiclassical matrix, whose eigenvalues are known to coincide with those provided by tunnelling theory, has the same diagonal elements as the exact matrix, but quite different off-diagonal elements.

4. COMPUTATIONAL RESULTS

The eigenvalues for the semiclassical and the exact Hamiltonian matrix have been computed near a sixth order resonance. The corresponding classical motion whould therefore be typical of resonances whose order is greater than four[2]. The sixth order resonance has, however, some computational advantages which were used in reference 6. Thus we have

$$\omega_1 = \frac{1}{6} - \lambda \ , \quad \omega_2 = 1 \quad , \tag{24}$$

Otherwise the choice of pararneters was

$$\lambda = 6^{-3} \ , \quad \alpha = 6^{-13} \quad , \quad b_{4,0} = 6^{-6}/2 \tag{25}$$

and all other coefficients b_{ij} were chosen to be zero. The further choice of

$$\hbar = 0.9917 \tag{26}$$

and the constant action

$$J_2 = \hbar(6^4 + \frac{1}{12}) \tag{27}$$

brought the resonant energy of the unperturbed system (with $\alpha = 0$) to $E = 1284.83$. It is near this energy that the effect of tunnelling becomes important. In table 1 we have subtracted out the term $\omega_2 J_2$ from the Hamiltonian, so the resonant energy becomes $E = -0.475292$ ($\alpha \neq 0$). Thus the resonant classical energy is close to the fifteenth quantum energy level. For this reason we only exhibit the thirty lowest levels, for which convergence was obtained by truncating the matrix at 80×80.

In general we obtain an agreement between the semiclassical levels and the levels of the exact matrix to within an order of 10^{-6}, whereas the spacing for this block is of order 10^{-3}. This contrasts strongly with the situation for Bohr-Sommerfeld quantization, which was found[6] to be in error by the same order of magnitude as the level spacing in the resonant energy. The lowest computed levels are in good agreement with the Bohr-Sommerfeld levels, corresponding to islands surrounding the stable periodic orbit.

6. CONCLUSION

Though we have not tested the effects of making further canonical transformations on the eigenvalues of the Hamiltonian, we have verified that the singular transformation to action-angle variables does not significantly alter the eigenenergies in the classically re-

Table 1 - 30 lowest levels of the Hamiltonians eqs. (14) and (23), with constants specified by eqs. (24)-(27).

a) Exact Matrix	b) Semiclassical Matrix
- 0.528903	- 0.528906
- 0.524276	- 0.524278
- 0.519769	- 0.519772
- 0.515386	- 0.515388
- 0.511131	- 0.511133
- 0.507006	- 0.507008
- 0.503018	- 0.503019
- 0.499171	- 0.499172
- 0.495473	- 0.495474
- 0.491933	- 0.491934
- 0.488563	- 0.488563
- 0.485377	- 0.485377
- 0.482409	- 0.482409
- 0.479634	- 0.479634
- 0.477472	- 0.477471
- 0.474582	- 0.474582
- 0.474067	- 0.474056
- 0.469234	- 0.469233
- 0.469182	- 0.469182
- 0.462897	- 0.462896
- 0.462812	- 0.462811
- 0.455590	- 0.455590
- 0.455457	- 0.455457
- 0.447410	- 0.447410
- 0.447216	- 0.447215
- 0.438403	- 0.438403
- 0.438134	- 0.438134
- 0.428597	- 0.428597
- 0.428240	- 0.428240
- 0.418011	- 0.418011

sonant region. In this region tunnelling is a strong effect, wherefore the evidence is that it is legitimate to use action angle variables in the study of resonant tunnelling.

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Resumo

Sabe-se que aproximação semiclássica da Mecânica Quântica são invariantes com relação a transformações canônicas clássicas, apesar de estas não serem em geral isomorficas a transformações unitárias em Mecânica Quântica. No entanto, esta regra não é a priori extensível a efeitos envolvendo tunelamento, já estes próprios efeitos podem ser semiclassicamente pequenos. Uma classe importante de transformações canônicas traz o sistema-para variáveis de-ação-angulo, o que facilita o estudo de tunelamento próximo a uma ressonancia clássica. Verificamos numericamente que os níveis de auto-energias de um sistema ressonante calculados em uma base de oscilador harmônico estão em bom acordo com os valores semiclássicos obtidos através do uso de variáveis de ação-ângulo.