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CLASSICAL PROPERTIES AND SEMICLASSICAL CALCULATIONS IN A SPHERICAL NUCLEAR AVERAGE POTENTIAL

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Résumé - Nous étudions la relation entre les propriétés classiques d'un potentiel nucléaire moyen et ses propriétés spectrales. Nous avons tracé la surface d'énergie-action de ce potentiel et relié ses propriétés à celles du spectre dans le cadre de la méthode semi-classique EBK. Nous décrivons aussi une méthode permettant d'obtenir l'évolution du spectre en fonction du nombre de masse.

Abstract - We study the relation between the classical properties of an average nuclear potential and its spectral properties. We have drawn the energy-action surface of this potential and related its properties to the spectral ones in the framework of the EBK semiclassical method. We also describe a method allowing us to get the evolution of the spectrum with the mass number.

I - INTRODUCTION

This work is part of a study regarding classical dynamics of an average nuclear potential and their relation, in the frame of EBK method /1/, with the quantum properties of this potential. Certain of these properties will appear naturally as a consequence of the dynamics of the underlying classical systems. This is the case, for example,of the spectral properties (degeneracy, anharmonicities) which can be related in a transparent way to the classical dynamics when it is described in the action-angle variables.

The potential considered is a slightly modified version of the Saxon-Woods one in order to avoid the singularity at r = 0 which is unsuitable for a classical treatment. It was introduced in /2/ and is written

$$V(r) = - V_o \frac{Ch \frac{R}{a} + 1}{Ch \frac{R}{a} + Ch \frac{r}{a}} \qquad (1)$$

The parameters of the problem are $\lambda = \frac{R}{a}$ which measures the size of the nucleus and $\eta = 1+(E/V_o)$.The relation between R and the mass number A is given by $R=r_oA^{1/3}$ and we fix the values a = 0.65 fm, r_o = 1.26 fm and V_o = 52 MeV.

We have also introduced an ellipsoidal deformation, and a new parameter μ with it, by the change

$$\frac{r}{a} \longmapsto \lambda \sqrt{x^2+y^2 + \left(\frac{z}{\mu}\right)^2}$$

By doing this we have shown /3,4,5/ that the potential loses its integrability and the particle may wander chaotically in the regions of the phase space of which the size depends strongly on the three parameters of the problem : λ,μ,η.

In this paper, however, one will only be concerned with the simplest case : that is the spherical integrable case ($\mu = 1$) which needs to be understood fully before considering the non integrable situation.

II - EBK QUANTIZATION OF INTEGRABLE HAMILTONIANS

It is well known /6/ that the phase trajectories of an hamiltonian dynamical system, integrable in the Liouville sense, lie in a N-dimensional manifold M which is diffeomorphous to a torus. If $C_1,\ldots,C_2$ are N irreductible and independent contours on M we can associate with each phase trajectory the N quantities defined by

$$I_i = \frac{1}{2\pi} \cdot \oint_{C_i} \sum_{\alpha=1}^{N} p_\alpha . dq_\alpha \qquad (2)$$

We can also choose a certain parametrisation on M, $\{\phi_1 \ldots \phi_N\}$ in such a way that $\{ I_1,\ldots I_N,\phi_1,..,\phi_N\}$ is a set of canonical coordinates with the very interesting property that the hamiltonian, when expressed in these coordinates, depends only on Is. The quantities I and ϕ are called respectively action and angle variables.

For a given energy E, the actions are not independent but must satisfy the equation

$$H(I_1,\ldots I_N) - E = 0 \qquad (3)$$

We thus define a N-dimensional surface in the $(E,I_1,..,I_N)$ space : the energy-action surface (EAS). Each trajectory is represented by a point on this surface and all the dynamics of the system is contained on it.

In the case of a single particle in a spherical potential V(r), the usual angular actions I_θ and I_ϕ /7/ appear in the hamiltonian only via their sum. This allows us to reduce the EAS to a bidimensional one by defining a new action $I_L = I_\theta + I_\phi$ which must be identified with the classical angular momentum l_C. We can therefore represent this surface in the 3-dimensional space (E,I_r,I_L). Its equation $E = H(I_r , I_L)$ is implicitly given in the definition of the radial action :

$$I_r = \frac{1}{2\pi} \cdot \oint_{C_r} p_r(r;E,I_L)dr \qquad (4)$$

which is nothing but the volume of the radial phase space accessible to the particle for a given energy and angular momentum.

The EBK method consists in looking for the trajectories the actions of which satisfy

$$\begin{aligned} I_r &= (n_r + \tfrac{1}{2})\hbar \qquad & n_r &= 0,1,2,\ldots \\ I_L &= (L + \tfrac{1}{2})\hbar \qquad & L &= 0,1,2,\ldots \end{aligned} \qquad (5)$$

The energies of these "quantum" trajectories are either the same or slightly different from the eigenvalues of the Schrödinger equation. Usually this semiclassical method is understood as an approximate means of calculating a spectrum. Nevertheless if we take into account the fact that the scattered quantum trajectories are in fact part of a continuum (the EAS) we can also expect that the properties of the spectrum could be interpretated and, in a certain sense, understood through the properties of this continuum. In fact to solve /5/ merely means choosing a lattice in the action-surface and searching the image of this lattice in the purely classical energy surface : it is the properties of this surface which will therefore determine those of the spectrum.

III - APPLICATION TO THE NUCLEAR AVERAGE POTENTIAL

We have studied the EAS associated with the average nuclear potential (1). In order to make the study of its properties easier, this surface will be represented either by its sections η = cte ($I_r = F_\eta(I_L)$ or I_L = cte ($I_r^L(\eta)$). All the actions are given in $\hbar$ units.

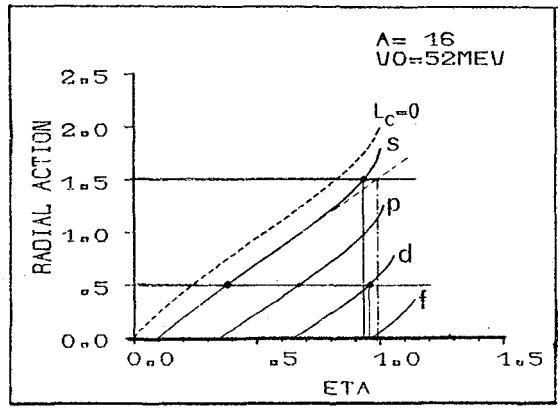

Fig. 1 - Radial action versus energy (η) for A = 16

	η_Q	η_{SC}	$\Delta\eta$
1s	.3733	.3756	.61
1p	.6534	.6683	2.28
2s	.9149	.9301	1.66
1d	.9271	.9515	2.63

Table I - Comparison between quantum (η_Q) and EBK semiclassical energies for A = 16.

$$\Delta\eta = \frac{\eta_{SC} - \eta_Q}{\eta_Q} \times 10^2$$

Figure 1 shows the results for A=16. It shows the $I_r^L(\eta)$ sections for the values L = 0,1,2,3 defined in (5). The dotted line corresponds to $I_L = 0$ and, therefore, does not contain any quantum trajectory. We notice the remarkable linearity of these sections except, perhaps, at the extreme $\eta \simeq 1$ where the slope increases greatly. The EBK spectrum is obtained by making the intersection of these curves with the straight lines $I_r = n_r + \frac{1}{2}$. There are only 4 bound states and the semiclassical energies thus obtained (η_{SC}) are given in Table I. They are compared with the exact quantum results (η_Q) which we have calculated by using the Numerov-Cooley method /8/.

The linearity of a section, the S-section for example, is related to the harmonicities of the S-states in the spectrum. If we consider all of these sections we see that it is their relative position which explains the formation of the multiplets. The degeneracies of the harmonic oscillator (H.O.) would be obtained with linear, parallel and equidistant sections, the distance between them being determined by their common slope ($1/2\hbar\omega$). This is what happens for A = 16 as a good approximation. The difference, that is the way in which an H.O. multiplet splits, is explained by the different curvature of the sections at the energy of the multiplet : the 2 s state which is situated below the 1d state would be situated above it if the corresponding radial action was linear in this region.

The curvature of a given L-section is therefore manifested either by a compression of the L-spectrum, when the slope increases, or by a dilatation in the opposite case. We can easily understand this fact by realizing that the slope of an L-section is related to the classical radial frequency ω_r^L by.

$$\frac{d}{d\eta}\left(\frac{I_r^L}{\hbar}\right) = \frac{1}{\hbar\omega_r^L} \qquad (6)$$

and that the level spacing is given approximatively by $\Delta E = \hbar\omega_r^L$. We can also see that it is these curvature properties which explain both the gaps and the order of levels when an H.O. multiplet splits. Obviously this curvature is related to the potential in a more or less direct way. In our case it is the effect of the asymptotic region of the potential which gives the particle an extra radial phase space.

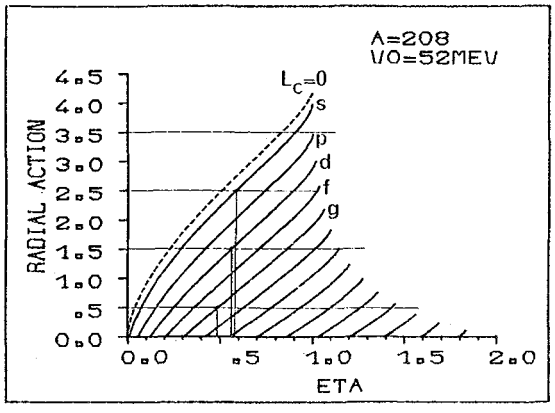

Fig. 2 - Radial action versus energy (η) for A = 208

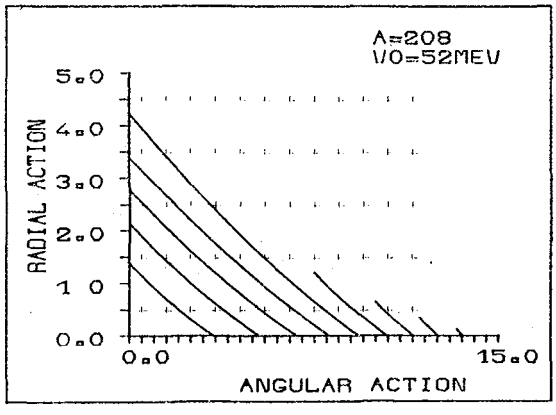

Fig. 3 - η= cte section of the EAS for A = 208.The values represented are η = 0.2, 0.4, 0.6,0.8,1.0, 1.2, 1.4, 1.6,1.8.

	η_Q	η_{SC}	$\Delta\eta$
1s	.0807	.0728	-9.74
1p	.1598	.1540	-3.62
1d	.2555	.2521	-1.31
2s	.2911	.2900	- .35
1f	.3656	.3651	- .15
2p	.4204	.4224	+ .49
1g	.4888	.4913	+ .52
2d	.5587	.5638	+ .91
3s	.5841	.5899	+1.00
1h	.6235	.6294	+ .95
2f	.7036	.7117	+1.15
3p	.7387	.7473	+1.17
1i	.7683	.7780	+1.25
2g	.8520	.8630	+1.30
3d	.8877	.8982	+1.19
4s	.8986	.9083	+1.09
1j	.9217	.9354	+1.48
Resonances			
2h	.9982	1.0125	
3f	1.0187	1.0255	
1k	1.0845	1.0999	
2i	1.1467	1.1463	
1l	1.2548	1.2688	
1m	1.4355	1.4368	

Table II - The same as for table I,but for A = 208.

In Fig. 2 we have represented the $I_r^L(\eta)$ sections of the EAS for A = 208. The complexity of the spectrum is much greater. In any case the anharmonicity of the states with the same angular momentum and the splitting of the H.O. multiplets, much more important here, can be explained as for A = 16. We see in this figure the relation between the curvature properties and the splitting of the 3s-2d-1g shell. The same EAS is represented in Figure 3 by its sections η = cte. The semiclassical energies are given in Table II and compared to the exact quantum results. Unlike the A = 16 case there exist semiclassical bound states with positive energy (η>1). The latter are a consequence of the attractive pocket of the effective potential and they constitute a semiclassical way to define a resonance. The energies of these

semiclassical resonances are compared with the quantum energies calculated as in the Gamov α-decay theory /9./.

We also remark that it is the linearity of the $I_r^L(\eta)$ curves which allows one to define a mean slope, and therefore a mean frequency, for the potential (1). It is this frequency which one must use to replace, as is usually done, a nuclear average potential by an H.O. From a classical point of view this approximation is justified as far as the frequencies of the classical motion present a weak dispersion with respect to a constant mean value, at least in the energy interval containing the eigenvalues. In Fig. 4 we have plotted the classical radial frquencies versus the energy for different values of L and for the two cases previously treated. The $\omega_r^L(\eta)$ curves shows the energy regions inside of which the H.O. approximation is classically justified. We see that the weak dispersion condition is far from being satisfied for A = 208.

In all cases the radial mean frequency ω_r obtained from the $\omega_r^L(\eta)$ curves has nothing to do with the one which is obtained by a Taylor expansion of the potential at r = 0.

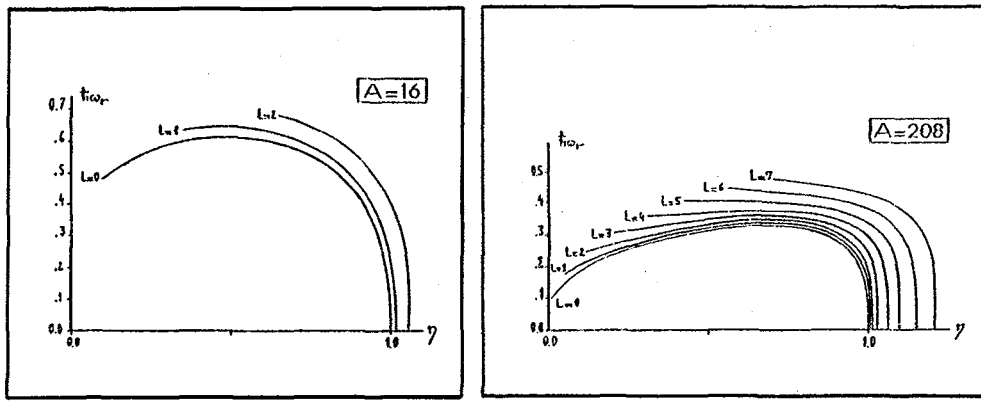

Fig. 4 - Classical radial frequencies of the potential (1). They are given by $\hbar\omega$ in V_o units.

The study we have just exposed for the A = 16 and A = 208 cases has also been performed for intermediate values of the mass number. The evolution of the EBK spectrum with this parameter will be given in the next section where we develop a more straightforward method than the step-by-step one. Let us remark only here that this evolution is the EAS one. In Fig. 5 we have drawn at the same scale the whole EAS for the A = 16, A = 90 and A = 208 values. Some of the features of the spectrum evolution can be understood just by looking at this figure. Thus, the number of eigenvalues will increase because the EAS is more and more extended, the splitting of the H.O. multiplets will become more and more important because the curvature of the EAS increases also with A, the fact that the properties of the surface does not change in a similar way will produce the level crossings.

Concerning the accuracy of the EBK method in the nuclear potential we have plotted in Fig. 6 the relative difference between the EBK and the exact eigenvalues versus the energy for various values of A. This difference is about 1% on the average but this value is greatly exceeded for the states near the bottom of the well. It is well known that the semiclassical methods give a result all the better that the quantum numbers are high and that the size of the system is large (small h). Anyway in our problem the range of variation of the parameters is not sufficient for these effects to be predominant. Thus the 3s state is less well approached than the

4s, just the contrary of what we could expect. Likewise, the relative error in the 1p state increases with A. The only conclusion we can draw for our results is that, independently of A, there exists two regions in the spectrum inside of which the quantum EBK differences has a constant sign.

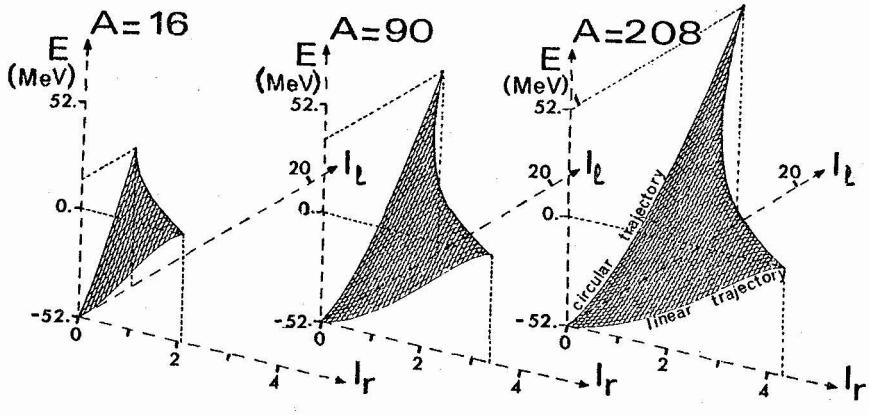

Figure 5 : Energy-action surface , E = H (I_r,I_L), for A = 16, A = 90 and A = 208.

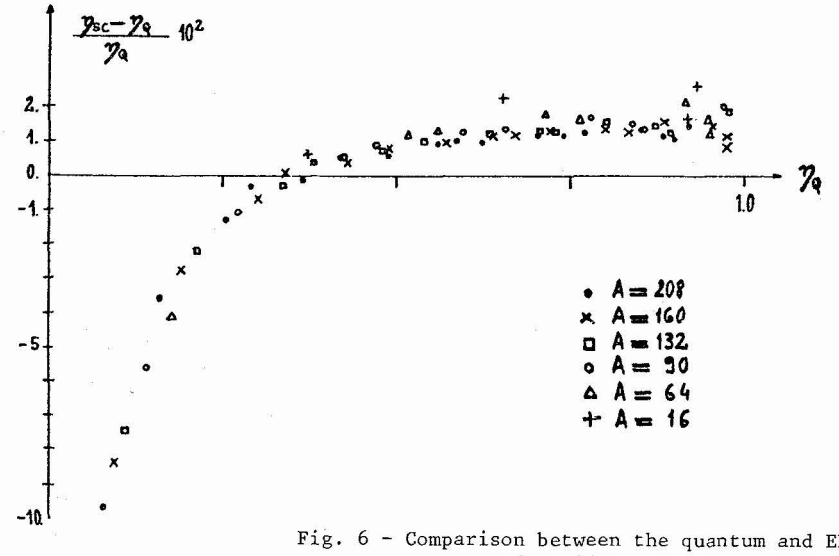

Fig. 6 - Comparison between the quantum and EBK spectrum for different values of A.

This difference which is minimum at the boundary of the two regions ($\eta \simeq 0.35$) is practically stationnary at 1% above it and increases exponentially below. It is therefore the fact that an eigenvalue belongs to one of these regions which will determine mainly the error.

IV - FROM LEAD TO OXYGEN

In order to avoid the repetition of the preceding work for each value of A it would be very interesting to develop a method allowing us to follow each eigenvalue when A is changing. The perturbation theory of quantum mechanics is excluded beyond small variations of A, which is far from being the case. The EBK method seems more adequate in order to solve such a problem. In its framework we have developed a technique which allows one to follow a semiclassical eigenvalue continuously as a function of A, for any domain of variation and with the required precision. The idea consists in following the quantum tori defined in (5) when A is changing. In other words suppose that for a given A the particle is at some semiclassical energy E_{n_L}. That means that quantum conditions (5) are fulfilled. Let us change A into A+dA and the question is : what is the energy variation dE in order to satisfy the same quantum conditions ?

We can answer this question by considering the radial action for a given angular momentum, I_r^L , as a function of E and A. If this function satisfy

$$I_r^L (E,A) = (n + \frac{1}{2})\hbar \tag{7}$$

and if we impose to keep the same value under small variations of its arguments we obtain the relation

$$(\frac{\partial I_r^L}{\partial E})_A \, dE + (\frac{\partial I_r^L}{\partial A})_E \, dA = 0 \tag{8}$$

This is the differential equation of the $E_{n_L}(A)$ curves giving the EBK eigenvalues as a function of A. We can rewrite this equation, in view of (6), in a more useful way

$$dE = - \omega_r^L(E,A) \cdot (\frac{\partial I_r^L}{\partial A})_E \, dA \tag{9}$$

It only remains now to know the spectrum of a heavy nucleus in order to get, by integrating numerically equation (9), the spectrum of the whole chart. This is what we have done by starting from A = 208. The results are shown in Fig. 7, which was obtained with an integration step $\Delta A = -0.2$. We have drawn, together with the bound states the semiclassical resonances. The energies are given here in MeV by $E = (1-\eta) \cdot V_o$.

We see, from equation (9), that the evolution of the EBK spectrum is commanded by a product of two functions. One of them is the classical frequency represented in Fig. 4. The other one can be written from equation (4), in the more explicit way

$$(\frac{\partial I}{\partial A})_E = - \frac{1}{2\pi} \oint \frac{m}{p_r} \left(\frac{\partial V}{\partial A}\right) dr$$

This function has a constant positive sign which explains us the uniform sloping down of each energy level in Fig. 7.

We also remark that the crossings of energy levels occur only in the upper part of the spectrum. There the states with smaller L tend to be at a lower energy. Below this region the evolution of the spectrum with A occurs in a more regular, quasi parallel way. We can understand this, through the $\omega_r^L(\eta)$ curves showed in Fig. 4. Indeed, when one of the $E_{n_L}(A)$ curves approach the values E = 0 (η= 1), the difference between the classical frequencies corresponding to two contiguous states is greater and greater. This difference produces, from (9), a rather different slope in

the E_{nL} (A) curves and a crossing occurs.

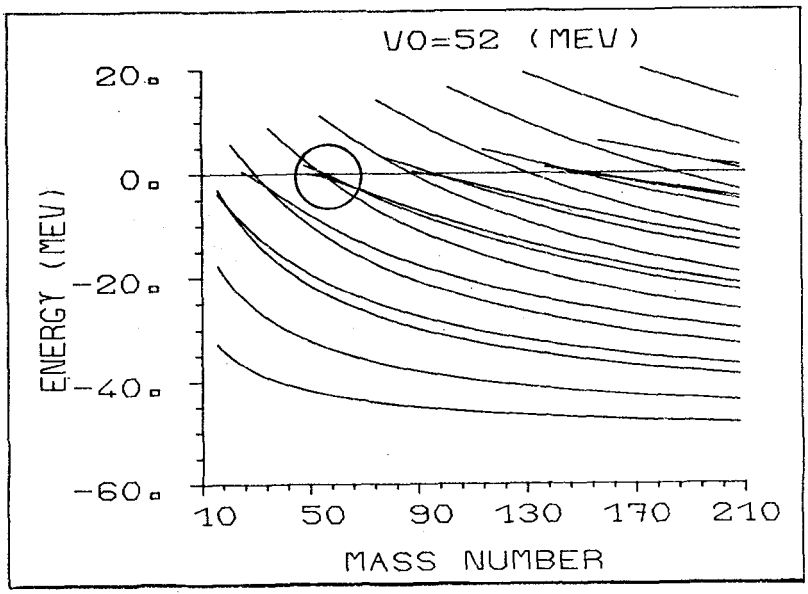

Fig. 7 - Evolution of the EBK spectrum with the mass number.

In Fig. 8 an enlargement of the encircled part of Fig. 7 is presented. The semiclassical energies can be compared to the exact quantum mechanical eigenvalues (dotted lines). All the crossings predicted by considering the energy action surface are seen to be produced in quantum mechanics a few units of A away.

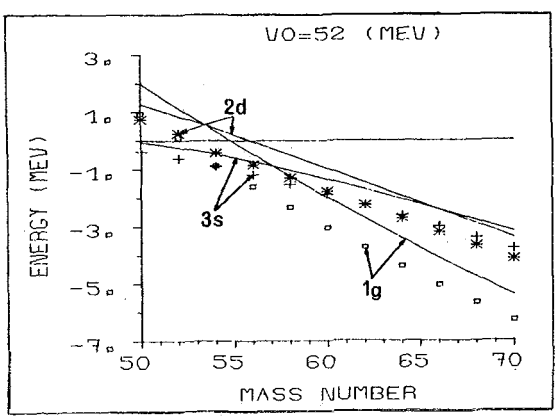

Fig. 8 - The encircled region of Fig. 7 (full line) is compared to the exact quantum results (dotted lines).

The precision of the method we have just exposed in following the semiclassical EBK spectrum depends on the integration step and on the length of the integration

interval. In table III we have compared the energies obtained with equation (8), (η'_{sc}), to the semiclassical values, (η_{sc}), for two, not time expensive, integration steps $\Delta A = -0.2$ and $\Delta A = -1.0$.

	A = 16		A = 90		A = 132		A = 160	
	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
1s	201.6	41.0	35.3	7.1	16.4	3.3	8.7	1.8
1p	148.3	29.9	30.6	6.2	14.4	2.9	7.8	1.6
1d	92.1	18.2	27.3	5.5	13.1	2.7	7.2	1.5
2s	54.3	10.6	24.1	4.8	11.8	2.4	6.4	1.3

Table III - Relative error between the exact EBK eigenvalues (η_{sc}) and those obtained by integrating equation (8), (η'_{sc}). We give the quantity $(\eta_{sc}-\eta'_{sc})/\eta_{sc}$ x 10^4 for two integration steps : (a) $\Delta A = -1.0$, (b) $\Delta A = -0.2$

The outline of the level spectrum of Fig. 7 has been obtained long time ago by Green et al. /10/ by solving the Schrödinger equation with slightly modified potentials. We see that the main features of the spectral evolution can be explained through the classical properties.

V - CONCLUSION

In this work we have shown, through the example provided by the nuclear average potential (1), that the EBK semiclassical method can be used not only to obtain the quantum spectrum with a good approximation but to understand its properties. They are carried by the energy-action surface which summarizes all the dynamics of the classical system. The geometrical properties of this surface, on the other hand, are directly related to the level spacing, ordering and crossings. In this way we see that the main features of a quantum spectrum appear as being assigned by the classical properties.

We have also shown that the EBK method seems very appropriate in order to follow the spectrum of an hamiltonian which depends on one parameter if the classical system remains integrable.

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