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1993 J. Phys. A: Math. Gen. 26 4767

(http://iopscience.iop.org/0305-4470/26/18/036)

J. Phys. A: Math. Gen. 26 (1993) 4767–4783. Printed in the UK

Semiclassical quantization in a prolate cavity via the adiabatic switching method: evolution of the classical actions

F Brut

Institut des Sciences Nucléaires, F-38026 Grenoble Cédex, France

Received 13 July 1992, in final form 24 February 1993

Abstract. Invariance of the actions which are the classical counterparts of the quantum numbers is very often postulated in adiabatic switching calculations but never checked carefully. In the particular case of a free particle moving in a prolate cavity deformed adiabatically at constant volume, time evolution of the classical actions is presented. Starting from semiclassical energies in a spherical cavity, the classical actions are calculated for each trajectory at each step of the switching procedure. This can be performed for any deformation since the system is separable in suitable coordinates. Invariance of the actions is not well verified for few values of the deformation. If it is easily understood why the actions invariance fails when the semiclassical solution cross the separatrix for the $L_z=0$ levels, such failures are in principle not expected for the $L_z\neq 0$ levels for which the trajectories belong to only one topology. The intrinsic frequencies of the motion are thus calculated for each trajectory at each step of the switching. Then, it is shown that failures in the action invariance occur exactly for values of the deformation for which two intrinsic frequencies become commensurate. For these particular values, the semiclassical trajectories are resonant for the $L_z\neq 0$ levels and periodic for the $L_z=0$ levels. By an appropriate canonical transformation on the action variables, a better invariant than the actions themselves has been built in the neighbourhood of each resonance. Apart from the particular values of the deformation where the radial and the angular frequencies become commensurate, action invariance is verified with a very good accuracy during the adiabatic switching.

1. Introduction

In the preceding paper [1], referred to as I, the adiabatic switching approximation was applied successfully to obtain the semiclassical eigenenergies in a simple but non-trivial two-dimensional system. Here, we study the same system, namely the motion of a free particle inside a spheroidal prolate cavity which is adiabatically deformed at constant volume, to determine how the classical actions are conserved during the switching. This paper is to be read in conjunction with paper I, whose notation is extensively used and whose equations are denoted as (I-1). (I-2), etc.

The system we study is always separable in a suitable system of coordinates for any deformation of the prolate cavity; thus classical tori are present everywhere in phase space and the classical actions can be calculated for any deformation. Under adiabatic changes of the shape of the cavity classical actions which are the classical equivalents of quantum numbers must in principle remain constant as a consequence of the Ehrenfest, hypothesis [2]. In many adiabatic switching calculations—see numerous references in I—invariance of the actions is more often postulated than numerically

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verified. In the particular system studied here, it is possible to calculate in a reasonable amount of computing time the classical actions at each step of the switching and for every trajectory. One of the possible tests of the validity of the method is based on a comparison between the exact semiclassical or quantum energy and the energy obtained by using the adiabatic switching method. As we saw in I, randomly chosen initial conditions are used to cancel the small oscillations around the mean energy which are linked to the finite switching time used in practical calculations. This necessary method of averaging over different energies obtained for each random initial condition gave a second test of confidence in the method: in previous calculations a small standard deviation around the averaged energy calculated at the end of the switching was considered as good evidence of the validity of the method. In fact, this standard deviation can be reduced by increasing the switching time, on one hand, and by increasing the number of initial conditions, on the other hand. Thus, a small standard deviation on the energy at the end of the switching procedure is not a sufficient criterion to ensure the validity of the method. In fact, we will show surprising results on some unexpected behaviour of classical quantities for the adiabatically changed prolate cavity even when the standard deviations on the energy remain small.

Starting in a spherical cavity with an initial condition which fulfils the EBK quantization conditions [3], the cavity is changed adiabatically in a prolate shape at constant volume. Of course, the dynamical quantities which define the motion of the particle are only changed at bounces on the moving boundary. Therefore, the energy, the angular momentum, but not its projection on the symmetry axis, are modified as well as any other quantities which depend on the velocity. After each bounce on the boundary, the particles restart on a new trajectory for which it is possible again to calculate the turning points needed for the determination of classical actions. In section 2, we present the time evolution of the two actions which are specific to the system, for different initial conditions and during the adiabatic switching. For the $L_z=0$ levels, the crossing of separatrix by the adiabatic semiclassical solution is seen by a failure of the conservation of classical actions. This feature is present as expected, although we showed in I, that being in the neighbourhood of the separatrix does not affect the quality of agreement between exact and adiabatic semiclassical energies. For $L_z \neq 0$ levels, as well as for $L_z=0$ levels but for other deformations than the special value corresponding to the crossing of separatrix, strange behaviours of the classical actions are still present during the switching procedure in well localized areas. Explanation of these facts requires the determination of intrinsic frequencies of the system which is presented in section 3. For some precise values of the deformation in the prolate cavity, two intrinsic frequencies of the motion become commensurate and correspond exactly to the regions where classical quantities have strange behaviours. Only primary resonances notably affect the conservation of actions. For these particular values, by a canonical transformation on the actions and angles variables, it is possible to build other invariants which are less sensitive to crossings of resonance zones than the primitive actions of the systems. These new invariants depend on the primary resonance which is considered and will be studied in section 4.

2. Time evolution of classical quantities during adiabatic switching

For every starting point in phase space, after each bounce of the particle on the boundary during the adiabatic switching, turning points can be determined in spheroidal prolate coordinates. These turning points are needed to calculate the classical actions given by equations (I-9).

The upper limit ε_1 of the ε variable is given by the boundary of the prolate cavity

$$\varepsilon_1 = \frac{1}{2}\ln\frac{\mu+1}{\mu-1} \tag{1}$$

where μ is the deformation of the cavity defined by the semi-axis ratio (I-4). For the other turning points of the canonical momenta, $L_z \neq 0$ levels are distinguished from $L_z = 0$ levels.

For $L_z \neq 0$ levels we have

$$\varepsilon_0 = \cosh^{-1}\left\{\frac{1}{2}\left(\frac{1}{e^2}+1\right)+\frac{1}{2}\left[\left(\frac{1}{e^2}-1\right)^2+4\lambda^2\right]^{1/2}\right\}^{1/2} \tag{2a}$$

$$\xi_0 = \cos^{-1}\left\{\frac{1}{2}\left(\frac{1}{e^2}+1\right)-\frac{1}{2}\left[\left(\frac{1}{e^2}-1\right)^2+4\lambda^2\right]^{1/2}\right\}^{1/2} \tag{2b}$$

with

$$\lambda = \frac{L_z}{kf} \tag{3a}$$

$$e = \frac{kf}{\sqrt{C}} \tag{3b}$$

where k, f and C are defined by (I-5), (I-2) and (I-6), respectively. Of course, the separation constant C is always positive for levels with $L_z \neq 0$ [4].

For levels $L_z = 0$ we have still two different cases depending on the topology of the classical trajectory.

$e<1$ corresponds to the classical trajectory with an ellipsoidal caustic; in this case we have

$$\varepsilon_0 = \cosh^{-1}\left(\frac{1}{e}\right) \tag{4a}$$

$$\xi_0 = 0. \tag{4b}$$

$e>1$ corresponds to the classical trajectory with a hyperboloidal caustic which happens after crossing the separatrix, then

$$\varepsilon_0 = 0 \tag{4c}$$

$$\xi_0 = \cos^{-1}\left(\frac{1}{e}\right) \tag{4d}$$

where e is always defined by (3b).

Starting from one particular initial condition it is thus possible to take snapshots of the canonical momenta $p_\varepsilon(\varepsilon)$ and $p_\xi(\xi)$, defined by (I-6), as functions of ε and ξ, at different time of the adiabatic switching. Figures 1(a) and 1(b) correspond, respectively to the $L_z = 2$ and $L_z = 0$ levels belonging to the spherical (1h) multiplet. Figure 1(a) shows that the turning point coordinate ε_0 is decreasing as the deformation or the

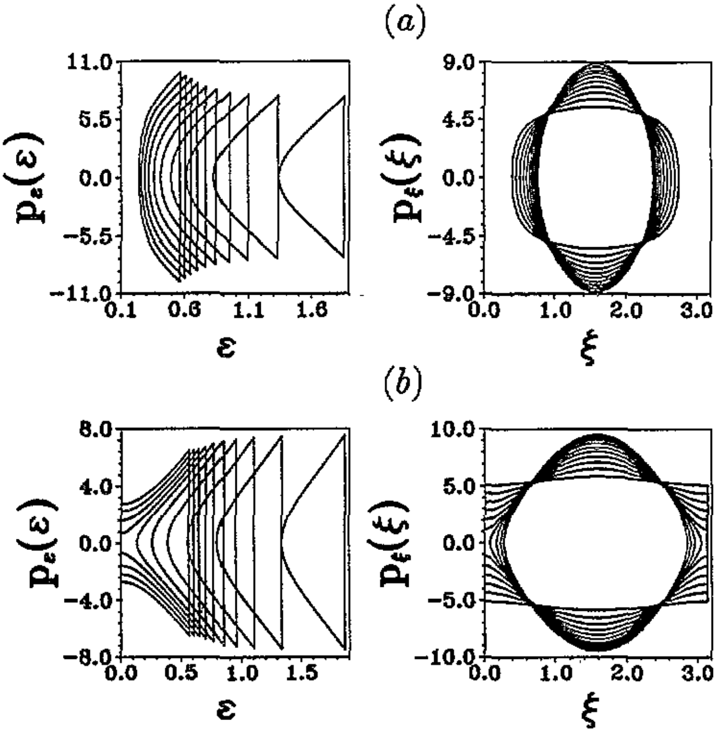

Figure 1. The canonical momenta $p_\varepsilon(\varepsilon)$ and $p_\xi(\xi)$ are drawn at ten different steps of the adiabatic switching, namely for ten different deformations, for two levels starting from the $(1h)$ spherical multiplet. Invariance of classical actions imply that each curve surrounds a constant surface which is precisely proportional to the corresponding action. (a) $L_z=2$ level; (b) $L_z=0$ level. In the latter case, the crossing of the separatrix is obvious.

switching time increases, even though the corresponding coordinate ξ_0 is increasing. The maximum values of the canonical momenta $p_\varepsilon(\varepsilon)$ and $p_\xi(\xi)$ evolve in just the opposite direction of ε_0 and ξ_0, respectively, to ensure conservation of the area, which in principle represents the associated actions. The momentum $p_\varepsilon(\varepsilon)$ changes abruptly its sign when the particle hits the boundary for $\varepsilon=\varepsilon_1$.

The semiclassical trajectories associated with levels $L_z=0$ start with an ellipsoidal caustic at the beginning of the switching, thus $\xi_0=0$ and ε_0 is non zero, as can be seen in figure 1(b). Thus the momentum $p_\xi(\xi)$ takes its lowest maximum value. During switching, ξ_0 remains zero when ε_0 decreases as the deformation increases until the crossing of separatrix for which the two turning points ξ_0 and ε_0 are both zero. After the separatrix, ξ_0 is never zero and ε_0 is always zero. In order to conserve the area enclosed in each curve, the maximum value of $p_\xi(\xi)$ must increase as seen in figure 1(b). The variations of the maximum value of $p_\varepsilon(\varepsilon)$ depend on the level under consideration. Obviously, the actions are calculated by numerical integration of the analytical functions corresponding to the canonical momenta given by (I-6) between the turning points and the boundary, at each step of the adiabatic switching.

Figures 2 and 3 show the time evolution of the two classical actions I_ε and I_ξ defined by (I-9), in a probate cavity during the adiabatic switching, i.e. when the deformation μ is increased from its spherical value $\mu=1$ to the final value $\mu=2$. This time evolution is presented for five randomly chosen initial points in phase space, which all together fulfil the EBK quantization conditions [3–5] in a spherical cavity.

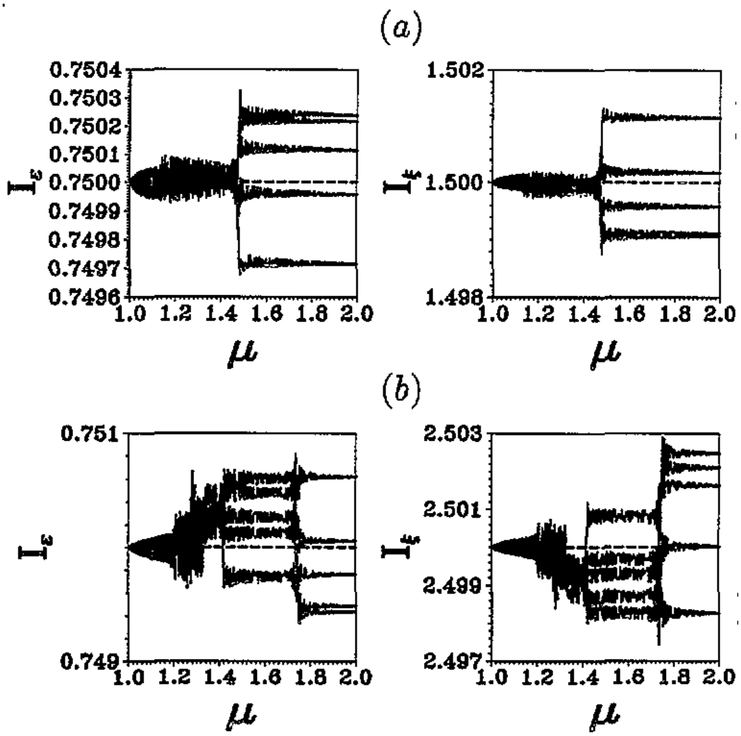

Figure 2. Time evolution of the classical actions during adiabatic switching, corresponding to five different initial conditions in the spherical cavity. If the actions were exactly conserved, they should take the constant value materialized by the dashed line. Frame 2(a) corresponds to the $L_z=1$ level, frame 2(b) to the $L_z=0$ level, each of them starts from the ($1d$) spherical multiplet. The switching time corresponds to about 24 000 and 20 000 bounces of the particle for the $L_z=1$ and $L_z=0$ levels, respectively.

The time dependence of the two actions I_ε and I_ξ is obviously presented for the same starting initial conditions. Exact invariance of the actions during adiabatic switching means that they take constant values which are materialized by dashed lines in each frame.

First, let us look for the $L_z \neq 0$ levels in figures 2(a) and 3(a). For any initial conditions, the actions I_ε and I_ξ change abruptly for the particular values of the deformation around $\mu=1.48$ and $\mu=1.42$ for the $L_z=1$ and $L_z=2$ levels, respectively. However, the relative deviations from the exact semiclassical values are small, less than a few 10^{-3} in the most unfavourable case. Moreover, the actions I_ε and I_ξ evolve in opposite directions after crossing these special deformations in relation to the exact semiclassical actions. Before the discontinuity, we can see that the actions are oscillating around an average value very close to the expected constant values—the relative deviations are now less than a few 10^{-4}. The small oscillations, around the exact semiclassical values, are due to the necessary choice of a finite switching time in practical calculations. Their amplitudes could be reduced significantly by increasing switching time. After the discontinuity, the actions are still oscillating but now around different values reached during the crossing of this discontinuity.

The situation is more confused for the $L_z=0$ levels shown in figures 2(b) and 3(b). There, the crossing of the separatrix is expected when the semiclassical solution changes from trajectories having an elliptical caustic—for small deformation—to

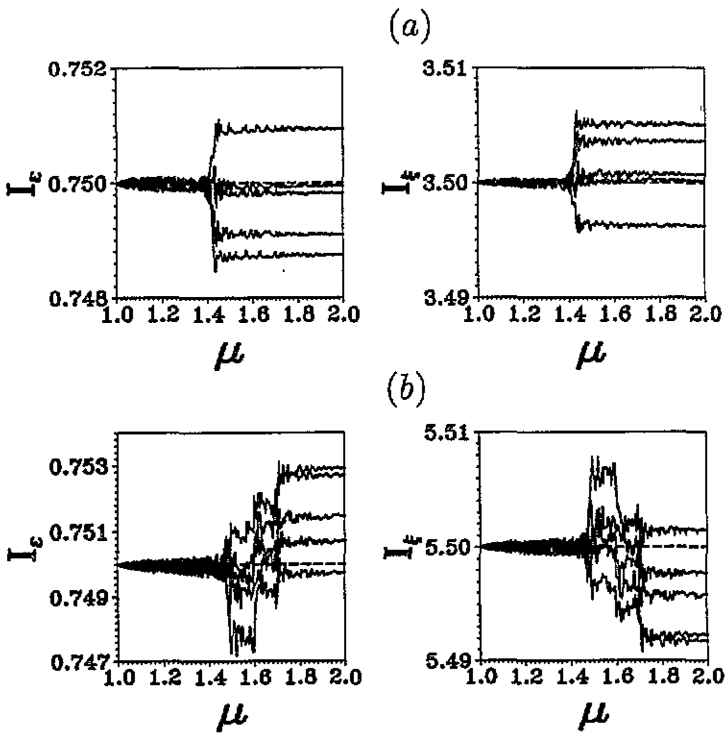

Figure 3. As figure 2, but for two levels starting from the ($1h$) spherical multiplet, namely $L_z=2$ in 3(a) and $L_z=0$ in 3(b). Now, the particle bounces 23 000 and 28 800 times on the boundary for the $L_z=0$ and $L_z=2$ levels, respectively.

trajectories having a hyperbolical caustic—for large deformations—and consequently the adiabatic approximation must fail. Thus, at the crossing of the separatrix, as one intrinsic period of the system becomes infinite, the switching time is then not greater than the two characteristic periods of the system, as required. The separatrix is crossed [4] for $\mu_{sep}=1.281\,025$ and for $\mu_{sep}=1.616\,581$ for the two $L_z=0$ levels presented in figures 2(b) and 3(b), respectively. For these two deformations, we observe sudden variations of the actions, and we notice that relative deviations around the exact semiclassical values are small, less than a few 10^{-3}, in the most unfavourable case on the whole deformation range. But, in figure 2(b), for the $L_z=0$ level issued from the (1d) spherical multiplet, other abrupt variations of the two actions occur for values of the deformation around $\mu=1.42$ and 1.74. These large deviations from exact invariance occur also for the $L_z=0$ level shown in figure 3(b), around $\mu=1.48$ and $\mu=1.71$. This phenomenon, shared with the $L_z\neq 0$ levels previously discussed, appears always for particular values of the deformation and simultaneously for the two actions, it is independent on the initial conditions. Again, we must notice opposite behaviour of I_ε and I_ξ with respect to the values of reference. This generic behaviour is clearly shown in figures 2(b) and 3(b). Another striking feature is that the fluctuations of the actions which occur around these specific values of the deformation are of the same order of magnitude as those which correspond to the separatrix crossing. In addition, we have also small oscillations around an average mean outside the particular set of deformations discussed above.

In order to enlighten all our previous comments let us draw the classical trajectories in the vicinity of the values of the deformation corresponding to the more abrupt changes. Figures 4 and 5 show the classical trajectories that have been reached during adiabatic switching for some specific values of deformation. The switching is of course stopped during the evolution of the particle. Figure 4 shows the classical trajectories in the (ρ, z) plane which is rotating with the particle around the symmetry axis Oz. On the left of figure 4, the classical trajectory drawn for the deformation $\mu = 1.421\,594$ which corresponds to the $L_z = 2$ level issued from the $(1h)$ spherical multiplet has clearly two frequencies which become resonant in the ratio 4:1. It is similar this time for $\mu = 1.475\,011$ for the $L_z = 1$ level, shown on the right of figure 4, which is issued from the $(1d)$ spherical multiplet. These two values of μ are very close to the points where the classical actions I_ε and I_ξ were changing abruptly (see figures 2 and 3).

Classical trajectories for the $L_z = 0$ levels, which are deduced from the $(1d)$ and $(1h)$ spherical multiplets are shown at the top and bottom of figure 5, respectively, for different values of the deformation μ. Each of them has been reached during adiabatic switching and corresponds to deformations for which the classical actions change abruptly (see figures 2(b) and 3(b)). Again trajectories are drawn in an arbitrary (x, z) plane perpendicular to the angular momentum of the particle, while adiabatic switching has been stopped the particle bounces 50 times on the boundary before one ends the calculation. The trajectories corresponding to the $L_z = 0$ level belonging to the $(1d)$ spherical multiplet clearly have a hyperbolical caustic which means that the corresponding deformation values $\mu = 1.416\,556$ and $\mu = 1.739\,113$ are greater than the value μ_{sep} for which the semiclassical level lies on the separatrix. This is in agreement with our previous discussion of figure 2(b) where the crossing of the separatrix is located at $\mu_{\mathrm{sep}} = 1.281\,025$. It is also obvious that the trajectory drawn for $\mu = 1.416\,656$ is a resonant one, the ratio of the radial frequency over the angular frequency is 3:1. The same ratio is now 4:1 for the trajectory corresponding to $\mu = 1.739\,113$. Similar conclusions hold for the $L_z = 0$ level starting from the $(1h)$ spherical multiplet, but now the classical trajectories have either an elliptical caustic or a hyperbolical caustic corresponding, respectively, to the deformation values $\mu = 1.479\,654$ and $\mu = 1.705\,591$ which enclose the value $\mu_{\mathrm{sep}} = 1.616\,58$ for which the semiclassical level lies on the separatrix. The frequencies ratio is 3:1 for both trajectories in this case. We should notice that all these trajectories for the $L_z \neq 0$ levels are resonant but not periodic, because there is not necessarily commensurability with the motion around the z axis.

In this section, we have shown that classical actions are very well conserved during adiabatic switching, except for some deformation values for which sudden changes of the actions occur. Some of them could be understood by the crossing of a separatrix in

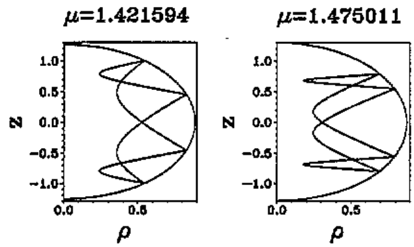

Figure 4. Classical trajectories corresponding to values of the deformation where the semiclassical actions change abruptly, in figures 2 and 3, during adiabatic switching. Two trajectories for two $L_z \neq 0$ levels are shown here they are drawn in the (ρ, z) plane which is rotating with the particle around the symmetry axis Oz. Left: $L_z = 2$ level starting from the $(1h)$ spherical multiplet. Right: $L_z = 1$ level starting from the $(1d)$ spherical multiplet.

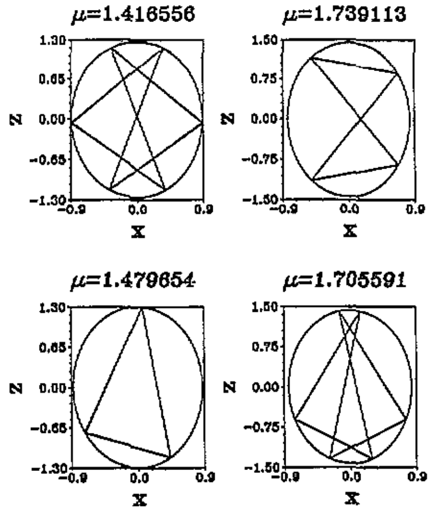

Figure 5. As figure 4 but for the $L_z=0$ levels. We study here the trajectories that occur at resonance, i.e. apart from the separatrix at the place where the classical actions change abruptly during adiabatic switching in figures 2 and 3. The classical trajectories are drawn in the neighbourhood of these two deformations on a plane (x, z) perpendicular to the angular momentum of the particle. Top: trajectory for the $L_z=0$ level that starts from the $(1d)$ spherical multiplet. The two periodic trajectories have the same topology with a hyperbolic caustic. Bottom: trajectory for the $L_z=0$ level that starts from the $(1h)$ spherical multiplet. For the lower deformation, the periodic trajectory has an elliptic caustic and for the greater deformation, the periodic trajectory has a hyperbolic caustic.

the case of the $L_z=0$ levels. Other changes correspond to some resonant trajectories where the ratio of two intrinsic frequencies of the motion become commensurate as 3:1 or 4:1. The prolate cavity is one of few systems for which intrinsic frequencies of the motion could be calculated analytically, which will be done in the next section.

3. Frequencies of the motion in a prolate cavity

The components of the frequency vector in an integrable system are just the first derivatives of the Hamiltonian function with respect to the classical actions. Here we are dealing with a system which remains integrable during adiabatic switching. We will start with motion inside a spherical cavity and we will extend our results to the prolate cavity.

3.1. Intrinsic frequencies of the motion in a spherical cavity

For a free particle of unit mass inside a spherical cavity of radius R_0, the radial action I_r of the motion is written as [5, 6]:

$$I_r=\frac{1}{\pi}\sqrt{2E}\,R_0\left\{\left(1-\left(\frac{R}{R_0}\right)^2\right)^{1/2}-\frac{R}{R_0}\cos^{-1}\left(\frac{R}{R_0}\right)\right\} \tag{5}$$

where E is the energy of the particle and R is the radius of the spherical caustic fixed by the conservation of classical angular momentum [5]

$$l_c \equiv l + \tfrac{1}{2} = \sqrt{2E}\,R. \tag{6}$$

Using (5) and (6), a straightforward calculation gives the radial frequency

$$\omega_r \equiv \frac{\partial E}{\partial I_r} = \pi \frac{\sqrt{2E}/R_0}{\left[1 - \dfrac{l_c^2}{2E R_0^2}\right]^{1/2}} \tag{7}$$

In order to calculate the angular frequencies we must notice that in a spherical cavity the particle covers its trajectory which is lying on a plane perpendicular to the angular momentum. Therefore, we can choose two different systems of coordinates, the usual spherical one (r, θ, ϕ) and the other (r, ψ) on the plane of the trajectory. As the kinetic energy T of the particle is a constant in any system and a polynomial of degree 2 under the momenta p, we can write

$$2T = \sum_i p_i \dot{q_i} \tag{8}$$

thus

$$p_\theta \, \mathrm{d}\theta + p_\phi \, \mathrm{d}\phi = p_\psi \, \mathrm{d}_\psi \tag{9}$$

where p_θ, p_ϕ and p_ψ are the canonical momenta associated with the coordinate θ, ϕ and ψ, respectively. In a plane (ρ, z) which is rotating with the particle around the z axis, the motion is confined by the boundary of the cavity, of course, by a caustic circle of radius R, given by (6) and by two straight lines which make an angle θ_0 and $\pi - \theta_0$ with the z axis given by

$$\sin\theta_0 = \frac{L_z}{l_c}. \tag{10}$$

If we integrate (9) over one cycle of the angular motion, we get

$$\frac{1}{\pi}\int_{\theta_0}^{\pi-\theta_0} p_\theta \, \mathrm{d}\theta = \frac{1}{2\pi}\int_0^{2\pi} p_\psi \, \mathrm{d}\psi - \frac{1}{2\pi}\int_0^{2\pi} p_\phi \, \mathrm{d}\phi \tag{11a}$$

which could be read as

$$I_\theta = I_\psi - I_\phi. \tag{11b}$$

Obviously, in this simple case, we may identify I_ψ and I_ϕ with l_c and L_z, respectively, thus we have a first relation by using (6):

$$\frac{\partial E}{\partial I_\theta} = \frac{\partial E}{\partial I_\phi} \Leftrightarrow \omega_\theta = \omega_\phi. \tag{12}$$

The motion is singly degenerate as it is for all central forces [7]. A straightforward calculation using (5)–(11) gives

$$\omega_\theta \equiv \frac{\partial E}{\partial I_\theta} = -\frac{\dfrac{\partial I_r}{\partial l_c}}{\dfrac{\partial I_r}{\partial E}} = \frac{\sqrt{2E}/R_0}{\left[1-\dfrac{l_c^2}{2E\,R_0^2}\right]^{1/2}} \cos^{-1}\left(\frac{l_c}{\sqrt{2E}\,R_0}\right). \tag{13}$$

Finally, the ratio of the radial and angular frequencies is written as

$$\frac{\omega_r}{\omega_\theta} = \frac{\pi}{\cos^{-1}\left(\dfrac{\lambda_c}{\sqrt{2E}\,R_0}\right)} = \frac{\pi}{\cos^{-1}\left(\dfrac{R}{R_0}\right)}. \tag{14}$$

In the preceding equation, the radius R of the spherical caustic is never zero due to the Langer correction in the definition of the classical angular momentum. The upper limit of R is of course the radius R_0 of the boundary giving the important relation

$$\frac{\omega_r}{\omega_\theta} > 2 \tag{15}$$

for any motion in a spherical cavity, corresponding to a semiclassical eigenstate.

3.2. *Intrinsic frequencies of the motion in a prolate cavity*

In this case, analytical dependence of the energy on the classical actions is not known, but the classical actions I_ε, I_ξ and I_ϕ, defined by (I-9) are functions of the three constants of motion, namely the energy E, the scalar product C defined by (I-6) and the projection L_z of the angular momentum along the symmetry axis. If $J(I_\varepsilon, I_\xi; E, C)$ and $J(I_\varepsilon, I_\xi; L_z, C)$ are the two Jacobians of the transformations associated with the variable changes (I_ε, I_ξ) to (E, C), and (I_ε, I_ξ) to (L_z, C), respectively:

$$J(I_\varepsilon, I_\xi; E, C) = \frac{\partial I_\varepsilon}{\partial E}\frac{\partial I_\xi}{\partial C} - \frac{\partial I_\varepsilon}{\partial C}\frac{\partial I_\xi}{\partial E} \tag{16a}$$

$$J(I_\varepsilon, I_\xi; L_z, C) = \frac{\partial I_\varepsilon}{\partial L_z}\frac{\partial I_\xi}{\partial C} - \frac{\partial I_\varepsilon}{\partial C}\frac{\partial I_\xi}{\partial L_z}. \tag{16b}$$

Then, following Gutzwiller and Strutinsky [8], the frequencies of motion are defined by

$$\omega_\varepsilon \equiv \frac{\partial E}{\partial I_\varepsilon} = \frac{1}{J(I_\varepsilon, I_\xi; E, C)}\frac{\partial I_\xi}{\partial C} \tag{17a}$$

$$\omega_\xi \equiv \frac{\partial E}{\partial I_\xi} = \frac{-1}{J(I_\varepsilon, I_\xi; E, C)}\frac{\partial I_\varepsilon}{\partial C} \tag{17b}$$

$$\omega_\phi \equiv \frac{\partial E}{\partial I_\phi} = -\frac{J(I_\varepsilon, I_\xi; L_z, C)}{J(I_\varepsilon, I_\xi; E, C)}. \tag{17c}$$

In calculating the partial derivatives needed to know the radial and angular frequencies of the motion, defined by the preceding equations, we have to derive an integral, the limits of which depend on the variables. Fortunately, in our case these limits are precisely the turning points, defined by (2)–(4) for which the momenta vanish. Therefore, after a tedious but straightforward calculation, we obtain

$$\frac{\omega_\xi}{\omega_\varepsilon}=\frac{1}{2}\left\{1-\frac{F(\chi,m)}{F\left(\frac{\pi}{2},m\right)}\right\} \tag{18}$$

where $F(\chi, m)$ is an elliptic integral of the first kind [9], defined by

$$F(\chi,m)=\int_0^\chi (1-m\sin^2 x)^{-1/2}\,\mathrm{d}x \tag{19a}$$

with

$$\chi=\sin^{-1}\left[\frac{\cosh\varepsilon_0}{\cosh\varepsilon_1}\right] \tag{19b}$$

$$m=\frac{\cos^2\xi_0}{\cosh^2\varepsilon_0} \tag{19c}$$

where ε_0, ε_1 and ξ_0 are defined by (1)–(4). The ratio of the two angular frequencies is obtained in the same way:

$$\frac{\omega_\phi}{\omega_\xi}=\frac{2\left[\left(1-\frac{m}{m'}\right)(1-m')\right]^{1/2}}{\pi}\left\{\pi\left(\frac{\pi}{2},\frac{m}{m'},m\right)-F\left(\frac{\pi}{2},m\right)\right.$$
$$\left.+\left[\pi\left(\frac{\pi}{2},m',m\right)-\pi(\chi,m',m)\right]\left[1-\frac{F(\chi,m)}{F\left(\frac{\pi}{2},m\right)}\right]^{-1}\right\} \tag{20}$$

where $\pi\ (\chi, m', m)$ is an elliptic integral of the third kind [9] given by

$$\pi(\chi,m',m)=\int_0^\chi (1-m'\sin^2 x)^{-1}(1-m\sin^2 x)^{-1/2}\,\mathrm{d}x \tag{21a}$$

with

$$m'=\frac{1}{\cosh^2\varepsilon_0}. \tag{21b}$$

At each step of the adiabatic switching the prolate cavity remains integrable. The turning points of the momenta can be determined at every bounce with the boundary, and the classical actions are then defined. The knowledge of turning points, at each step allows calculation of the frequency ratios given by (18) and (20). Before giving the numerical results, let us notice some particular cases which are of interest for the $L_z=0$ levels.

First, the ratio of the two angular frequencies, given by (20), is always vanishing in this case. In fact, in more detail we found that ω_ϕ is proportional to L_z. It can be seen also in (20) that (4) gives the special values $m=m'=e^2$ for a classical trajectory with

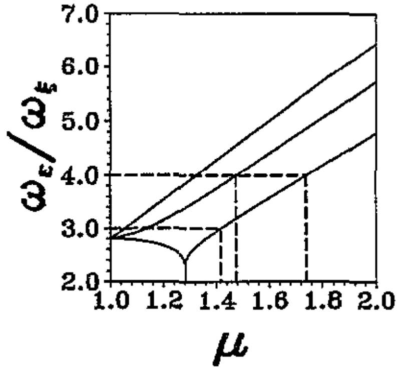

Figure 6. Ratio of the radial (ω_ε) to the angular (ω_ξ) intrinsic frequencies of the motion for the levels starting from the (1d) spherical multiplet, as a function of the deformation μ during adiabatic switching. For any fixed deformation, each curve is labelled by a definite value of L_z which increases with $\omega_\varepsilon/\omega_\xi$ ($L_z=0,1,2$). The dashed lines determine the deformations for which the two frequencies become commmensurate, in the ratios 3:1 and 4:1.

an elliptical caustic and $m=1/e^2$, $m'=1$ for a classical trajectory with a hyperbolical caustic. Thus

$$\frac{\omega_\phi}{\omega_\xi}=0 \qquad \forall\mu \text{ for the } L_z=0 \text{ levels.} \tag{22}$$

Second, the semiclassical level crosses the separatrix for the value $\mu=\mu_{\rm sep}$ which corresponds to $e=1$. Therefore, in this special case we have $m=1$ and thus $F(\pi/2, m)$ becomes infinite. The angle χ, given by (19b), is written as

$$\chi=\sin^{-1}\left(\left[1-\frac{1}{\mu_{\rm sep}^2}\right]^{1/2}\right)$$

which implies that χ is always less than $\pi/2$, in the deformation range under study.

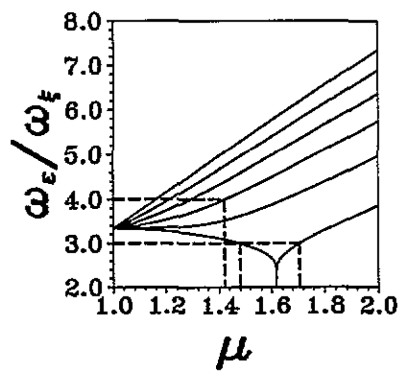

Figure 7. As figure 6 but for the (1h) spherical multiplet. Here the frequencies of levels with $L_z=0,1,2,3,4$ and 5 are plotted.

Finally, the ratio defined by (18) has a finite value when the semiclassical level lies on the separatrix:

$$\frac{\omega_\varepsilon}{\omega_\xi}(\mu=\mu_{\rm sep})=2 \qquad \text{for the } L_z=0 \text{ levels} \tag{23}$$

The ratio of interest for our purpose is given by (18), its limit for the spherical symmetry is given by (14). Figures 6 and 7 show the quantities $\omega_\varepsilon/\omega_\xi$ as a function of the deformation μ for the levels belonging to the ($1d$) and ($1h$) spherical multiplets, respectively. Each curve corresponds to a definite value of the projection L_z of the angular momentum; for any fixed deformation μ, increasing L_z correspond to an increase of the ratios $\omega_\varepsilon/\omega_\xi$. Each of the different curves is deduced from a single initial condition chosen among the 25 which were previously used in order to calculate the averaged energy as a function of μ. This frequency ratio is a function which is not sensitive to the initial conditions and its fluctuations can be neglected for our purpose. The ratios $\omega_\varepsilon/\omega_\xi$ begin at the value determined by ω_r/ω_θ, given by (14), for the spherical symmetry ($\mu=1$), this ratio does not depend on L_z. The dashed lines are drawn for the specific values encountered when the two frequencies ω_ε and ω_ξ become commensurate in the ratios 3:1 and 4:1. Figures 6 and 7 confirm the conclusions of the preceding section. More precisely, in figure 6, the $L_z=0$ level is associated with two intrinsic frequencies ω_ε and ω_ξ which become commensurate to 3:1 and 4:1 on the same side of the separatrix for which the ratio $\omega_\varepsilon/\omega_\xi$ is just 2. The corresponding values of the deformation were found more or less clearly in discussions of figures 2 and 5. When the two frequencies ω_ε and ω_ξ become commensurate to 3:1 and 4:1, it is clearly seen that the associated trajectories have the same topology with a hyperboloidal caustic. One peculiar event occurs for the $L_z=1$ level in figure 6. When the two frequencies become commensurate to 3:1, which occurs for a deformation around 1.14, the semiclassical actions I_ε and I_ξ are not very sensitive to the crossing of this resonance zone, as is seen in figure 2(a). On the contrary, the change is very abrupt exactly when the two frequencies are commensurate in the ratio 4:1. The same conclusion holds for the $L_z=2$ level belonging to the same spherical multiplet. In figure 7, we notice that the ratio ω_r/ω_θ for the spherical symmetry is now greater than 3:1 and therefore this resonance will act only on the $L_z=0$ level. For this level, the frequencies become commensurate to 3:1 before and after crossing the separatrix, which means that each of the trajectories associated with these particular values of the deformation must have different caustics, as shown by figure 5. The deformation range under study does not allow the semiclassical $L_z=0$ level to cross the resonant zone corresponding to the ratio 4:1 therefore, this zone has no effect on this level for $\mu<2$ as was the case for the previous multiplet. In the same way, as the ratio ω_r/ω_θ is always greater than 3 for all the other levels belonging to the same spherical multiplet, the $L_z=2$ level, in particular, crosses a resonance 4:1 for the deformation already found in the preceding discussion of figures 3 and 4. As mentioned before for the $L_z=1$ level, we notice that other resonances, like 5:1, seem to have no influence on the classical actions. The same conclusions are drawn for the other $L_z\neq 0$ levels which are sensitive only to the lowest 4:1 resonance, even if the semiclassical eigenstate crosses resonances of greater order (up to 7:1 for the $L_z=5$ level for example, in figure 7). We must underline also that all these effects are decreasing in intensity with increasing values of L_z inside the same spherical multiplet.

A careful analysis of the separatrix crossing was done by Skodje and Cary [10] in the case of a 1D-symmetric quartic double well varying with the time. In this onedimensional problem, where some approximations allow calculation of a crucial crossing parameter, it is possible to follow the instantaneous frequency and action during the switching. The separatrix crossing is seen by an increasing amplitude of the oscillating action and, as expected, by a discontinuity of the intrinsic frequency. The same general behaviour is qualitatively seen in the 2D problem studied here. Adiabatic switching for non-integrable systems, and especially crossings of resonances, was studied by Reinhardt [11] and Chirikov [12], for the standard map. In this 1D map the leading order correction to the action is determined and studied when a resonance is crossed during switching.

In the following section, we will verify the hypothesis [13, 14] that a canonical transformation on the action variables help to avoid such resonance zones. In the prolate cavity, we have already all the necessary quantities to construct numerically such a transformation and determine if the conservation of the new invariant is improved.

4. New invariants around resonance zones

For 2D Hamiltonian systems, it has been stated [13, 14] that by using appropriate canonical transformation on the action-angle variables a strategy could be implemented for avoiding resonance zones during adiabatic switching. In fact, deviations around exactly conserved invariants can be minimized when the semiclassical solution of the unperturbed Hamiltonian is closed to a resonance. In the preceding section, we found that the particular spherical multiplet levels under study were precisely closed to the resonances 3:1 and 4:1 which were clearly correlated to small non-conservation effects of the classical actions during adiabatic switching. Therefore, we have in this particular case—as the actions are calculated at each step of the switching—all the quantities needed to verify that we can numerically build a best invariant than the previous two actions I_ε and I_ξ.

It is shown in [13] and [14] when the two intrinsic frequencies ω_1, ω_2 of 2D Hamiltonian system become commensurate (in resonance), i.e. $\omega_1:\omega_2=s:r$, where s and r are integers, that a new action $\tilde{I}$ can be built

$$\tilde{I}=sI_1+rI_2$$

which becomes a proper adiabatic invariant. In the case of accidental degeneracy which is relevant here, the theory leads to a Hamiltonian which is isomorphic to that of the pendulum [12–14]; crossing of the resonance is then seen as crossing the separatrix in the appropriate new variables.

During adiabatic switching, we showed that intrinsic frequencies ω_ε and ω_ξ of the motion could be calculated at each step for the free particle inside a prolate cavity. Correlations between resonances and abrupt changes in the actions and I_ε and I_ξ are clearly established by the preceding section. We also noticed that, in the vicinity of a resonance, when one action I_ε is increasing (decreasing), the other I_ξ is decreasing (increasing), but these variations were not of the same amplitudes for a given level and depended on the semiclassical eigenstate under study. Thus, we can build at each step of the switching a new action $\tilde{I}$ defined by the following linear combination

$$\tilde{I}=sI_\varepsilon+rI_\xi \tag{24a}$$

when the semiclassical level crosses the resonance

$$\omega_\varepsilon:\omega_\xi=s:r \tag{24b}$$

during adiabatic switching; s and r are integer. Figure 8 shows the variation of $\tilde{I}$ as a function of the deformation μ for the $L_z=2$ and $L_z=0$ levels starting from the $(1h)$ spherical multiplct. First, we must notice that for the deformation range under interest here, $\tilde{I}$ is relatively a better invariant than the actions I_ε and I_ξ alone. In both cases, relative deviations of $\tilde{I}$ from the exactly conserved invariant are at least one order of magnitude less than they were for I_ε and I_ξ, as seen by comparing figure 8 with figure 3. Second, looking in more detail, the $L_z=2$ level has a very clear behaviour, but the situation is more confused with the $L_z=0$ level. For the deformation, which corresponds to the resonance ω_ε:$\omega_\xi=4$:1, which is indicated by an arrow on the right–hand part of figure 8(a), the new action defined by (24) is even better conserved than for other values of μ, and this for any initial conditions. The same behaviour occurs for other semiclassical $L_z\neq 0$ levels which cross only one resonance during adiabatic switching. For the $L_z=0$ level, shown in figure 8(b), the semiclassical eigenstate crosses the resonance ω_ε:$\omega_\xi=3$:1 twice: once before crossing the separatrix of the motion itself, located at $\mu_{\rm sep}=1.616\,581$, and the other after the separatrix. In figure 8(b), even if the global deviations from the exactly conserved value are smaller than those already obtained for each action I_ε or I_ξ, there is no clear signature of crossing a resonance in the zones indicated by arrows. Therefore, even if the system remains

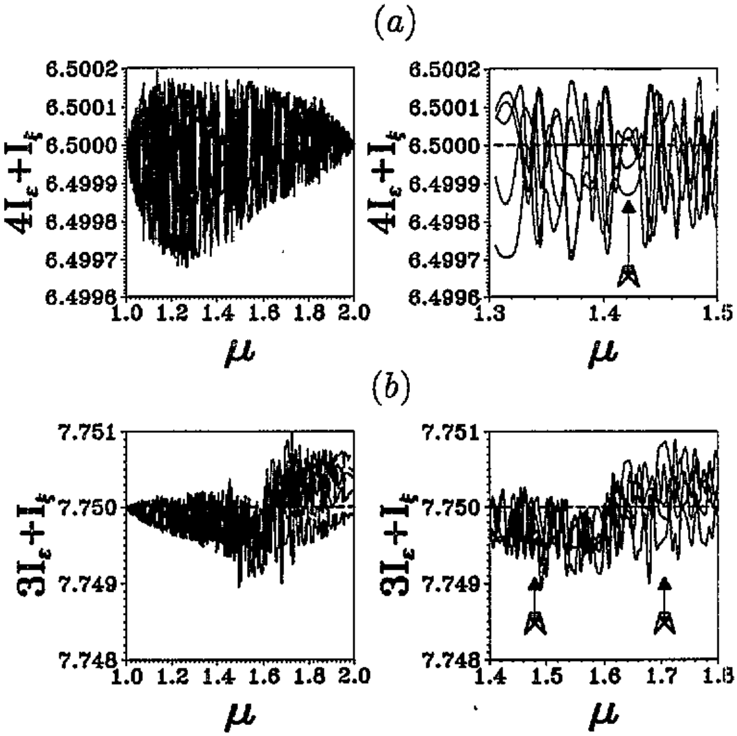

Figure 8. Two new invariants $\tilde{I}$ are studied during adiabatic switching; they are derived from the resonance ω_ε: $\omega_\xi=s$:r, where s and r are integers, which are crossed by the semiclassical level. The curves showing $\tilde{I}$ as a function of the deformation μ are drawn for the five randomly chosen initial conditions already used in figure 3. Frames (a) correspond to the $L_z=2$ level and 4:1 resonance, frames (b) to the $L_z=0$ level and 3:1 resonance, both belonging to the $(1h)$ spherical multiplet. The right-hand side is an enlargement of the left-hand side around the resonance zones. Resonance locations indicated by arrows, were exactly determined for figures 3, 4, 5 and 7.

integrable for any deformation, we are dealing with a special case where the two resonance zones are closed to the deformation for which the semiclassical eigenstate crosses the separatrix, which implies this unclear signature.

If we consider the $L_z=0$ level, starting from the (1*g*) spherical multiplet, for example, the semiclassical eigenstate crosses twice the resonance 3:1, before and after the separatrix and a little bit after the resonance 4:1; therefore, two different local invariants $\tilde{I}$ can be built. In this latter case, only the first invariant encountered during the adiabatic switching is significant. Indeed, after crossing the first resonance, the semiclassical trajectory crosses the separatrix and only later reaches the second resonance 4:1. Before this point, the variations of the actions around the exactly conserved value, due to the crossing of the first resonance and of the separatrix, are, relatively, too large, and a second invariant cannot be built.

5. Conclusion

The simple but non-trivial case of a free particle inside a prolate cavity gives us a good opportunity to test the adiabatic switching method in detail. In the present case, the classical actions associated with the motion were calculated at each step of the adiabatic switching, i.e. after each bounce of the particle on the boundary. Time evolution of the two classical actions during switching has shown many interesting features. First, as was expected from the beginning, the classical actions remain constant with a good accuracy as the deformation of the cavity is adiabatically changed from a spherical to a prolate shape. Second, small oscillations around the exactly conserved value arc related to the practical necessity of a finite switching time. In this way the solution depends on the initial conditions, i.e. on the angle variables. Third, crossing the separatrix, for the $L_z=0$ eigenstates, is clearly followed by abrupt changes of the actions in a small range sharply beginning at the semiclassical value of the deformation. Finally, abrupt changes on the actions could be seen for other values of the deformation, not only for the $L_z=0$ levels but also for the $L_z\neq0$ levels. The amplitudes of these changes are similar to those occurring for a separatrix crossing in the $L_z=0$ case. Such strange behaviour can be observed only once or more often, at special values of the deformation and depending on the eigenstate under study. It was shown that classical trajectories corresponding to such variations on the actions are all corresponding to resonances $\omega_\varepsilon:\omega_\xi=3:1$ and 4:1 between the radial ω_ε and angular ω_ξ frequencies. It was confirmed analytically that crossing of the primary resonances 3:1 and 4:1 are precisely correlated to abrupt variations of the classical action during adiabatic switching. Discontinuity on the ratio $\omega_\varepsilon:\omega_\xi$, for the $L_z=0$ levels, is exactly related to separatrix crossing. For other levels, $\omega_\varepsilon:\omega_\xi$ is a smooth function of the deformation which crosses resonance zones other than 3:1 and 4:1; the other resonances do not produce any effect on the action conservation. In conclusion, we have clearly shown how to understand the classical actions behaviour during adiabatic switching in the particular case of a prolate cavity. The method proposed to build a new invariant [11] is well verified in the case of levels for which there is an isolated crossing during adiabatic switching. Unfortunately, the method is of less interest when several are either closed together or are present with a separatrix during adiabatic switching. Finally, by checking carefully at each step every quantity, we have been able to study the domain of validity of the adiabatic switching method in the case for which it is more appropriate: an integrable system with simple separatrix crossings. In this case, as shown in I, the method provides a physically interesting classical frame with which one is able to follow the behaviour of the whole spectrum with deformation. There are, however, cases not discussed in our paper for which the crossing of the separatrix involves a semiclassical approximation that goes one step beyond the EBK approximation, as in the oblate cases. There it is known [15] that one has either two solutions or zero solution at the separatrix crossing and that it is necessary to use a uniform approximation. Such crossings are outside the field of a simple theory like ASM.

Acknowledgment

The author would like to acknowledge the Lawrence Berkeley Laboratory hospitality where part of this work was done and where the good working conditions and fruitful discussions in the nuclear theory group were greatly appreciated.

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