Semiclassical trace formula for truncated spherical well potentials – towards the analyses of shell structures in nuclear fission processes

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Contributions of degenerate families of periodic orbits to the semiclassical level density in truncated spherical hard-wall potentials are considered. In addition to the portion of the continuous periodic-orbit family contribution which persists after truncation, end-point correction to the truncated family should be taken into account. We propose a formula to evaluate this end-point correction as separate contributions of what we call marginal orbits. Applications to the two-dimensional billiard and three-dimensional cavity systems with the three-quadratic-surfaces shape parametrization, initiated to describe the nuclear fission processes, reveal unexpectedly large effects of the marginal orbits.

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I. INTRODUCTION

In quantum many-body systems such as nuclei and microclusters, the fluctuations in the physical quantities like energy and deformations as functions of the constituent particle number are essentially governed by the single-particle shell effects. In many cases, gross structures in the single-particle spectrum show regularly oscillating patterns. The origins of such patterns are clearly explained using the semiclassical periodic-orbit theory (POT), which expresses the quantum level density and shell energy in terms of the contributions of classical periodic orbits. This formula, known as the trace formula, immediately after its discovery by Gutzwiller[1, 2] and independently by Balian-Bloch[3, 4], has been recognized extremely useful in explaining the properties of gross shell structures in nuclei, shell and supershell structures in metallic clusters and so on. Degeneracies of levels in isotropic and anisotropic harmonic oscillator systems with rational frequency ratios are related to the conditions for most of the classical orbits to be periodic with short periods, which qualitatively explain the origins of spherical and superdeformed shell structures[5]. Strutinsky and coworkers applied the trace formula to explain the deformed shell structures in nuclear mean field[6]. Nishioka et al. have set out an elegant explanation of the supershell structures in metallic clusters as the interference of the contributions of triangle and square type periodic orbits in the spherical mean field[7].

In the low-energy fissions of the actinide nuclei, the appearance of double-humped structure in the fission barrier and the asymmetric fragment mass distributions are caused by the quantum shell effect[8]. According to the POT, shell structures associated with the periodic orbits which oscillate twice along the minor axis while they oscillate once along the major axis in strongly elongated mean-field potential play significant role in building the double-humped fission barrier[9–11]. Brack et al. have made a semiclassical analysis on the origin of the asymmetric fission using a simple cavity potential model[12]. They have found that the potential valley from symmetric normal-deformed minima towards strongly-elongated asymmetric shapes in the potential energy surface can be nicely explained by the contribution of the shortest periodic orbit.

More specifically, the fragment mass distribution in the low-energy nuclear fission experiments suggest strong effects of the fragment shell structures. In the fission of actinide nuclei, the mass numbers of the heavier fragments are around 140 independent on the mass of the parent nuclei, which is close to that of the doubly-magic $^{132}$Sn ($Z = 50, N = 82$). On the other hand, the recent experiment for the fission of neutron-deficient mercury isotope $^{180}$Hg shows asymmetric fragment-mass distribution in spite of the stability of the symmetric fragment $^{90}$Zr ($Z = 40, N = 50$) [13]. According to the theoretical analysis of the five-dimensional potential energy surface with macroscopic-microscopic model[14], the hindrance of symmetric fission in $^{180}$Hg is successfully interpreted as the result of large potential barrier along the symmetric path in the potential energy surface, which stem mainly from the shell effect. This implies the importance of the deformed shell effect in the fission process, rather than those of the final daughter nuclei, to understand the properties of the fragment mass distributions.

For the nucleus in the fission process whose mean-field potential consists of two fragment parts and the neck part between them, one may expect a kind of shell effect to stabilize the shapes and sizes of the fragment parts. Unexpectedly large fragment shell effect at early stage of the fission process was suggested by the two-center shell model calculation[17]. Emergences of the nascent fragments which have density profiles similar to those of stable spherical magic nuclei were found in a modern microscopic density-functional calculations[15, 16]. However, it is not a simple problem to extract the shell effect originated from the fragment parts out of those for the total system in purely quantum mechanical ways.

Here, we would like to put forward the idea of using the semiclassical POT to define the fragment shell effects. Formation of the neck in the potential generates periodic orbits which are confined in the fragment parts,
and the fragment shell effects are naturally identified as the contributions of those periodic orbits to the semiclassical level density. Based on this idea, we analyze the roles of fragment formation in stabilizing the shape of the nucleus in the fission process. In order to focus on the effect of shape evolution, a simple cavity potential model will be employed but with the ingenious three-quadratic-surfaces (TQS) shape parametrization which is useful in describing the nuclear fission processes. In this parametrization, two fragments and the neck part between them are represented by the quadratic surfaces, and their shapes are easily controlled by the shape parameters. Assuming spherical shapes for the fragments, we have to treat the classical periodic-orbit families confined in the truncated spheres for the semiclassical analysis of the deformed shell effect.

Periodic orbits which form a continuous family having the identical action and stability are called degenerate, and the order of degeneracy is defined by the number of independent continuous parameters for the family. In this paper, we derive the contribution of degenerate periodic-orbit families confined in the truncated spherical cavity potential based on the Balian-Bloch formula[4]. For simplicity, we begin with the two-dimensional (2D) bilayer system using the same shape parametrization. In Sec. II, the essence of the Balian-Bloch trace formula is briefly outlined, and then contributions of degenerate families of periodic orbits in 2D truncated circular bilayer and three-dimensional (3D) truncated spherical cavity are derived. They are applied to the TQS bilayer and cavity models in Sec. III. Sec. IV is devoted to summary and concluding remarks. Some details in derivations of the trace formulas are given in the Appendix.

II. TRACE FORMULA FOR DEGENERATE ORBITS IN HARD-WALL POTENTIALS

A. Balian-Bloch formula

In this section, we first outline the derivation of the Balian-Bloch formulas for semiclassical level density in hard-wall potential models[3, 4]. Consider a particle of mass $M$ which moves freely inside the closed surface $S$ and is reflected ideally on the wall. The energy of the particle is given by $E = \hbar^2 k^2 / 2M$ with the constant wave number $k$. The Green’s function for such a system is defined by

$$\left(-\frac{\hbar^2}{2M}\nabla^2 - E\right) G(r, r'; E) = \delta(r - r'), \quad (2.1)$$

with the Dirichlet boundary condition $G(r, r'; E) = 0$ for $r = r_s$ on the wall $S$. In terms of the Green’s function, level density $g(E)$ is expressed as

$$g(E) = \frac{1}{\pi} \Im \int_V dr G(r, r; E + i0) \quad (2.2)$$

where the volume integral is taken over the interior region $V$ of the closed surface $S$. By introducing a double-layer potential on the surface to ensure the boundary condition[18], multiple-reflection expansion formula for the Green’s function is derived[3], which is expressed as

$$G(r_0, r'_0; E) = G_0(0, 0') + \sum_{p=1}^\infty \left(\frac{\hbar^2}{M}\right)^p \int_S dS_1 \cdots dS_p \times \left.\frac{\partial G_0(0, p) \partial G_0(p, p - 1) \cdots \partial G_0(2, 1)}{\partial n_1} G_0(1, 0'). \quad (2.3)\right.$$  

Here, $G_0(b, a) = G_0(r_a, r_b; E + i0)$ denotes the Green’s function for a free particle, and $\partial / \partial n_a$ represents the component of the gradient normal to the surface $S$ at $r_a$. Each term on the right-hand side can be interpreted as the contribution of the wave which starts off $r'_0$ and hits $p$ times on the wall $S$ at $r_1, \ldots, r_p$ before arriving at $r_0$.

Substituting (2.3) into (2.2), one has

$$g(E) = g_0(E) + \frac{1}{\pi} \sum_{p=1}^\infty \left(\frac{\hbar^2}{M}\right)^p \int_V dV \int_S dS_1 \cdots dS_p \times \left.\frac{\partial G_0(0, p) \partial G_0(p, p - 1) \cdots \partial G_0(2, 1)}{\partial n_1} G_0(1, 0). \quad (2.4)\right.$$  

For sufficiently large $k$, integrations on the right-hand side can be carried out using the stationary-phase approximation (SPA), and the level density is expressed as the sum over contribution of the stationary paths, namely, the classical periodic orbits. The free-particle Green’s function $G_0$ is given by

$$\frac{\hbar^2}{2M} G_0(r_b, r_a; E) = \begin{cases} \frac{i}{4} H^{(1)}_\nu(kr_{ab}) \simeq \frac{e^{ikr_{ab}}}{\sqrt{8\pi k r_{ab}}}, & (2D) \\ e^{ikr_{ab}} / 4\pi r_{ab}, & (3D) \end{cases} \quad (2.5)$$

for the spatial dimension 2 and 3, with $r_{ab} = |r_b - r_a|$. In the expression for 2D billiard, $H^{(1)}_\nu$ denotes the $\nu$-th order Hankel function of the first kind, and the approximation on the right-hand side holds for the asymptotic limit $kr_{ab} \gg 1$. Using these expressions, one arrives at the general formula for the semiclassical level density

$$g(E) = g_0(E) + \text{Re} \sum_{\beta} a_{\beta}(k) \int_V dS_1 \cdots dS_p e^{ikl_{\beta}}. \quad (2.6)$$

$l_{\beta}$ denotes the total length of the polygon orbit with $p = p_{\beta}(\geq 2)$ vertices on the wall $S$,

$$l_p = r_{12} + r_{23} + \cdots + r_{p-1p} + r_{p1}, \quad (2.7)$$

which is expressed as a function of the local surface coordinates around the vertices of the stationary orbit $\beta$. The pre-exponential factor is evaluated for the stationary orbit $\beta$ and is put out of the integral into $a_{\beta}(k)$ as usual.
in the SPA (see Ref. [4] for its explicit form in the 3D case). For an isolated periodic orbit, all the surface integrals in (2.6) are carried out by expanding the length $l_p$ with respect to the surface coordinates up to the second order around the stationary point, and the integrals are reduced to the Fresnel type. The result can be translated to the Gutzwiller trace formula [1, 2]

$$g(E) = g_0(E) + \sum_{\beta} \sum_{m=1}^{\infty} \frac{T_\beta}{\pi h \sqrt{\text{det} (M_\beta^m - I)}} \times \cos \left( m k L_\beta - \frac{\pi}{2} \mu_{m\beta} \right).$$

On the right-hand side, the sum is taken over all the primitive periodic orbits and the numbers of their repetitions $m$ ($m = 1$ corresponds to the primitive orbit). $T_\beta$ is the period of the primitive orbit $\beta$.

$$T_\beta = \frac{dS_\beta}{dE} = \frac{M L_\beta}{\pi k^2 k}.$$ (2.9)

with the wave number $k = \sqrt{2ME}/h$ and the orbit length $L_\beta$. In Eq. (2.8), $M_\beta$ represents the monodromy matrix which describes the stability of the orbit, and $\mu_{m\beta}$ is the Maslov index related to the number of focal and caustic points along the orbit [1, 2]. The level density in terms of the wave-number variable $k$ is written as

$$g(k) = g(E) \left| \frac{dE}{dk} \right| = g_0(k) + \sum_{\beta} \sum_{m=1}^{\infty} \frac{L_\beta}{\pi \sqrt{\text{det} (M_\beta^m - I)}} \times \cos \left( m k L_\beta - \frac{\pi}{2} \mu_{m\beta} \right).$$ (2.10)

In a Hamiltonian system with continuous symmetries, generic periodic orbits form continuous families generated by the symmetry transformations. For such degenerate periodic orbits, some of the integrals in (2.6) should be carried out exactly with respect to the continuous parameters for the family. The extensions of the Gutzwiller trace formula to systems with continuous symmetries are presented in [6, 19].

In a 2D circular billiard with radius $R_0$, there are regular polygon orbits labeled by two integers $(p, t)$ where $p$ is the number of vertices and $t$ is the number of turns around the center ($p \geq 2t$). A primitive orbit is specified by an incommensurable pair of $p$ and $t$, and the repeated orbit with repetition number $m$ is denoted by $m(p, t)$. Each of those orbits forms a one-parameter family due to the rotational symmetry. Then, integrals in Eq. (2.6) are done exactly for the one surface coordinate associated with the degeneracy and the others using the SPA. The analytic expression of the result for the orbit $(p, t)$ is obtained as [20, 21]

$$g_{m(p, t)}^{(\text{circ})}(k) = 2R_0 \sqrt{kR_0} A_{m(p, t)}^{(\text{circ})}(k) \sin \left( km L_{pt} - \frac{\pi}{2} \mu_{m(p, t)}^{(\text{circ})} \right).$$ (2.11)

with the dimensionless energy-independent amplitude factor $A$, orbit length $L$ and the Maslov index $\mu$ given by

$$A_{m(p, t)}^{(\text{circ})} = w_{pt} \sqrt{\frac{\sin^3 \varphi_{pt}}{mp \pi}}, \quad \varphi_{pt} = \frac{\pi t}{p},$$

$$L_{pt} = 2pR_0 \sin \varphi_{pt}, \quad \mu_{m(p, t)}^{(\text{circ})} = 3mp - \frac{3}{2}. \quad (2.12)$$

Here, $w_{pt}$ represents the time-reversal factor: It takes the value 2 for polygon orbits ($p > 2t$) to take into account the orbits turning clockwise and anti-clockwise, while it takes the value 1 for diameter orbits ($p = 2t$) whose time reversals are equivalent to the original ones.

In a 3D spherical cavity potential with radius $R_0$, there exist the same set of periodic orbits as those in the circular billiard but with different degeneracies [4]. Polygon orbits ($p > 2t$) form three-parameter families generated by the three-dimensional rotations. To obtain the contribution of such a family, the integrals in Eq. (2.6) are done exactly for three surface coordinates associated with the degeneracy and others by using the SPA. The result is expressed as [4]

$$g_{m(p, t)}^{(\text{sph})}(k) = 2R_0(kR_0)^{3/2} A_{m(p, t)}^{(\text{sph})} \sin \left( km L_{pt} - \frac{\pi}{2} R_0^{(\text{sph})} \right),$$ (2.13)

with

$$A_{m(p, t)}^{(\text{sph})} = \sin(2\varphi_{pt}) \sqrt{\frac{\sin \varphi_{pt}}{mp \pi}}, \quad \mu_{m(p, t)}^{(\text{sph})} = m(2t - p) - \frac{3}{2}. \quad (2.14)$$

On the other hand, the diameter orbit ($p = 2t$) forms a two-parameter family since the rotation about the diameter itself does not generate a family. The contribution of the diameter family $m(2, 1)$ is also derived from Eq. (2.6) in the same manner as the polygon orbits, and is expressed as [4]

$$g_{m(2, 1)}(k) = 2R_0(kR_0)^{3/2} A_{m(2, 1)}^{(\text{sph})} \sin \left( km L_{21} - \frac{\pi}{2} \mu_{m(2, 1)} \right) \quad (2.15)$$

with

$$A_{m(2, 1)}^{(\text{sph})} = \frac{1}{2km}, \quad \mu_{m(2, 1)} = 2. \quad (2.16)$$

In general, gross shell structure is governed by the contribution of some shortest periodic orbits. In Fig. 1, oscillating part of the level density averaged with the width $\gamma$

$$\delta g_{\gamma}(k) = \int dk' [g(k') - \bar{g}(k')] \exp \left[ -\frac{1}{2} \left( \frac{k - k'}{\gamma} \right)^2 \right] \quad (2.17)$$

is shown for the 2D circular billiard and the 3D spherical cavity. The smoothing width $\gamma = 0.3$ is taken, for which
only the orbits with length $L \lesssim \pi/\gamma \approx 10$ contribute. In the 2D circular billiard, all the periodic orbits form one-parameter family and the dominance of their contribution to the gross shell structure is mainly determined by the shortness of the length. In the upper panel of Fig. 1, one sees that the quantum result of $\delta g_\theta(k)$ for 2D circular billiard is nicely reproduced by the semiclassical formula (2.11) with the contribution of two shortest orbits, diameter (2,1) and triangle (3,1). In the 3D spherical cavity, the shortest orbit is the diameter, but it plays a minor role compared with the other polygon families due to the low degeneracy. In the lower panel of Fig. 1, the quantum result of $g_\theta(k)$ for 3D spherical cavity is compared with the semiclassical trace formula (2.13) taking the contributions of triangle (3,1) and square (4,1) families into account. One sees that the outstanding beating pattern called supershell structure is successfully reproduced as the interference effect of those two orbits[4]. The agreements of the semiclassical trace formula with the quantum results are already fine with the above two main orbits, and become much better when the contributions of other remaining orbits are incorporated.

B. Two-dimensional truncated circular billiard

Now we consider a 2D billiard system with the wall partly consists of a circular arc whose central angle is larger than $\pi$. In such a billiard potential, one has a degenerate family of diameter orbit confined in the circle part. In general, there exists a family of regular polygon orbit with $p$ vertices when the central angle of the arc is larger than $2\pi(1 - 1/p)$. As an example shown in Fig. 2, the rotation around the center O generates a continuous family of the triangle orbit (3,1) ranges from ABC to A′B′C′. To avoid the complication due to singularities, we assume that the circle part of the wall is smoothly connected to the neighboring walls AP and C′Q as illustrated in Fig. 2.

Let us consider the contribution of this orbit family to the semiclassical level density based on Eq. (2.6). Fixing the position of the first vertex $P_1$, the positions of the other vertices of the stationary path are uniquely determined. We take $s_1 = R\theta$ as the position of $P_1$ and $s_j$ ($j \geq 2$) as the displacement of the $j$-th vertex from its position in the stationary path for given $s_1$. Figure 3 schematically shows the distribution of periodic orbits on the surface coordinate space $s = (s_1, \cdots, s_p)$. The panel (a) illustrates the contour plot of the length $l_{pt}$ near the truncated periodic-orbit family. The stationary points of the length $l_{pt}$ give the periodic orbits, and the thick solid line represents the continuous set of stationary points corresponding to the degenerate periodic-orbit family parameterized by the rotation angle $\theta$. It is truncated at $\theta = \theta_A$ and $\theta_A$ indicated by the dots, which correspond to what we call the marginal orbits. We evaluate the integrals in Eq. (2.6) by dividing the integration range into two parts: the interior portion (principal term) and the area around the end points (marginal term). In the interior portion of the family, $\theta_A < \theta < \theta_A$, the orbit length $l_{pt}$ is expanded with respect to $s_\perp = (s_2, \cdots, s_p)$ as

$$l_{pt}(s) = L_{pt} + \frac{1}{4R} \sum_{a,b \geq 2} K_{ab} s_a s_b + O(s_\perp^4),$$  \hspace{1cm} (2.18)
where the orbit length become as shown Fig. 3(c), and the orbits at the end of the family become isolated. For these hypothetical isolated orbits, which we call marginal orbits, it is possible to calculate their monodromy matrices and Maslov indices in a standard numerical prescription. Thus, the end-point correction to the truncated family contribution, from the shaded area shown in Fig. 3(c), is given by the half of the Gutzwiller formula (2.10) for each of those isolated marginal orbits $\beta$ as

$$g^{(mg)}_{pt,\beta}(k) = 2RA_{pt,\beta}^{(mg)} \sin \left( kL_{pt} - \frac{2}{2} \theta_{pt,\beta} \right),$$  \hspace{1cm} (2.23)

with

$$2RA_{pt,\beta}^{(mg)} = \frac{w_{pt}L_{pt}}{2\pi \sqrt{|\det(M_{pt,\beta} - I)|}}.$$  \hspace{1cm} (2.24)

In Eq. (2.23), we took sine, in contrast to cosine in Eq. (2.10), for the definition of the Maslov index in suit with Eq. (2.11).

Finally, the total contribution of the family of orbit $(p, t)$ confined in the circle part is given by the sum of the principal and marginal terms as

$$g^{(tot)}_{pt}(k) = g^{(pr)}_{pt}(k) + \sum_{\beta} g^{(mg)}_{pt,\beta}(k),$$  \hspace{1cm} (2.25)

where the sum in the second term is taken over the two marginal orbits.

C. Three-dimensional truncated spherical cavity

Next we consider a 3D cavity potential whose wall partly consists of a truncated sphere with radius $R$. As shown in Fig. 4, the spherical part is centered at O, truncated with the plane perpendicular to the axis OZ, and smoothly connected to the neighboring part of the surface which is assumed to be axially symmetric about the axis OZ. In the truncated spherical cavity, one has the same set of periodic-orbit families as those in the complete (non-truncated) spherical cavity, but with the restricted ranges of the parameters.
by Peral, the maximum angle the entire orbit fits the confines in the spherical part. In general, the maximum angle \( \vartheta_B \) for the orbit \((p, t)\) is given by

\[
\vartheta_B = \begin{cases} 
\pi - \vartheta_A & \text{for even } p, \\
\pi & \text{for odd } p \text{ with } \vartheta_A \leq \frac{\pi}{p}, \\
\cos^{-1} \left[ \frac{\cos \vartheta_A}{\cos(\pi/p)} \right] & \text{Id. but } \vartheta_A > \frac{\pi}{p}.
\end{cases}
\]

We consider the principal part of the integrals in Eq. (2.6) taking into account the degeneracies of the orbit. As illustrated in Fig. 5, we define the local surface coordinates \((x_a, y_a)\) on the surface \(S\) around the vertex \(P_a\) of a given periodic orbit, where \(x_a\) is taken along the orbital plane \(N_a\), and \(y_a\) perpendicular to it.

Let us first consider a diameter family (2.1). In this case, the orbit in the family is uniquely determined by fixing the position of the first vertex \(P_1\), and the coordinates \((x_1, y_1)\) are varied in the available range which fix the orbit in the family. Then, in the Eq. (2.6), the integrals over \((x_1, y_1)\) are done exactly in the available range to cover all the members of the family, and the other \((2p - 2)\) integrals are carried out using the SPA. The integration over \((x_1 = R\vartheta_1, y_1 = R\varphi_1 \sin \vartheta_1)\) gives

\[
\int dx_1 dy_1 = \int R^2 \vartheta_1 \cdot R \sin \vartheta_1 d\varphi_1 = 2\pi R^2 \int_{\vartheta_A}^{\pi-\vartheta_A} \sin \vartheta d\vartheta = 4\pi R^2 \cos \vartheta_A. \tag{2.27}
\]

We define \(f_2\) as the relative volume of the parameter space occupied by the truncated diameter family compared with that for the complete (non-truncated) spherical cavity, which will be called “occupation rate” in short. Since the same integral as (2.27) in the complete spherical cavity gives the factor \(4\pi R^2\), one obtains

\[
f_2 = \cos \vartheta_A. \tag{2.28}
\]

Since the remaining \((2p - 2)\) integrals using the SPA gives the result equivalent to that for the complete spherical cavity, the principal contribution of the truncated diameter family is given by

\[
\vartheta_{m(2,1)}^{(pr)}(k) = f_2 \vartheta_{m(2,1)}^{(sph)}(k), \tag{2.29}
\]

with \(\vartheta_{m(2,1)}^{(sph)}(k)\) given by Eq. (2.15).

For polygon family \((p, t)\) \((p > 2t)\), after fixing the first vertex \(P_1\), one can further rotate the orbit about the axis \(OP_1\) as shown in Fig. 4(b). We define \(\psi\) by the rotation angle of the orbit from its position where the orbital plane is perpendicular to the plane defined by the symmetry axis \(OZ\) and the axis of rotation \(OP_1\). Its maximum value \(\psi_p\) is given by

\[
\sin \psi_p(\vartheta) = \frac{\cos \vartheta_A - \cos(2\pi j/p) \cos \vartheta}{\sin(2\pi j/p) \sin \vartheta}, \tag{2.30}
\]

if the vertex \(P_{j+1}\) with \(\angle P_1OP_{j+1} = 2\pi j/p\) touches the joint circle in first by the above rotation. If no vertices touch the joint with the rotation, one simply has \(\psi_p = \pi/2\). Thus, for the polygon family, the integrals in (2.6) should be done exactly for three coordinates, \(x_1 = R\vartheta_1, \)

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y_1 = R\varphi_1 \sin \vartheta_1 \text{ and } y_2 = R\psi \sin(2\varphi_{pt}). \text{ For a given (x_1, y_1), the integral over } \psi \text{ simply gives } 4\psi_p(\vartheta_1), \text{ and one obtains}
\[ \int dx_1 dy_1 dy_2 = \int R d\vartheta_1 \cdot R \sin \vartheta_1 d\varphi_1 \cdot R \sin(2\varphi_{pt}) d\psi = 8\pi R^3 \sin(2\varphi_{pt}) \int_{\vartheta_A}^{\vartheta_B} \psi_p(\vartheta) \sin \vartheta d\vartheta. \quad (2.31) \]

Since the same integral for the complete spherical cavity gives \(8\pi R^3 \sin(2\varphi_{pt})\), one obtains the occupation rate \(f_p\) for the family \((p, t)\) as
\[ f_p = \int_{\vartheta_A}^{\vartheta_B} \psi_p(\vartheta) \sin \vartheta d\vartheta. \quad (2.32) \]

The remaining \((2p - 3)\) integrations in (2.6) using the SPA give exactly the same results as those for the complete spherical cavity, and the principal contribution of the polygon family \((p, t)\) to the level density is expressed as
\[ g_{pt}^{(pr)}(k) = f_p g_{pt}^{(ph)}(k) \quad (2.33) \]

with \(g_{pt}^{(ph)}(k)\) given by Eq. (2.13).

In addition to the above principal terms, one should consider the end-point corrections. They are associated with the marginal orbits whose first vertex \(P_1\) is on the joint of the spherical and the neighboring walls as shown in Fig. 6. For such orbits, we transform the local surface coordinate \((x_1, y_1)\) to \((\xi_1, \eta_1)\) so that \(\xi_1\) is along the joint circle and \(\eta_1\) perpendicular to it along the surface outside the spherical wall as indicated in Fig. 6. Then, the integral over \(\vartheta_1 > 0\) is executed using the SPA. The contribution of the marginal orbit is obtained, just in the same manner as the billiard case, by extending the wall neighboring the spherical part into the inner region around \(P_1\) so that the curvature of the surface is continuous there. It makes the marginal orbit to be a family with reduced degeneracy whose symmetry-reduced monodromy matrices and the Maslov indices can be calculated in the standard prescription. For the marginal diameter family, which forms a one-parameter family generated by the rotation about the symmetry axis, the integral over \(\xi_1\) is executed exactly and the rest of the \((2p - 1)\) integrals are carried out using the SPA. The contribution to the level density is expressed as
\[ g_{21}^{(mg)}(k) = 2R\sqrt{kR A_{21}^{(mg)}} \sin \left( kL_{21} - \frac{\pi}{2} \mu_{21}' \right), \quad (2.34) \]

where \(A_{21}^{(mg)}\) represents the dimensionless energy-independent amplitude factor. For the marginal polygon family, which forms a two-parameter family, the integrals with respect to \((\xi_1, y_j)\) are executed exactly and the rest of 2\(p\) integrals are carried out by using the SPA. The result is expressed as
\[ g_{pt}^{(mg)}(k) = 2R(kR A_{pt}^{(mg)}) \sin \left( kL_{pt} - \frac{\pi}{2} \mu_{pt}' \right). \quad (2.35) \]

See Appendix A for the explicit form of the amplitude factor \(A_{pt}^{(mg)}\).

For a marginal polygon family for which Eq. (2.30) gives the angle \(\psi_p(\vartheta_A) < \pi/2\), one should consider a secondary marginal orbit which have two vertices \(P_1\) and \(P_j\) on the joint. It forms a one-parameter family, and its contribution is evaluated by executing the integral over \(\xi_1\) exactly and the other \((2p - 1)\) integrals through the SPA to obtain
\[ g_{pt}^{(mm)}(k) = 2R\sqrt{kR A_{pt}^{(mm)}} \sin \left( kL_{pt} - \frac{\pi}{2} \mu_{pt}'' \right). \quad (2.36) \]

The explicit form of the amplitude factor \(A_{pt}^{(mm)}\) is also given in Appendix A.

Finally, the total contribution of the family of orbit \((p, t)\) confined in the spherical part of the wall is given by
\[ g_{pt}^{(tot)}(k) = g_{pt}^{(pr)}(k) + g_{pt}^{(mg)}(k) + g_{pt}^{(mm)}(k). \quad (2.37) \]

### III. APPLICATIONS TO THE THREE-QUADRATIC-SURFACES POTENTIALS

#### A. The three-quadratic-surfaces parametrization

As applications, we consider the 2D billiard as well as axially symmetric 3D cavity with three-quadratic-surfaces (TQS) parametrization[22], which is designed to describe the nuclear fission processes. The potential wall consists of three parts, two fragments and neck between them as shown in Fig. 7, and each of them is given by the axially-symmetric quadratic surface \(\rho = \rho_s(z)\) expressed as
\[ \rho_s^2(z) = \begin{cases} \alpha_1^2 - \frac{\alpha_2^2}{a_1}(z - l_1)^2 & (z_{\min} < z < z_1) \\ \alpha_2^2 - \frac{\alpha_3^2}{a_2}(z - l_2)^2 & (z_1 < z < z_2) \\ \alpha_3^2 - \frac{\alpha_4^2}{a_3}(z - l_3)^2 & (z_2 < z < z_{\max}) \end{cases} \quad (3.1) \]

On the right-hand side, first and third lines describe the left and right fragments centered at \(z = l_1\) and \(l_2\). The
second line describes the neck part which is smoothly connected to the left and right fragments at $z = z_1$ and $z_2$, respectively. Note that the neck part is concave in most cases, for which one has $c_3^2 < 0$. The continuity of $\rho_s(z)$ and $\rho'_s(z)$ at the joints $z = z_1$ and $z_2$ impose four constraints to the eleven parameters $\{a_{1-3}, c_{1-3}, l_{1-3}, z_{1,2}\}$, and the center-of-mass and volume conservation conditions impose two more constraints. (The last two conditions are imposed assuming the 3D axial cavity, and we use the same values of the parameters also in the 2D billiard.) Thus, one eventually has five free parameters which describe the shape of the potential. One of the useful choice for the shape parameters are $\{\sigma_{1-3}, \alpha_{1-3}\}$ defined by

$$
\sigma_1 = \frac{l_2 - l_1}{u}, \quad \alpha_1 = \frac{l_1 + l_2}{2u}, \quad \text{with} \quad u = \sqrt{\frac{a_1^2 + a_2^2}{2}},
$$

$$
\sigma_2 = \frac{a_3}{c_3}, \quad \alpha_2 = \frac{a_2 - a_3^2}{n^2},
$$

$$
\sigma_3 = \frac{1}{2}\left(\frac{a_1^2 + a_2^2}{c_1^2 + c_2^2}\right), \quad \alpha_3 = \frac{a_1^2}{c_1^2} - \frac{a_2^2}{c_2^2}.
$$

The parameter $\sigma_1$ describes the elongation, $\sigma_2$ gives the neck curvature, $\alpha_2$ is related to the fragment mass asymmetry, $\sigma_3$ and $\alpha_3$ determine the shapes of the fragments. The parameter $\alpha_1$ represents the asymmetry of the positions of the fragments from the center of mass, and it is automatically determined by the other 5 parameters.

Here, we limit ourselves to the case of symmetric shapes ($\alpha_{1-3} = 0$) with fixed neck curvature ($\sigma_2 = -0.6$) and spherical fragments ($\sigma_3 = 1$). The shapes of the wall for several values of $\sigma_1$ are shown in Fig. 8.

We discuss here the properties of classical periodic orbits in the TQS wall.

### B. Classical periodic orbits in the TQS wall

The parameter $\sigma_1 = 2.0$, $\sigma_2 = -0.6$ and $\sigma_3 = 1$. The name of the orbits are given after the number of vertices, the type of the shape (acronym of linear, rotational, butterfly or V-shaped), and an alphabetic identifier.
ment parts. As in the complete spherical cavity, the polygon orbits \((p > 2t)\) form three-parameter families and the diameter orbits \((p = 2t)\) form two-parameter families. The orbits shown in Fig. 9 in this case will form one-parameter families generated by the rotation about the symmetry axis, except the diameter 2La which remains isolated. In addition, one has orbits on the equatorial plane in the neck surface and three-dimensional orbits, which also form one-parameter families. From the view point of the semiclassical expansion with respect to the degeneracy, shell effect might be mainly governed by the three-parameter polygon families in the fragments, with relatively small contribution of the two-parameter diameter family, and the other one-parameter families might play only minor roles.

C. Fourier analysis

In the billiard and cavity systems, action integral along the orbit is given by a simple product of the wave number \(k\) and the orbit length \(L_\beta\). Owing to such a simple energy dependence of the phase part, one obtains a clear correspondence between the classical periodic orbits and quantum level density through the Fourier analyses. We consider the Fourier transform of the level density defined by

\[
F(L) = \sqrt{\frac{2}{\pi}} \int_0^\infty dk \frac{g(k)e^{ikL}e^{-(k/k_c)^2/2}}{\sqrt{|\det[M_\beta - I]|}},
\]

where we have introduced a Gaussian factor with the cutoff momentum \(k_c\) in the integrand to truncate the high energy part \(k \gg k_c\) of the level density which is unavailable in the numerical calculation. Inserting the quantum level density \(g(k) = \sum_i \delta(k - k_i)\), one has

\[
F^{(qm)}(L) = \sqrt{\frac{2}{\pi}} \sum_i e^{ik_i L}e^{-(k/k_c)^2/2},
\]

which can be easily evaluated using the quantum spectrum. The semiclassical level density is expressed in a form

\[
g(k) = g_0(k) + 2R_0 \sum_{\beta} (kR_0)^{D_\beta/2} A_\beta \sin \left( kL_\beta - \frac{\pi}{2} \mu_\beta \right),
\]

where \(D_\beta\) is the degeneracy of the orbit family \(\beta\). Inserting (3.6) into (3.4), one has

\[
F^{(sc)}(L) = F_0(L) + i \sum_{\beta} (k_cR_0)^{1+D_\beta/2} A_\beta e^{i\pi \mu_\beta/2} \times A_{D_\beta}(k_c(L - L_\beta)),
\]

where

\[
A_D(y) = \sqrt{\frac{2}{\pi}} \int_0^\infty dx x^{D/2} e^{iyx} e^{-x^2/2}
\]

is a function whose modulus has a peak at the origin \(y = 0\) as shown in Fig. 11. Thus, the Fourier amplitude of the quantum level density calculated with Eq. (3.5) will exhibit successive peaks at the lengths of classical periodic orbits, whose heights are proportional to the amplitude factor \(A_\beta\) of the semiclassical level density. If the cutoff momentum \(k_c\) is large enough to single out the peak of the orbit \(\beta\) from those of the other orbits, the modulus of the Fourier transform at \(L = L_\beta\) is given by

\[
|F(L_\beta)| = (k_cR_0)^{1+D_\beta/2} A_D(0) A_\beta,
\]

\[
A_D(0) = \frac{2^{D/2} \Gamma(1 + D/2)}{\sqrt{\pi}}.
\]

Taking account of all the marginal families, the contribution of the orbit \((p, t)\) to the level density of the truncated circular billiard or the truncated spherical cavity is written as

\[
g_{pt}(k) = 2R \sum_D (kR)^{D/2} A_{pt}^{(D)} \sin \left( kL_{pt} - \frac{\pi}{2} \mu_{pt}^{(D)} \right)
\]
where the sum is taken over the degeneracy parameter $D$ (see Appendix A). It can be written in a more compact form as

$$ g_{pt}(k) = 2R|A_{pt}(kR)|\sin\left(\frac{k L_{pt} - \frac{\pi}{2} \mu_{pt}^{(\text{eff})}}{D/2}\right), \quad (3.12) $$

with the complex amplitude $A_{pt}$ and effective Maslov index $\mu_{pt}^{(\text{eff})}$ defined by

$$ A_{pt}(x) = \sum_{D} x^{D/2} A_{pt}^{(D)} e^{-i\pi \mu_{pt}^{(D)}/2}, \quad (3.13) $$

$$ -\frac{\pi}{2} \mu_{pt}^{(\text{eff})}(x) = \arg A_{pt}(x). \quad (3.14) $$

The Fourier transform at $L = L_{pt}$ is then given by

$$ F(L_{pt}) = i \sum_{D} (k_{c} R)^{1+D/2} e^{i\pi \mu_{pt}^{(D)}/2} A_{D}(0) A_{pt}^{(D)} \quad (3.15) $$

$$ \approx 0.8 i k_{c} R A_{pt}^{(0)}(k_{c} R). \quad (3.16) $$

In the last approximation, we used $A_{D \geq 1}(0) \approx 0.8$ as seen in Fig. 11. Thus, the Fourier transform of the quantum level density provides us the direct information on the amplitude $A_{pt}$ which represents the combined contribution of the principal and marginal terms.

**D. Two-dimensional TQS billiard**

In this section, we investigate the quantum-classical correspondence in the 2D TQS billiard system using the Fourier transformation technique discussed above. In the top panel of Fig. 12, moduli of the quantum Fourier transform $|F^{(\text{qu})}(L; \sigma_1)|$ is displayed as the functions of $L$ and $\sigma_1$. In the bottom panel, lengths of some classical periodic orbits are plotted as functions of $\sigma_1$. As expected from the semiclassical trace formula, Fourier amplitude of the quantum level density show peaks at the lengths of the classical periodic orbits. For the circular shape ($\sigma_1 = 0$), one sees strong Fourier peaks at $L = L_{21}(= 4)$, $L_{31}(= 3\sqrt{3} = 5.19)$ and $L_{41}(= 4\sqrt{2} = 5.66)$ corresponding to the diameter, triangle and square orbits, respectively. Those peaks decay with increasing $\sigma_1$, but the peak of the diameter orbits confined in the fragments (labeled “2F”) grows up again at large $\sigma_1$.

Figure 13 shows the Fourier amplitude $|F(L_{21}(\sigma_1))|$ evaluated at the length of the diameter orbit as functions of the deformation parameter $\sigma_1$. The quantum mechanical result is compared with the semiclassical one given by (3.16). It is found that the principal term considerably underestimates the quantum result in the energy region considered, especially for the case of small $\sigma_1$. After taking into account the contributions of the marginal orbits, the quantum result is reasonably reproduced for $\sigma_1 \gtrsim 1.0$. For smaller $\sigma_1$, the breaking of the total rotational symmetry should be treated appropriately using a kind of uniform approximation, but it is beyond the scope of the current work.

Figure 14 shows the oscillating part of the quantum and semiclassical level densities (2.17) for TQS billiard with the deformation parameter $\sigma_1 = 1.0, 2.0$. Values of the averaging width $\gamma = 0.2$ and 0.5 are used to see the fine and gross shell structures, respectively. In each panel, one sees that the quantum results are nicely reproduced by the semiclassical trace formulas taking account of the contribution of short isolated orbits shown in Fig. 9 as well as the diameter orbit family confined in the fragments. The contribution of the isolated orbits are calculated with the Gutzwiller formula (2.10). In the contribution of the diameter family confined in the fragments, both principal and marginal terms are taken into account. As shown in the plots for $\gamma = 0.5$, the contribution of the primitive diameter orbit family dominates the gross shell structures.
E. Three-dimensional TQS cavity

Next, we consider the 3D TQS cavity systems. Unlike the 2D billiard, one has all \((p, t)\) families confined in the spherical fragments for all values of \(\sigma > 0\). The principal contribution of the three-parameter polygon families \((p > 2t)\) and two-parameter diameter families \((p = 2t)\) are obtained with the occupation rate \(f_p\) given by Eq. (2.32) and (2.28) as

\[
g_{pt}^{(pr)}(k; \sigma) = 2 \sum_{pt} f_p g_{pt}^{(sph)}(k; R(\sigma)), \quad (3.17)
\]

where \(g_{pt}^{(sph)}(k; R)\) represents the contribution of the orbit family \((p, t)\) in the spherical cavity with radius \(R\), and the overall factor 2 counts the families in two fragments which are equivalent for the symmetric shapes. Numerical results of the occupation rate \(f_p\) for the symmetric TQS cavity with \(\sigma_2 = -0.6, \sigma_3 = 1, \alpha_{1-3} = 0\) and several values of \(\sigma_1\) are shown in Table I. With increasing \(\sigma_1\), the angle \(\vartheta_A\) indicated in Fig. 4 becomes smaller. Then the occupation rates \(f_p\) increases and it makes the contribution of the orbit family confined in the spherical fragments more important.

To quantify the contributions of the periodic orbits, we examine the Fourier transform of the level density (3.4) just as in the 2D billiard case. Figure 15 shows the Fourier amplitude \(|F(L; \sigma_1)|\) of the quantum level density as function of \(L\) and \(\sigma_1\) (upper panel) and the lengths of the classical periodic orbits (lower panel). At the spherical shape \((\sigma_1 = 0)\), one finds especially large peaks corresponding to the triangle and square orbits, and the peak of the diameter orbit is relatively small due to the lower degeneracy [note the factor \((k, R)\delta_{1/2}\) in Eq. (3.7)]. With increasing \(\sigma_1\), those peaks promptly decay, and then the peaks corresponding to the orbit families confined in the fragments begin to grow up. Espe-

| \(\sigma_1\) | 1.0 | 1.5 | 2.0 | 2.5 | 3.0 |
|---|---|---|---|---|---|
| \(\vartheta_A\) [deg] | 79.193 | 73.665 | 67.975 | 62.047 | 55.771 |
| \(f_2\) | 0.18760 | 0.28088 | 0.37562 | 0.46851 | 0.56190 |
| \(f_3\) | 0.02962 | 0.06823 | 0.12650 | 0.21112 | 0.34345 |
| \(f_4\) | 0.02266 | 0.05169 | 0.09436 | 0.15204 | 0.22924 |
| \(f_5\) | 0.02055 | 0.04683 | 0.08504 | 0.13652 | 0.20416 |
Quantum and semiclassical results for the Fourier amplitude at the lengths of classical periodic orbits \((p,t)\), \(|F(L_{pt})|\), relative to those for the spherical cavity are shown in Fig. 16. Similarly to the 2D billiard case, the principal term considerably underestimate the quantum Fourier amplitude. By taking into account the marginal terms, quantum results are nicely reproduced for both diameter and triangle orbits. In the figure for diameter orbit, ragged behavior of the quantum Fourier amplitude might be due to the interference with the other periodic orbits, since the lengths of some equatorial orbits on the neck surface cross with the fragment diameter around \(\sigma_1 \sim 2\) as seen in Fig. 15(b).

As shown in Fig. 16(b), contribution of the secondary-marginal orbit is considerably smaller than the principal and marginal contributions. The contributions of other one-parameter families such as shown in Fig. 9 are expected to be the same order of the secondary-marginal family, and it may not be so bad just to ignore them for simplicity. It is also justified from the Fourier spectrum shown in Fig. 15(a) where one finds no significant peaks along those orbits. Thus, we can consider the semiclassical level density simply with the periodic-orbit families confined in the fragments.

In Fig. 17, quantum level density is compared with the semiclassical trace formula including the contributions of diameter \((2,1)\) and polygon families \((p,1)\) with \(3 \leq p \leq 5\) confined in the fragment parts. In these calculations, averaging width is taken as \(\gamma = 0.3\). For every values of deformation \(\sigma_1\), quantum results are nicely reproduced by the contributions of those fragment-orbit families. One also sees that the quantum fluctuations are mostly attributed to the contribution of the triangle family for large \(\sigma_1\) where the neck is well developed. This can be
Based on the Balian-Bloch formula, we have derived the contribution of degenerate family of orbits confined in 2D truncated circular billiard and 3D truncated spherical cavity. In addition to the truncated portion of the original families, contributions of the marginal orbits should be considered independently as the end-point correction to the former. In applications to the 2D billiard and 3D cavity potentials with TQS shape parametrization, our formulas successfully reproduce the quantum mechanical results. Although the contributions of the marginal orbits are expected to play minor roles in the semiclassical limit due to the lower degeneracies, it turns out that they play significant role on the shell effects in the energy region of nuclei. Their effect is important especially for small deformation where only a small portion of the parameter space is occupied by the fully-degenerate periodic-orbit families, and will be responsible for a fragment shell effect emerging at an early stage of the fission deformation process.

Using our trace formula, shell effect associated with the fragments is extracted in simple and natural way and can be evaluated quantitatively through the nuclear fission processes. In this way, the periodic-orbit theory provides us a powerful tool to investigate the nuclear fission dynamics. Detailed analysis of the potential energy surface taking into account the asymmetric shape degree of freedom in the TQS cavity model and discussions on the origin of asymmetric fission will be presented in a separate paper[23].

IV. SUMMARY AND CONCLUSION

Based on the Balian-Bloch formula, we have derived the contribution of degenerate family of orbits confined in 2D truncated circular billiard and 3D truncated spherical cavity. In addition to the truncated portion of the original families, contributions of the marginal orbits should be considered independently as the end-point correction to the former. In applications to the 2D billiard and 3D cavity potentials with TQS shape parametrization, our formulas successfully reproduce the quantum mechanical results. Although the contributions of the marginal orbits are expected to play minor roles in the semiclassical limit due to the lower degeneracies, it turns out that they play significant role on the shell effects in the energy region of nuclei. Their effect is important especially for small deformation where only a small portion of the parameter space is occupied by the fully-degenerate periodic-orbit families, and will be responsible for a fragment shell effect emerging at an early stage of the fission deformation process.

Using our trace formula, shell effect associated with the fragments is extracted in simple and natural way and can be evaluated quantitatively through the nuclear fission processes. In this way, the periodic-orbit theory provides us a powerful tool to investigate the nuclear fission dynamics. Detailed analysis of the potential energy surface taking into account the asymmetric shape degree of freedom in the TQS cavity model and discussions on the origin of asymmetric fission will be presented in a separate paper[23].

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Appendix A: Trace formula for marginal orbits

A1. Three-parameter family contribution

For regular polygon orbit \((p,t)\) in the three-dimensional spherical cavity potential, the generic formula (2.6) can be written as [4]

$$g_{pt}(E) = \frac{2M}{\hbar^2} \Re \sin \frac{\varphi_{pt}}{\pi k R_p^{-1}} \left( \frac{ik}{4\pi} \right)^p \int dS_1 \cdots dS_p e^{ikl}. \quad (A1)$$

We define the local surface coordinate \((x_a, y_a)\) around the vertex \(P_a\) as explained in Sec. II C (see Fig. 5).

For three-parameter family of polygon orbits, the integrals over \(x_1, y_1\) and \(y_2\) should be exactly done, which gives the factor

$$\int dx_1 dy_1 dy_2 = 8\pi R^3 \sin(2\varphi_{pt}) f_p \quad (A2)$$

with the occupation rate \(f_p\) given by Eq. (2.32). The other integrals are carried out using the SPA in the following way. The length of the orbit is expanded in \((2p - 3)\)-dimensional surface coordinates \(R \mathbf{u} = (x_2; x_3, y_3; \cdots; x_p, y_p)\) up to the quadratic order as

$$l(1, \cdots, p) = L_{pt} + \frac{R}{4} \sum_{ab} K_{ab} u_a u_b,$$

$$K_{ab} = \frac{2}{R} \frac{\partial^2 L_{pt}(u)}{\partial u_a \partial u_b}. \quad (A3)$$
\( L_{pt} \) is the length of the orbit \((p, t)\). \( K \) represents the curvature matrix for the orbit, which is dimensionless, symmetric and independent on the radius of the fragment. Using the SPA, the integrals are evaluated as

\[
\int dx_2 dx_3 dy_3 \cdots dx_n dy_n e^{i kl(1-p)}
= R^{2p-3} e^{i kl R} \int d^{2p-3} u \exp \left[ \frac{ikR}{4} \sum_{ab} K_{ab} u_a u_b \right]
= \frac{(4\pi R/k)^{p-3/2}}{\sqrt{\det K}} e^{i kl R - i \nu/2},
\]

(A4)

where \( \nu \) denotes the number of negative eigenvalues of \( K \). Inserting (A2) and (A4) into Eq. (A1), one has

\[
g_{pt}^{(pr)}(E) = 2MR^2 \frac{f_p \sin \varphi_p \sin(2\varphi_{pt}) \sqrt{kR}}{\hbar^2 \sqrt{\det K}} \times \sin(kL_{pt} - \frac{\pi}{2} \mu_{pt}), \quad \mu_{pt} = 2p + n_+ + \frac{1}{2},
\]

(A5)

Taking \( j = t \), the following relations have been checked numerically for each \((p, t)\):

\[
| \det K | = p \sin \varphi_{pt}, \quad 2p + n_+ + \frac{1}{2} = 2t - p - \frac{3}{2} \quad (\text{mod } 4)
\]

(A6)

and \( g_{pt}^{(pr)} \) coincides with the Balian-Bloch formula \( g_{pt}^{(sph)} \) for \( f_p = 1 \) [see Eq. (2.14)]. Thus one has the contribution of three parameter family as

\[
g_{pt}^{(pr)}(E) = f_p g_{pt}^{(sph)}(E)
= 2MR^2 \frac{f_p \sqrt{kR}}{\hbar^2} A_{pt}^{(sph)} \sin(kL_{pt} - \frac{\pi}{2} \mu_{pt}),
\]

(A7)

\[
A_{pt}^{(sph)} = \frac{\sin \varphi_p \sin 2\varphi_{pt}}{\sqrt{\det K}} = \sin 2\varphi_{pt} \sqrt{\frac{\sin \varphi_p}{\pi p}},
\]

(A8)

\[
\mu_{pt} = 2t - p - \frac{3}{2},
\]

(A9)

where \( A_{pt} \) represents the dimensionless amplitude independent on \( k \) and \( R \).

**A2. Contribution of the Marginal orbit families with one vertex on the joint**

To evaluate the contribution of the marginal family to the integral (A1), any vertex can be put on the joint of the spherical surface and the neighboring surface, and each gives the identical contribution. Thus, we put the first vertex on the joint and multiply it with \( p \). The marginal orbit form a two-parameter family for polygon \((p > 2t)\) and a one-parameter family for diameter \((p = 2t)\). For a marginal polygon, the surface coordinates to be exactly integrated are \( \xi_1 \) and \( y_2 \). \( \xi_1 = R \varphi_1 \sin \theta_A \) deals with the rotation about the symmetry axis \((0 \leq \varphi_1 \leq 2\pi)\), and \( y_2 = R \psi \sin(2\varphi_{pt}) \) deals with the rotation about the axis \( OP_1 \) with angle \( \psi \) over the range \( 4\psi_p \). The integrations over these variables give the factor

\[
\int d_1 d_2 = 8\pi R^2 \psi_p(\theta_A) \sin \theta_A \sin(2\varphi_{pt}).
\]

(A10)

Integrating over the rest of \( 2p - 2 \) variables \( Ru = (\eta_1; x_2; x_3, y_3; \cdots; x_p, y_p) \) using the SPA by expanding the length \( l_p \) as (A3), one has

\[
\int dS_1 \cdots dS_p e^{i kl(1-p)}
= p \cdot \frac{1}{2} \cdot 8\pi R^2 \psi_p(\theta_A) \sin \theta_A \sin(2\varphi_{pt})
\times e^{i kl R} \int d^{2p-2} u \exp \left[ \frac{ikR}{4} \sum_{ab} K'_{ab} u_a u_b \right]
= \frac{4\pi p R^2 \psi_p(\theta_A) \sin \theta_A \sin(2\varphi_{pt}) \cdot (4\pi)^{p-1}}{\sqrt{\det K'}} \times e^{i kl R - i \frac{\pi}{2} n'_{-}}.
\]

(A11)

In the middle expression, the factor \( p \) appears because any of the \( p \) vertices can be put on the joint as stated above. The next factor \( 1/2 \) is to compensate the integration range of \( \eta_1 \) which is actually \( \eta_1 > 0 \) but extended to \((-\infty < \eta_1 < \infty)\) by assuming the surface around the vertex \( P_1 \) is the extension of the neighboring wall outside the spherical surface. \( n'_{-} \) counts the number of negative eigenvalues of the \((2p-2)\)-dimensional curvature matrix \( K' \). In consequence, we obtain

\[
g_{pt}^{(mg)}(E) = 2MR^2 \frac{f_p}{\hbar^2} A_{pt}^{(mg)} \sin \left( kL_{pt} - \frac{\pi}{2} \mu_{pt}^{(mg)} \right),
\]

(A12)

with

\[
A_{pt}^{(mg)} = \frac{p \psi_p(\theta_A) \sin \varphi_p \sin(2\varphi_{pt}) \sin \theta_A}{\pi \sqrt{\det K'}} \times \sin \left( kL_{pt} - \frac{\pi}{2} \mu_{pt}^{(mg)} \right),
\]

(A13)

\[
\mu_{pt}^{(mg)} = 2p + n'_{-}.
\]

(A14)

The above equation is valid for a primitive polygon family. For a repeated polygon \( m(p, t) \), the \( j(p+1) \)-th vertex \((1 \leq j < m)\) on the joint can be placed either on the spherical surface or on the neighboring surface. Therefore, one should sum over all \( 2^{m-1} \) combinations (labeled \( \beta \)) for the choice of the surfaces:

\[
g_{m(p, t)}^{(mg)}(E) = \frac{2MR^2}{\hbar^2} \sum_{\beta} A_{m(p, t), \beta}^{(mg)}
\times \sin \left( kmL_{pt} - \frac{\pi}{2} \mu_{m(p, t), \beta}^{(mg)} \right),
\]

(A15)

with

\[
A_{m(p, t), \beta}^{(mg)} = \frac{p \psi_p \sin \varphi_p \sin(2\varphi_{pt}) \sin \theta_A}{2^{m-1} \pi \sqrt{| \det K'_{\beta} |}}
\times \sin \left( kL_{pt} - \frac{\pi}{2} \mu_{m(p, t), \beta}^{(mg)} \right),
\]

(A16)

\[
\mu_{m(p, t), \beta}^{(mg)} = 2mp + n'_{\beta}.
\]

(A17)
The marginal diameter orbits \((2t, t) = t(2, 1)\) form a one-parameter family generated by the rotation about the symmetry axis. Their contribution to the level density is derived in the same way as above, and one has

\[
\tilde{g}^{(\text{mg})}_{t(2, 1)}(E) = \frac{2MR^2}{\hbar^2} \sum_{\beta} A_{t(2, 1), \beta}^{(\text{mg})} \sin\left(kL_2 - \frac{\pi}{2} \mu_{t(2, 1), \beta}^{(\text{mg})}\right),
\]

with

\[
A_{t(2, 1), \beta}^{(\text{mg})} = \frac{\sin \theta_A}{2^{t-1} \sqrt{\pi |\det K'_{\beta}|}},
\]

\[
\mu_{t(2, 1), \beta}^{(\text{mg})} = n'_{\beta} - \frac{1}{2}.
\]

A3. Marginal polygon family with two vertices on the joint

For a polygon orbit family, there are possibility of two vertices to be placed on the joint. It forms one-parameter family according to the rotation about the symmetry axis. The integration with respect to \(x_1 = R \varphi_1 \sin \theta_A\) gives the factor \(2\pi R \sin \theta_A\), and other \(2p - 1\) integrals are carried out by using the SPA. The curvature \(K''\) is calculated under assumption that the two vertices are on the neighboring surface. Taking account of the \(2p\) possible ways of selecting the two vertices on the joint, and the extensions of surface integration ranges for the two surface coordinates from \((0, \infty)\) to \((-\infty, \infty)\), one has

\[
\int dS_1 \cdots dS_p e^{ik(1 \cdots p)} = 2^p \cdot \frac{1}{4} \cdot 2\pi R^{2p} \sin \theta_A \cdot (4\pi i/kR)^{p-1/2} \cdot e^{i\pi \varpi_1/2}.
\]

Thus, the contribution to the level density is given by

\[
g_{pt}^{(\text{mm})}(E) = \frac{2MR^2}{\hbar^2} A_{pt}^{(\text{mm})} \sin\left(kL pt - \frac{\pi}{2} \mu_{pt}^{(\text{mm})}\right),
\]

\[
A_{pt}^{(\text{mm})} = \sum_{\varpi_1} p \sin \varphi \sin \theta_A \cdot 2^{\pi |\det K''|},
\]

\[
\mu_{pt}^{(\text{mm})} = 2p + n'' - \frac{1}{2}
\]

for a primitive orbit family. In cases of repeated orbits, one has to consider all the possible combinations of the surfaces for intermediate reflections on the joint as in Eq. (A15).

A4. Total contribution of the fragment-orbit family

Summarizing the above contributions, total contribution of the orbit family \((p, t)\) confined in the spherical fragment is given by

\[
g_{pt}^{(\text{frag})}(E) = \frac{2MR^2}{\hbar^2} \sum_{D=1}^{3} (kR)^{D/2} A_{pt}^{(D)} \sin\left(kL pt - \frac{\pi}{2} \mu_{pt}^{(D)}\right),
\]

where the summation is taken over the degeneracy \(D\). The amplitudes and Maslov indices are given by

\[
\begin{align*}
A_{pt}^{(3)} &= f_p A_{pt}^{(sph)}, & \mu_{pt}^{(3)} &= \mu_{pt}^{(sph)}, \\
A_{pt}^{(2)} &= A_{pt}^{(sph)}, & \mu_{pt}^{(2)} &= \mu_{pt}^{(sph)}, \\
A_{pt}^{(1)} &= A_{pt}^{(mm)}, & \mu_{pt}^{(1)} &= \mu_{pt}^{(mm)}
\end{align*}
\]

for a polygon \((p > 2t)\), and

\[
\begin{align*}
A_{2t, t}^{(3)} &= 0, & \mu_{2t, t}^{(3)} &= \mu_{2t, t}^{(sph)}, \\
A_{2t, t}^{(2)} &= f_2 A_{2t, t}^{(sph)}, & \mu_{2t, t}^{(2)} &= \mu_{2t, t}^{(sph)}, \\
A_{2t, t}^{(1)} &= A_{2t, t}^{(mm)}, & \mu_{2t, t}^{(1)} &= \mu_{2t, t}^{(mm)}
\end{align*}
\]

for a diameter. The level density with the wave-number variable is expressed as

\[
g_{pt}^{(\text{frag})}(k) = \frac{\hbar^2 k}{M} g_{pt}^{(\text{frag})}(E)
\]

\[
= 2R \sum_{D=1}^{3} (kR)^{D/2} A_{pt}^{(D)} \sin\left(kL pt - \frac{\pi}{2} \mu_{pt}^{(D)}\right)
\]

\[
= 2R \text{Im} \left[ \sum_{D} (kR)^{D/2} A_{pt}^{(D)} e^{-i\pi \mu_{pt}^{(D)}/2} \right] e^{ikL pt}
\]

\[
= 2R \text{Im} \left[ A_{pt}(k) e^{ikL pt} \right].
\]

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