Perturbative Semiclassical Trace Formulae for Harmonic Oscillators

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September 2, 2014

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Abstract

Already 100 years ago Bohr used classical mechanics to build a model for a quantum system, the hydrogen atom. Although Bohr only included the circular classical orbits, the calculated energy spectrum from his model showed remarkable agreement with measurements. In this article we expand the known semiclassical models by including more general perturbative potentials of the harmonic oscillator in arbitrary spatial dimensions. Our starting point is a radial harmonic potential with an arbitrary even monomial perturbation, which we use to study the resulting $U(D)$ to $O(D)$ symmetry breaking. We derive the gross structure of the semiclassical spectrum from periodic orbit theory, in the form of a perturbative ($\hbar \to 0$) trace formula. We then show how to apply the results to even order polynomial potentials, possibly including mean-field terms. We have drawn the conclusion that the gross structure of the quantum spectrum is determined from only classical circular- and diameter-orbits for this class of systems.

1 Introduction

In 1913 Niels Bohr published his seminal work on the Hydrogen atom \cite{1} where he depicted the electron orbiting the proton as planets orbits the sun. Bohr’s pictorial model is used in logotypes of research institutions and companies world wide, and is still the most popular way to draw an atom. With the vocabulary of today, Bohr obtained the quantum mechanical energy levels of the Coulomb potential. But 100 years ago, there was hardly any established quantum theory.
Bohr’s way of combining well known classical mechanical laws with an innovative quantization of the electron radius (or equivalently, its angular momenta), together with the correspondence principle, had a tremendous influence on the development taking place the two decades to follow. Bohr did only include circular orbits, although the corresponding classical system have elliptic solutions [2]. It must be considered of great historical importance for the development of quantum mechanics that Bohr obtained the correct quantum spectrum from his simple model. First the development of the Heisenberg-Schrödinger quantum theory seemed to be unrelated to Bohr’s semiclassical treatment. However, work by the EBK trio [3] and by Van Vleck [4], and Feynman [5], have pointed onto relations between the action for the classical orbits of a particle and the corresponding quantum spectrum. The interest of these so called semiclassical relations, i.e., between classical systems and their quantum counterpart, boosted again in the 60s and 70s with the study of quantum chaos [6]. Finally a more mature periodic orbit theory (POT) was introduced by Gutzwiller [7], where the study of the periodic classical orbits were related to quantum mechanical observables through so called trace formulae (TF), which had already been studied in the 50s by Selberg [8]. From a mathematical point of view, a TF can express the spectrum of a differential operator, as in the time independent Schrödinger equation, as a train of delta functions. Several principally important quantum systems: the harmonic oscillator; the cavity; and again, the hydrogen atom, were soon solved within POT [9, 10]. These systems could be connected by a principle trace formula for integrable systems given by Berry and Tabor [11]. At the same time, semiclassical approximations were succesful in describing shell structures of different quantum many-body systems from atomic and nuclear physics [12]. This have been one motivation to refine the POT also to classical chaotic systems. Studies of (super-) shell structures have now also been undertaken in new man-made systems: the abundance in atomic metal clusters [13], that have been confirmed experimentally [14]; in solid state devices, like the conductance of quantum wires [15]; in weakly repulsive atomic Fermi gasses [16]; and pairing gaps of attractive Fermi gasses [17] and nano-grains [18]; and recently also in triangular flakes of graphene [19].

In this article we treat a class of quantum systems of principal importance in approximations, the isotropic perturbed harmonic oscillator (HO) in arbitrary dimensions. We here present a TF for $U(D)$ to $O(D)$ symmetry breaking that gives the gross structure of density of states (DOS), sometimes called the level density, to leading order in $\hbar^{-1}$ for the perturbed system and that recovers the exact quantum mechanical TF in the limit of no perturbation to leading order in $\hbar^{-1}$. Special cases have been presented before: the quartically perturbed two-dimensional HO was treated by Craigh in [20]; and the three-dimensional counterpart by Brack et al. in [21]. The present treatment follows a similar perturbative technique as pioneered by Craigh [20], but is implemented with a mathematical beauty that generalize the special case of quartic perturbation and allows the treatment of arbitrary dimensions simultaneously.
We consider the Hamiltonian of the $D$-dimensional harmonic oscillator (HO), as given by the following Hamiltonian function defined from the classical space and momentum coordinates $q, p \in \mathbb{R}^D$

$$H_0(q, p) = \sum_{j=1}^{D} \left( \frac{p_j^2}{2m} + \frac{1}{2} m \omega_j^2 q_j^2 \right).$$

We consider an isotropic HO, $\omega \equiv \omega_j$, $j = 1, 2, ..., D$, with unit mass, $m = 1$, such that the characteristic length scale of the oscillator is $R_0 = \sqrt{2E/\omega}$.

### 2.1 Classical mechanics of the Harmonic Oscillator

From the Hamiltonian (1) we can deduce Hamilton’s equations, with solutions

$$\begin{cases}
\dot{q}(t) = p(t) \\
\dot{p}(t) = -\omega^2 q(t)
\end{cases}, \quad \begin{cases}
q(t) = q_0 \cos(\omega t) + p_0 \omega \sin(\omega t) \\
p(t) = p_0 \cos(\omega t) - \omega q_0 \sin(\omega t)
\end{cases},$$

where $q_0, p_0$ are constant vectors. The solutions are circles in some two-dimensional hyper-plane of the $(q, p)$ phase-space, which projects to ellipses in the $D$-dimensional $(q)$ configuration space. Note that many different choices of $p_0, q_0$ give rise to the same orbit. For a constant energy $E = H_0(q_0, p_0)$ we have from (1) and (2)

$$H_0(q(t), p(t)) = \frac{1}{2} \left( |p_0|^2 + \omega^2 |q_0|^2 \right) = E.$$  

That is, energy is conserved along orbits. Consequently the normalised solutions $(q(t)/R_0, p(t)/\omega R_0)$ live on the unit sphere $S^{2D-1}$ in phase-space.

Identifying $\mathbb{R}^{2D} \simeq \mathbb{C}^D$ by $z \sim (q, p)$ with $q = \text{Re}(z)/\omega$ and $p = -\text{Im}(z)$, the Hamiltonian (1) can be rewritten to

$$H_0(z) = \frac{1}{2} z^T z.$$  

Here $z^T$ denotes transposition of the (column) vector $z \in \mathbb{C}^D$, and a bar means complex conjugation. It then directly follows that the system has $U(D)$-symmetry (invariant under the action of a $D$ dimensional unitary matrix), since given a matrix $A \in U(D)$ we obtain from (1)

$$H_0(Az) = \frac{1}{2} \overline{A} z^T A z = \frac{1}{2} z^T \overline{A}^T A z = H_0(z).$$  

Now Hamilton’s equation and solution (2) simply reads

$$\dot{z} = i\omega z, \quad z(t) = e^{i\omega t} z_0.$$  

The formulation of the orbits in the phase-space are then simply

$$q(t) = \text{Re} \left\{ e^{i\omega t} z_0 \right\}/\omega, \quad p(t) = -\text{Im} \left\{ e^{i\omega t} z_0 \right\}.$$
and an alternative real parametrisation to \[2\] is
\[
\begin{align*}
q(t) &= R_0 \cos (\omega t + \nu), \quad \nu_1, ..., \nu_D \in [0, 2\pi) \\
p(t) &= \dot{q}(t)
\end{align*}
\]
where \(R_0 = (\sqrt{2E_1}/\omega, ..., \sqrt{2E_D}/\omega)\) with \(E_1 + ... + E_D = E\). We now choose the initial time (e.g.) by setting \(\nu_1 = 0\), such that we determine the initial values of the first components of the phase-space coordinates to be \(q_1(0) = \sqrt{2E_1}/\omega\) and \(p_1(0) = 0\). Then the constant vector \(z_0/\omega R_0\) can be viewed as living in the complex projective space \((n_1, n_2 e^{i\nu_2}, ..., n_D e^{i\nu_D}) \in CP^{D-1}[22]\). Here the \(D-1\) complex parameters in \(CP^{D-1}\) corresponds to \(D-1\) real angles that parametrise part of \(S^{D-1}\), i.e., for \(R_0 > 0\) we have \(n_1, ..., n_D \in [0, 1]\), with \(n_1^2 + ... + n_D^2 = 1\) due to the energy conservation, together with the \(D-1\) phase angles \(\nu_2, ..., \nu_D \in [0, 2\pi)\) remaining free when \(\nu_1 = 0\). This explains the background for the two possible alternative calculations outlined in \[21\] for \(D = 3\).

As mentioned earlier, many different choices of \((q_0, p_0)\) leads to the same orbits. As we will see the high dimensional symmetry allows the short mathematical description of all orbits of the same energy. The discussion below will be short and informal, as the details of the spaces and identifications we mention are covered in standard literature on symplectic geometry and classical mechanics, see for example \[23\]. According to (6), \(U(1)\) acts on solutions \(z(t)\) by time. The remaining symmetry is hence \(SU(D) \simeq U(D)/U(1)\), corresponding to the space of "special" unitary matrices of determinant one. As (6) also shows; an orbit is completely contained in some complex "line" (a real two-dimensional hyper-plane), which we without loss of generality might assume to be the line spanned by the first complex coordinate. The group of matrices which fixes the first coordinate of a vector while preserving the energy is \(U(D-1)\). Removing this symmetry finally gives us \(CP^{D-1} \simeq SU(D)/U(D-1)\). So the space of all solutions of the same energy can indeed be parametrized by the complex projective space, in agreement with the specific parametrisation \[5\] with \(\nu_1\) fixed. A dimension count shows that this is exactly all of the solutions.

Finally, another way to describe this manifold of solutions, which will be of particular use for us, is the following: \[6\] shows that \(S^1\) acts on the energy sphere \(S^{2D-1}(H_0 = E)\); the well known quotient space \(S^{2D-1}/S^1 \simeq CP^{D-1}\) is realized by the famous Hopf map, which end up being a so-called Riemannian submersion when equipping \(CP^{D-1}\) with the Fubini-Study (FS) metric \[24\]. Hence schematically it reads
\[
(R^{2D}, g_R) \xrightarrow{H_0=E} (S^{2D-1}, g_{can}) \xrightarrow{(S^1, \pi_{Hopf})} (CP^{D-1}, g_{FS}).
\]
In local coordinates, this allows us to write the volume measure on \(S^{2D-1}\) as
\[
d\text{vol}_{S^{2D-1}} = d\text{vol}_{CP^{D-1}} dt
\]
which will be used in sections \[3.1\] and \[3.4\]. Here \(d\text{vol}\) is the Riemannian volume form: the canonical choice of volume measure induced by the metric.
2.2 Trace formula for the HO

The well known quantum mechanical energy spectrum of the $D$-dimensional harmonic oscillator is

$$E_n = \hbar \omega (n + D/2), \quad n = 0, 1, 2, \ldots,$$

(11)

where each energy has a degeneracy factor

$$d_n = \frac{1}{(D - 1)!} \prod_{j=1}^{D-1} (n + j).$$

(12)

An energy spectrum can be expressed in the form of a trace formula for the density of energy states (DOS) \[7, 8, 10\]

$$g(E) \equiv \bar{g} + \delta g = \text{g}_{ETF}(E) + \sum_{\gamma} A_{\gamma}(E) \cos \left( \frac{S_{\gamma}(E)}{\hbar} - \mu_{\gamma} \frac{\pi}{2} \right).$$

(13)

The first term in (13) is the extended Thomas-Fermi DOS \[10, 25\], which is a smoothly varying function of energy $\bar{g}$, while the second term, built up by the summation over classical periodic orbits $\gamma$ with amplitudes $A_{\gamma}$, produce the shell oscillations $\delta g$ investigated semiclassically in this article. The frequencies are determined by the classical actions $S_{\gamma}$ for the orbits, while the phase is determined by the so called Maslov index $\mu_{\gamma}$ \[10\]. Specifically for the isotropic HO in $D$ dimensions, we can write the trace formula representing the energies (11) and (12) on a complex form to be used later \[10, 25\]

$$g(E) = \frac{1}{\hbar \omega (D - 1)!} \prod_{j=1}^{D-1} \left( \frac{E}{\hbar \omega} - \frac{D}{2} + j \right) \Re \left\{ \sum_{k=\infty}^{\infty} (-1)^k e^{2\pi i k E/\hbar \omega} \right\}, \quad E > 0.$$  

(14)

Comparing (13) with the $k = 0$ term in (14) shows that the prefactor in (14) is the extended Thomas-Fermi DOS \[26\], which can be obtained directly from (11) and (12) by viewing the spectrum as a train of delta spikes, each centered at the positions (11), and normalized to the degeneracy factor (12). Moreover, the exponent of the sum in (14) is in agreement with the classical action of a primitive HO orbit being $S_0 = 2\pi E/\omega$, and the Maslov index of the HO being zero \[10\].

3 Perturbation of the Harmonic oscillator

In this article we consider perturbations to the HO of the form

$$\Delta H = \varepsilon |q|^{2\alpha}, \quad \alpha \in \mathbb{N}, \quad |q|^2 = \sum_{j=1}^{D} q_j^2,$$

(15)
where the small parameter $\varepsilon$ has the dimension of $E/R_0^{2\alpha}$. From (1) and (15) we obtain the full Hamiltonian under study here

$$H(q, p) = H_0 + \Delta H = \frac{1}{2} (|p|^2 + \omega^2 |q|^2) + \varepsilon |q|^{2\alpha}. \quad (16)$$

Note that for the special case of quartic perturbation, $\alpha = 2$, the Hamiltonian (16) have been studied in two spatial dimensions ($D = 2$) in [20], and for $D = 3$ in [21]. In the present article we treat in detail an arbitrary even monomial perturbation in $|q|$, in any dimension $D$, and in addition give an example of a realistic polynomial perturbation for $D = 3$. The key observation for this Hamiltonian, is that the original energy preserving matrix symmetries, see (5), is reduced to the set of orthogonal matrices $O(D)$. Taking out the orientation, reduces this to the positive ones in $SO(D)$. The resulting space $SO(D)/SO(2)$ is not so simple to describe, and the lack of an explicit solution to (16) makes it impossible to completely describe the manifold of the constant energy solutions in the general case.

### 3.1 Perturbative Trace Formula

We now turn our focus to the quantum mechanical energy spectrum of the perturbed HO, with the goal to obtain a semiclassical trace formula for the DOS of the Hamiltonian (16) within first order perturbation theory. Starting from the HO trace formula (14) and including a complex modulation factor $M_k$ in the sum, we define the perturbative trace formula to (16) according to [20]

$$g_{\text{pert}}(E) \equiv \left( \frac{\hbar \omega}{E} \right)^{-D} \frac{E^{D-1}}{(D-1)!} \operatorname{Re} \left\{ \sum_{k=-\infty}^{\infty} (-1)^D M_k e^{2\pi i k E/\hbar \omega} \right\}, \quad E > 0. \quad (17)$$

The prefactor above only contains the leading order term in $\hbar^{-1}$ of the extended Thomas-Fermi DOS for the unperturbed HO, see the prefactor in (14), in accordance with the order of the perturbative theory in use. The modulation factor in (17) is generally defined according to [10, 20]

$$M_k(E, \varepsilon, D, \alpha, \omega) = \langle e^{ik\Delta S_{\gamma}/\hbar} \rangle_{\gamma \in \mathbb{CP}^{D-1}}, \quad (18)$$

where $\gamma$ ranges over all classical periodic orbit of energy $E$ for the unperturbed HO, the last four variables are system dependent parameters. $\Delta S$ is a lowest order term, with respect to $\varepsilon$, of the action in the perturbed system, see section 3.3. In the following we shall calculate this expression explicitly. Using the Hopf map briefly described in section 2.4, $\Delta S(\gamma)$ induces a map on $S^{2D-1}$, given by $(\Delta S \circ \pi_{\text{Hopf}})$. Notationally we shall not distinguish between the two. Notice that $\Delta S$ is constant on the fiber $S^1$. Rewriting,

$$M_k = \frac{1}{\operatorname{Vol(\mathbb{CP}^{D-1})}} \int_{\mathbb{CP}^{D-1}} e^{ik\Delta S_{\gamma}/\hbar} d\text{vol}_{FS}$$

$$= \frac{1}{\operatorname{Vol(S^1)} \operatorname{Vol(\mathbb{CP}^{D-1})}} \int_{S^{2D-1}} e^{ik\Delta S_{\gamma}/\hbar} d\text{vol}_{\text{can}}, \quad (19)$$
where $d\text{vol}_{FS}$ is the Fubini-Study volume form, $d\text{vol}_{can}$ is the volume form of the canonical round metric on $S^{2D-1}$, $\text{Vol}(S^1) = 2\pi$, and $\text{Vol}(\mathbb{C}P^{D-1}) = \pi^{D-1}/(D-1)!$. The spherical integral is significantly easier to compute, see section 3.3.

### 3.2 Generalised angular momentum

To analyse the perturbed system, we will use conserved quantities. Since $SO(D)$ is a Lie group, i.e., a continuous group of symmetries, one can utilize Noethers theorem to directly compute conserved quantities. To this end we define a generalised angular momentum operator $L: \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{(D-1)/2}$ according to

$$L(q,p) = (\ldots, p_j q_k - p_k q_j, \ldots), \quad j,k = 1 \ldots D, j \neq k.$$  

That is, all combinations of the coordinates from $q$ and $p$. Using the theory of momentum maps and Noethers theorem as given in [27], one can show that all the coordinates are conserved for systems with $SO(D)$ symmetry. Hence, this is just a generalization of the well known situation where angular momentum is preserved in three dimensional systems ($D = 3$) with the rotational symmetry expressed by $SO(3)$ invariance. Explicitly calculating the length of $L$ from (20) reveals that the following identity

$$|L|^2 = |q|^2 |p|^2 - (q \cdot p)^2 = |q|^2 |p|^2 \left(1 - \cos^2 \theta\right) = \sin^2 \theta |q|^2 |p|^2,$$

(21)

generally holds, just as in the common case where $q, p \in \mathbb{R}^3$. Hence, we can define the conserved total angular momentum in $D$ dimensions as the area spanned by $q, p \in \mathbb{R}^D$:

$$L \equiv |L| = \sin \theta |q| |p|,$$

(22)

where $\theta$ is the angle between the two vectors $q$ and $p$.

### 3.3 The perturbative action

We here concentrate on the perturbative classical action $\Delta S_{\gamma}$, that occurs in the exponent of (18).

In order to obtain a scaling for the perturbative action, we consider the following expansion

$$S = \oint_{\gamma} p dq \sim 4 \int_0^{R_0} \sqrt{2E - \omega^2 r^2 - 2\varepsilon r^{2\alpha}} dr \simeq S_0 + \Delta S + O(\varepsilon^2)$$

$$= \frac{2\pi E}{\omega} - \varepsilon \frac{2^{\alpha+1}\sqrt{\pi\Gamma(\alpha + \frac{1}{2})} E^{\alpha}}{\Gamma(\alpha + 1) \omega^{\alpha+1}} + O(\varepsilon^2),$$

(23)

i.e., with the curve $\gamma$ corresponding to a classical diameter orbit. From the above result, we define the following scale of the first order perturbative action $\Delta S$ to be used later

$$\sigma_\alpha \equiv \varepsilon \frac{2\pi E^{\alpha}}{\omega^{\alpha+1}} = \varepsilon \frac{\pi R_0^{2\alpha}}{2^{\alpha-1} \omega},$$

(24)
Figure 1: Illustration of a coordinate system for which the orbits in configuration space can be written on the form (26).

such that $\sigma_\alpha/\hbar$ is dimensionless.

According to the first order semiclassical perturbation theory given in [20], we generally have

$$\Delta S_\gamma = -\oint \Delta H dt = -\varepsilon \int_0^{2\pi} |\mathbf{q}(t)|^{2\alpha} dt.$$  \hspace{1cm} (25)

In earlier work, more specific perturbations have been treated, the calculation of (25) have been performed with brute force methods. Involving for example specific parameterisations of the periodic orbits on a hyper-sphere or a complex projective space [21], depending on the dimension $D$. The intention here is to avoid these technical calculations and use a more geometrical approach, independent of $\alpha$ and $D$. Ending with a reduced version of the trace formula in (17), with an explicit dependence on the parameter space.

To compute the circulation integral (25) for classical periodic orbits $\mathbf{q}(t)$ [such as (2) or (8)], consider a change of coordinates to a canonical form. As discussed in section 2.1, the orbits are ellipses in the configuration space. Hence for any orbit there exists an orthogonal change of coordinates, such that $\mathbf{q}(t)$ can be written

$$\tilde{\mathbf{q}}(t) = [a \cos(\omega t), b \sin(\omega t), 0, ..., 0],$$  \hspace{1cm} (26)

for some constants $a, b \in \mathbb{R}$, see figure 1.

The energy and the total angular momentum are still conserved for the perturbed Hamiltonian (16). Using (26) they are easily found to be

$$R_0^2 = a^2 + b^2, \quad L^2 = a^2 b^2 \omega^2.$$  \hspace{1cm} (27)
Solving for \( a \) and \( b \) in terms of the conserved quantities \( R_0 \) and \( L \) yields
\[
a^2 = \frac{R_0^2}{2} + \sqrt{\frac{R_0^4}{4} - \frac{L^2}{\omega^2}}, \quad b^2 = \frac{R_0^2}{2} - \sqrt{\frac{R_0^4}{4} - \frac{L^2}{\omega^2}}.
\] (28)

The action integral (25) calculated in the \( \tilde{q} \)-coordinates becomes
\[
\Delta S = -\epsilon \int_0^{2\pi} \left[ a^2 \cos^2(\omega t) + b^2 \sin^2(\omega t) \right] \alpha \ dt.
\] (29)

We substitute \( s = \omega t \) and apply the Binomial theorem
\[
\Delta S = -\epsilon \int_0^{2\pi} \sum_{k=0}^{\alpha} \binom{\alpha}{k} a^{2k} \cos^{2k} (s) b^{2\alpha-2k} \sin^{2\alpha-2k} (s) \ ds.
\] (30)

Using the following identity for \( 0 \leq k \leq \alpha \)
\[
\frac{1}{2\pi} \int_0^{2\pi} \cos^{2\alpha-2k} (s) \sin^{2k} (s) \ ds = \frac{(2k-1)!! [2\alpha - (2k + 1)]!!}{(2\alpha)!!},
\] (31)
we have from (30) above
\[
\Delta S = -\frac{2\pi \epsilon}{\omega} \sum_{k=0}^{\alpha} \binom{\alpha}{k} a^{2k} b^{2\alpha-2k}.
\] (32)

For a more convenient notation, we define coefficients \( I^k_\alpha \) in (32), such that
\[
\Delta S = -\frac{2\pi \epsilon}{\omega} \sum_{k=0}^{\alpha} I^k_\alpha a^{2k} b^{2\alpha-2k},
\] (33)
where we note that \( I^k_\alpha = I^\alpha_{\alpha-k} \). Due to this symmetry we can reduce the expression (32), depending on whether \( \alpha \) is even or odd. As we are interested in integrating this expression over the orbits of the HO, we would like to use (27) to rewrite this into an expression in \( R_0 \) and \( L \), since these are easily obtained given a specific orbit. To this end let \( \lfloor x \rfloor \) denotes the floor of \( x \), i.e., the largest integer fulfilling \( \lfloor x \rfloor \leq x \), and we can then write
\[
\Delta S = \begin{cases} 
-\frac{2\pi \epsilon}{\omega} \sum_{k=0}^{\lfloor \alpha/2 \rfloor} I^k_\alpha a^{2k} b^{2\alpha-2k} & \text{, } \alpha \text{ odd}, \\
-\frac{2\pi \epsilon}{\omega} \sum_{k=0}^{\alpha-1} I^k_\alpha a^{2k} b^{2\alpha-2k} + I^{\alpha/2}_\alpha a^{\alpha} b^{\alpha} & \text{, } \alpha \text{ even}.
\end{cases}
\] (34)

Here combinations of \( a^2 \) and \( b^2 \) can be replaced by the expressions in (28), such that
\[
a^{2k} b^{2\alpha-2k} + a^{2\alpha-2k} b^{2k} = \frac{R_0^2}{2\alpha} \sum_{l=0}^{\alpha-k} \sum_{p=0}^{\alpha-k} K^{a,k}_{l,p} \left( 1 - \frac{4L^2}{\omega^2 R_0^4} \right)^{\frac{l+p}{2}},
\] (35)

with the constants
\[
K^{a,k}_{l,p} = \binom{k}{l} \binom{k-l}{p} \left[ (-1)^l + (-1)^p \right].
\] (36)
The expression (35) is in fact a polynomial in the two constants of the motion, \(R_0^2\) and \(L^2\). Observe that \(K_{\alpha,k}^{\ell,p}\) = 0 if the parity of \(l\) and \(p\) is not the same. Hence only terms in the double sum with \(l + p\) even will be non-zero. The last term in (34), for \(\alpha\) even is

\[a_{\alpha}b^\alpha = \frac{L^\alpha}{\omega^\alpha}.\]  
(37)

Defining a dimensionless angular momentum

\[\tilde{L} \equiv \frac{2L}{\omega R_0^2},\]  
(38)

and inserting (35) and (37) into (34), we can transform (33) into the form

\[\Delta S = -\sigma_{\alpha} \sum_{j=0}^{\lfloor \alpha/2 \rfloor} a_j \tilde{L}^{2j},\]  
(39)

for some coefficients \(a_j(\alpha)\), which only depends on the order of the perturbation \(\alpha\), but not on the spatial dimension \(D\) of the system, see Table 1 for examples. First, we can see that for \(\alpha = 1\), we have \(\lfloor \alpha/2 \rfloor = 0\), such that \(ik\Delta S = 0\) and then (38) gives \(\mathcal{M}_k \equiv 1\) in any dimension \(D\). Hence, the perturbative trace formula (17) for the oscillating part of the DOS naturally give no information about the frequency shift \(\omega_{\text{eff}} \equiv \sqrt{\omega^2 + 2\varepsilon}\) of a harmonic perturbation [17].

The shift of the main HO levels can be taken into account by a (perturbative) calculation of the smooth TF DOS of the system as outlined in appendix C of [21]. Clearly \(\mathcal{M}_k \equiv 1\) also for \(\varepsilon = 0\) by definition, and the corresponding perturbed trace formula uniformly restores the unperturbed TF in the limit \(|\varepsilon| \to 0\). As a non-trivial example, take \(\alpha = 2\), i.e., a quartic perturbation, to obtain

\[\Delta S = -\varepsilon \pi R_0^4 \left( 3 - \frac{4L^2}{\omega^2 R_0^2} \right) = -\sigma_2 \frac{1}{2} \left( 3 - \tilde{L}^2 \right),\]  
(40)

with \(\sigma_2\) from (24) and \(\tilde{L}\) from (38). This is in agreement with what have implicitly been derived by Brack et. al. in three-dimensions [21] and by Craig in two-dimensions [20]. However, the approach presented here has no limitations for \(\alpha\) in any dimension, such that for example \(\alpha = 3\) gives

\[\Delta S = -\varepsilon \frac{\pi R_0^6}{8\omega} \left( 5 - \frac{12L^2}{\omega^2 R_0^2} \right) = -\sigma_3 \frac{1}{2} \left( 5 - 3\tilde{L}^2 \right).\]  
(41)

We summarize the rest of the first ten cases in Table 1. A pattern seem to emerge, and in the general case we conjecture that the following identity holds

\[\Delta S = -\sigma_{\alpha} \tilde{L}^\alpha P_\alpha \left( \frac{1}{\tilde{L}} \right),\]  
(42)

where \(P_\alpha\) denote the Legendre polynomial of order \(\alpha\). This provides an explicit form of the coefficients \(a_j\) in (39). We have not proven (42) but confirmed that it holds for \(\alpha \leq 1000\) with a CAS software. In section 3.5 the zeros of \(\Delta S(\tilde{L})\) will be important, and we can then utilize that the zeros of \(P_\alpha\) are well understood.
Table 1: Results for the perturbative action $-\Delta S/\sigma = \sum_{j=0}^{\lfloor \alpha/2 \rfloor} a_j \tilde{L}^{2j}$, for a monomial potential $\varepsilon r^{2\alpha}$ in arbitrary dimensions.

| $\alpha$ | $\frac{1}{8} (35 - 30\tilde{L}^2 + 3\tilde{L}^4)$ | $\frac{1}{8} (63 - 70\tilde{L}^2 + 15\tilde{L}^4)$ | $\alpha = 5$ |
|---|---|---|---|
| 4 | | | 
| 6 | $\frac{1}{16} (231 - 315\tilde{L}^2 + 105\tilde{L}^4 - 5\tilde{L}^6)$ | $\frac{1}{16} (429 - 693\tilde{L}^2 + 315\tilde{L}^4 - 35\tilde{L}^6)$ | 
| 8 | $\frac{1}{128} (6435 - 12012\tilde{L}^2 + 6930\tilde{L}^4 - 1260\tilde{L}^6 + 35\tilde{L}^8)$ | $\frac{1}{128} (12155 - 25740\tilde{L}^2 + 18018\tilde{L}^4 - 4620\tilde{L}^6 + 315\tilde{L}^8)$ | 
| 10 | $\frac{1}{256} (46189 - 109395\tilde{L}^2 + 90090\tilde{L}^4 - 30030\tilde{L}^6 + 3465\tilde{L}^8 - 63\tilde{L}^{10})$ | 

3.4 Reduction of the modulation factor

Recall that we are holding $E$ fixed (hence also $R_0$), so only $L$ changes in (39) as $\gamma$ varies in the family of fixed energy periodic orbits. In particular a so called diameter orbit have $L = 0$, while the maximum of $L$ is obtained for a circular orbit, where $a^2 = b^2 = R_0^2/2$, corresponding to zero radial momentum.

Now focusing on calculating the orbit invariant $L(q_0, p_0)$, for the variables $(q_0/R_0, p_0/\omega R_0) \in S^{2D-1}$, used in the spherical integral for the modulation factor in (19). It will be beneficial to consider the sphere $S^{2D-1}$ as the following set

$$S^{2D-1} = \left\{ \left[ \cos \left( \frac{\varphi}{2} \right) \mathbf{e}_q, \sin \left( \frac{\varphi}{2} \right) \mathbf{e}_p \right] | \mathbf{e}_q, \mathbf{e}_p \in S^{D-1}, \varphi \in [0, \pi] \right\}. \quad (43)$$

Using (43), we can rewrite (22) according to

$$L(q, p) = \omega R_0^2 \cos \left( \frac{\varphi}{2} \right) \sin \left( \frac{\varphi}{2} \right) L(\mathbf{e}_q, \mathbf{e}_p) = \frac{\omega R_0^2}{2} \sin (\varphi) \sin (\theta), \quad (44)$$

where $\theta$ is the angle between the two vectors $\mathbf{e}_q$ and $\mathbf{e}_p$ of unit length. That is, taking a $\Delta S$ polynomial in $\tilde{L}$ from (40), (41), (42), or table 1, one should interchange $\tilde{L} \rightarrow \sin (\varphi) \sin (\theta)$ to obtain the form to be used in this section.

Given an energy $E$, the integrand of $M_k$ in (19), is now only dependent on $L(\varphi, \theta) = |L|$. The integration measure for the splitting of the sphere in (43), is given by

$$d\text{vol}_{S^{2D-1}} = \frac{1}{2D} \sin^{D-1} (\varphi) d\text{vol}_{\mathbf{e}_q} d\text{vol}_{\mathbf{e}_p} d\varphi. \quad (45)$$

To integrate over the two smaller spheres, we use the observation that in the integrand, the only dependence of the variables is given by (44), and then only
the angle between \( \mathbf{e}_q \) and \( \mathbf{e}_p \). With this in mind, consider \( S^n \) as the set

\[
S^n = \{ \cos(\theta), \sin(\theta) \mid \mathbf{e} \in S^{n-1}, \theta \in [0, \pi] \},
\]

see figure 2 for an illustration. In the case of \( S^2 \) this reduces to the usual spherical coordinates. In the general case, the metric arising in this fashion is called a warped product structure of \( S^n \), see [28]. Notice that \( \theta \) exactly corresponds to the angle appearing in (44). The integration measure induced by (46) is

\[
d\text{vol}_{S^n} = \sin^{n-1}(\theta)d\text{vol}_{S^{n-1}}.
\]

Collecting our results, with \( n = D - 1 \), yields the following double integral in \( \varphi \) and \( \theta \)

\[
\mathcal{M}_k(E) = \frac{2(D-1)}{\pi} \int_0^{\pi/2} \int_0^{\pi/2} \sin^{D-1}(\varphi) \sin^{D-2}(\theta) e^{ik\Delta S(\varphi,\theta)/\hbar} d\varphi d\theta,
\]

where

\[
\Delta S(\varphi,\theta) = -\sigma_{\alpha} \sum_{j=0}^{[\sigma/2]} a_j \sin^{2j}(\varphi) \sin^{2j}(\theta),
\]

according to (39) and (44). The pre-factor in (48) was obtained by evaluating

\[
\frac{4}{2\pi} \frac{\text{Vol}(S^{D-1}) \text{Vol}(S^{D-2})}{\text{Vol}(\mathbb{C}P^{D-1})^{2D}} = \frac{2(D-1)}{\pi},
\]

where the factor 4 to the left above is due to the reduction of the two remaining upper integration limits that follows from the symmetry of the integrand.

In order to reduce (48) to a single integral we use new variables \( \ell \in [0, 1] \) and \( \vartheta \in [0, \pi/2] \), defined according to

\[
\ell = \sin(\varphi) \sin(\theta), \quad \cos(\varphi) = \sqrt{1 - \ell^2} \sin(\theta).
\]
Simplifying the corresponding Jacobian to \( \sin(\varphi)d\varphi d\theta = d\ell d\vartheta \), and using (42) for \( \Delta S(\ell) \), we are left with

\[
\mathcal{M}_k = (D - 1) \int_0^1 \ell^{D-2} e^{-ik\sigma_a \ell^a \phi(\ell)/\hbar} \ell \, d\ell.
\]

Generally, exponentials of high orders, \( \alpha \geq 4 \), do not have known integrals. Restricting the discussion for a moment to the case where \( a_j = 0 \) for \( j \geq 2 \), i.e., according to table 1, to perturbations with \( \alpha = 2, 3 \). One can show that (52) can be expressed with help of a generalized hypergeometric function \( \pFq \)

\[
\mathcal{M}_k = \frac{1}{\hbar} e^{-ik\sigma_{a_1} \varphi_0} \left[ 1 + \frac{2z}{D+1} + \frac{4z^2}{(D+1)(D+3)} \right],
\]

where the argument is \( z = ik\sigma_{a_1} \varphi_0 / \hbar \).

As specific examples we give in table 2 the modulation factors valid for perturbations with \( \alpha = 2, 3 \) for different dimensions \( D = 2, 3, \ldots, 7 \). For odd dimensions \( D \), the integral seems to always be expressible using elementary functions, and for even \( D \) the error function (erf) can be used.

We note that the two-dimensional \( (D = 2) \) case was in [20] equivalently expressed in terms of Fresnel integrals.

### Table 2: Modulation factors \( \mathcal{M}_k \) according to (53), valid for the two monomial potential \( \varepsilon \varphi^4 \) and \( \varepsilon \varphi^6 \) in different dimensions \( D \).

| \( D \) | \( D = 2 \) | \( D = 3 \) |
|---|---|---|
| \( \sqrt{2} \) \( \text{erf} \left( \frac{\sqrt{ik\sigma_{a_1} \varphi_0}}{\hbar} \right) \) | \( \frac{1}{\hbar} e^{-ik\sigma_{a_1} \varphi_0} \left( e^{-ik\sigma_{a_0+a_1}/\hbar} - e^{-ik\sigma_{a_0}/\hbar} \right) \) |
| \( \frac{3\hbar}{ik\sigma_{a_1}} \) \( e^{-ik\sigma_{a_0+a_1}/\hbar} \sqrt{\pi} \) | \( \text{erf} \left( \frac{\sqrt{ik\sigma_{a_1} \varphi_0}}{\hbar} \right) e^{-ik\sigma_{a_0}/\hbar} \) |
| \( \frac{2\hbar}{k^2\sigma_{a_1}^2} \left( ik\sigma_{a_1} \varphi_0 + \hbar \right) e^{-ik\sigma_{a_0+a_1}/\hbar} - \hbar e^{-ik\sigma_{a_0}/\hbar} \) |
| \( \frac{5\hbar}{8k^2\sigma_{a_1}^2} \) \( \left[ 4ik\sigma_{a_1} \varphi_0 + 6\hbar \right] e^{-ik\sigma_{a_0+a_1}/\hbar} - 3\sqrt{\pi} \hbar \text{erf} \left( \frac{\sqrt{ik\sigma_{a_1} \varphi_0}}{\hbar} \right) e^{-ik\sigma_{a_0}/\hbar} \) |
| \( \frac{\hbar}{k^2\sigma_{a_1}^2} \left( ik^2\sigma_{a_1}^2 \varphi_0^2 + 2\hbar k\sigma_{a_1} \varphi_0 - 2i\hbar^2 \right) e^{-ik\sigma_{a_0+a_1}/\hbar} + 2i\hbar^2 e^{-ik\sigma_{a_0}/\hbar} \) |

### 3.5 Stationary phase approximation

The perturbative POT in use in this article is valid to leading order in \( \hbar^{-1} \). Therefore we promote an analytic alternative to numerical integration, in the
focus the asymptotic approximation onto the boundary points which gives so-called upper- (and lower-) end-point corrections.

Let us stress that this situation is atypical for most potentials that are treated within POT, where stationary points correspond to so-called rational tori [11].

However, it was confirmed for the three-dimensional ($D = 3$) quartic perturbed HO in [21], that the leading order contributions came from those end-point corrections also in the exact trace formula. The end-point corrections could then be interpreted as corresponding to the classical diameter ($\ell = 1$) periodic orbits.

For the upper integration limit $\ell = 1$ (maximal angular momenta), we have $f(\ell) = 1$ and $h'(\ell) \neq 0$ in (54), such that the upper end-point contributes with a term

$$ I_1 = -\frac{i f(1)}{\lambda' h'(1)} e^{i h(1)} = \frac{i h}{k \sigma_\alpha \sum_j [\alpha/2]}_2 a_j e^{-ik \sigma_\alpha \sum_j [\alpha/2]_2 a_j \ell \lambda / h}. $$

cases where the integral [52] can not be given explicitly, the stationary phase approximation (SPA) to leading order in $\hbar^{-1}$. A few such examples are evaluated numerically in figure 8.

We can rewrite the integral (52) onto a standard form for Fourier integrals ($h = 1/\lambda \to 0$ in the classical limit), according to

$$ \mathcal{M}_k = (D - 1)e^{-ik \sigma_\alpha a_0 / h} \int_0^1 f(\ell) e^{i h(\ell)} d\ell, $$

$$ f(\ell) = \ell^{D-2}, \quad h(\ell) = -k \sigma_\alpha \sum_{j=1}^{[\alpha/2]} a_j \ell^{2j}. \quad (54) $$

The leading order contributions in the asymptotic expansion ($\lambda \to \infty$) of the integral, normally comes from the stationary points $\ell_0 \in (0, 1)$, i.e., for which

$$ \Delta S'(\ell) = -\sigma_\alpha \sum_{j=1}^{[\alpha/2]} 2j a_j \ell^{2j-1} = 0. \quad (55) $$

For the polynomials found in table 1, there are no stationary points within the interval $0 < \ell_0 \leq 1$, while for $\ell = 0$ we trivially have $\Delta S'(\ell) = 0$. Given that (52) holds, this is true for all $\alpha$. Since $x_0 \in (-1, 1)$ for all zeroes $x_0$ of the Legendre polynomials $P_\alpha(x)$, it follows from the Gauss-Lucas theorem that the zeroes of $P_\alpha'(x)$ also satisfy $x_0 \in (-1, 1)$, hence $P_\alpha'(1/\ell_0) = 0$ implies $\ell_0 \notin [-1, 1]$. The zeros are also simple, i.e. $P_\alpha'(x_0) \neq 0$. Using the recurrence relations for the Legendre polynomials, we find that (55) simplifies to

$$ \Delta S'(\ell) = -\sigma_\alpha \ell^{\alpha-1} P_\alpha \left(\frac{1}{\ell}\right) - \sigma_\alpha \ell^{\alpha-1} P_\alpha' \left(\frac{1}{\ell}\right) = \sigma_\alpha \ell^{\alpha-1} P_{\alpha-1} \left(\frac{1}{\ell}\right) = 0. \quad (56) $$

Hence, the only stationary point within the interval of the integral $\ell \in [0, 1]$ is $\ell_0 = 0$ coming from the factor $\ell^{\alpha-1}$ in the last part of (56). This means we can focus the asymptotic approximation onto the boundary points $\ell = 1$ ($\ell = 0$), which gives so-called upper- (and lower-) end-point corrections $I_\ell$, such that

$$ \mathcal{M}_k \approx (D - 1)e^{-ik \sigma_\alpha a_0 / h} (I_1 + I_0). \quad (57) $$

Let us stress that this situation is atypical for most potentials that are treated within POT, where stationary points correspond to so-called rational tori [11]. However, it was confirmed for the three-dimensional ($D = 3$) quartic perturbed ($\alpha = 2$) HO in [21], that the leading order contributions came from those end-point corrections also in the exact trace formula. The end-point corrections could then be interpreted as corresponding to the classical diameter- ($\ell = 0$) and circular- ($\ell = 1$) periodic orbits.

For the upper integration limit $\ell = 1$ (maximal angular momenta), we have

$$ I_1 \equiv -\frac{i f(1)}{\lambda' h'(1)} e^{i h(1)} = \frac{i h}{k \sigma_\alpha \sum_j [\alpha/2]}_2 a_j e^{-ik \sigma_\alpha \sum_j [\alpha/2]_2 a_j \ell \lambda / h}. \quad (58) $$
The lower integration limit $\ell = 0$ (minimal angular momenta) needs special attention for $D \geq 3$, since, first we then have $f(\ell) = 0$, secondly it is a stationary point, i.e., $h'(\ell) = 0$. In this case this lower end-point contributes with a leading order term

$$I_0 \equiv \int_0^\infty \ell^{D-2} e^{-ik_\alpha a_1 \ell^2/h} d\ell = \Gamma \left( \frac{D-1}{2} \right) \left( \frac{h}{k_\alpha a_1} \right)^{\frac{D-1}{2}} e^{-i(D-1)\frac{\pi}{4}}.$$ \hspace{1cm} (59)

Hence, from (57), (58), and (59) we can finally conclude that the asymptotic form of the modulation factor as obtained from SPA for an arbitrary monomial perturbation to a harmonic oscillator in $D \geq 2$ dimensions is

$$M_k \simeq (D-1) i \hbar e^{-i k_\alpha a_0/\hbar} \times \left[ e^{-i k_\alpha \sum_{j=1}^{\lceil |\alpha|/2 \rceil} a_j/\hbar} + O(\hbar) \right] + \Gamma \left( \frac{D-1}{2} \right) \left( \frac{h}{k_\alpha a_1} \right)^{\frac{D-1}{2}} e^{-i(D+1)\frac{\pi}{4}}.$$ \hspace{1cm} (60)

We observe that the SPA gives the exact integral in the $D = 3$ and $\alpha = 2, 3$ cases, see table 2, since then the only two terms are both of order $\hbar$. For $D = 2$ the circular orbit ($\propto e^{ik\Delta S(1)/\hbar}$) is suppressed by a factor $\sqrt{\hbar}$, while for $D \geq 4$ the diameter orbit ($\propto e^{ik\Delta S(0)/\hbar}$) is suppressed. From the exact integrals in table 2 it is seen that the next to leading order $\hbar^{-1}$ corrections of the circular orbit terms dominate the $\hbar^{-1}$ order of the leading diameter term already for $D > 5$. Further on, we can see from the cases in table 2 that (60) then seems to exactly reproduce the leading order circular term in any dimension, while the diameter term from (60) seems exact only in odd dimensions.

More important, the formula (60) is certainly not restricted only to $\alpha = 2, 3$, and we report on a few numerically investigated cases in figure 3.

### 3.6 Applications with radially symmetric polynomial perturbations

Following the same procedure as leading from (25) to (39) but for $N$ perturbative terms, it is straightforward to consider the more general polynomial perturbations

$$\Delta H = \sum_{j=1}^N \varepsilon_j |q|^{2\alpha_j}.$$ \hspace{1cm} (61)

We briefly discuss one such realistic example here. Motivated by the mean-field description of weakly interacting fermions in a harmonic trap \[17,31\], where the perturbation in $D = 3$ dimensions is proportional to a mean-field interaction parameter $|U_0| \ll 1$ times the following particle density in the Thomas-Fermi approximation

$$\rho_{TF} = \rho_0 \left( 1 - \frac{r^2}{R_{TF}^2} \right)^{3/2} \simeq \rho_0 \left( 1 - \frac{3}{2} \frac{r^2}{R_{TF}^2} + \frac{3}{8} \frac{r^4}{R_{TF}^4} + \frac{1}{16} \frac{r^6}{R_{TF}^6} + ... \right).$$ \hspace{1cm} (62)
Figure 3: Numerical evaluation of the modulation factor from the stationary phase approximation. The panels shows $|M_{k=1}|$ as a function of $\sigma_\alpha/\hbar$ for nine different cases of the dimension and the order of the perturbative potential (physical parameters are set to unity). Solid curves shows results from SPA \[\text{(60)},\] while thin black dashed curves shows the modulation factors calculated numerically from \[\text{(52)}.\] We have observed that the modulation factors calculated from SPA are generally indistinguishable from the numerical results in the $\hbar \to 0$ limit. For the two rows with the lowest perturbative potentials illustrated here ($\alpha = 2, 4$) this happens already during the first oscillation. An exception is the $D = 3, \alpha = 2$ panel, which is one of the cases where SPA is exact (see table 2). The fact that $|M_{k=1}| = 0$ in each oscillation also signals the perfect super-shell structure for this case, as observed in \[\text{[17, 21]}.\] When the order of the perturbation is increased substantially ($\alpha = 10$), the results from SPA are no longer close to the exact even after several oscillations (lowest row).
We then consider the perturbative semiclassical action for a HO, with a modified trap frequency \( \omega_{\text{eff}} = \sqrt{\omega^2 + 3U_0\rho_0/R_{TF}^2} \) due to the second term in (62), according to

\[
\Delta S = \frac{U_0\rho_0}{16R_{TF}^6} \int_0^{2\pi} \left( 6R_{TF}^2 \left[ a^2 \cos^2(\omega t) + b^2 \sin^2(\omega t) \right] \right)^2 dt.
\]

Hence, from the linearity of the integral, we have using (39) that

\[
\Delta S (\ell) = -\frac{U_0\rho_0\pi R_0^4}{32\omega R_{TF}^4} \left[ 36 + \frac{5R_0^2}{R_{TF}} - \left( 12 + \frac{3R_0^2}{R_{TF}} \right) \ell^2 \right].
\]

The fact that there is only one non-constant term in (64), is in agreement with an alternative perturbative semiclassical analysis for this mean-field potential performed using WKB wavefunctions [25, 31]. In particular this also means that the exact modulation factor is straightforward to obtain analytically in analogy to the case for \( D = 3 \) in table 2. Finally we note that similar polynomial perturbations can be constructed (e.g.) with the help of table 1.

## 4 Final trace formulae

Combining (17) and (52) we can generally write the exact perturbative trace formula on the following compact form

\[
g_{\text{pert}}(E) \simeq \frac{E^{D-1}}{(D-2)! \left( h\omega \right)^D} \text{Re} \left\{ \sum_{k=-\infty}^{\infty} (-1)^D k^D e^{\frac{E}{h} - ik\sigma,\ell^\alpha p_{\alpha}(\frac{1}{2})/h} \right\},
\]

where \( S_0 = 2\pi E/\omega \), and the role of the order \( \alpha \) of the perturbative potential \( \varepsilon r^{2\alpha} \) enters through the polynomial in the exponent, see table 1 for examples.

For quartic- and sextic-perturbations \( (\alpha = 2, 3) \), the one-dimensional Fourier integral in (65) can be expressed by the generalised hypergeometric function of (53), see table 2 for examples.

Finally, in all cases we can approximate the Fourier integral in (65) with SPA (60) such that the modulation factor only contains the leading order \( h^{-1} \) contributions for the diameter- and circular-orbits respectively in elementary functions.

### 4.1 Super-shell structures

The cases \( D = 3 \) and \( \alpha = 2, 3 \) (including the polynomial application discussed in section 3.6) is special, since, according to table 2, the modulation factor then only have two terms, both of the same order in \( h \). We now use the \( D = 3 \) case
Figure 4: Numerical illustration of trace formulae for the gross structure of the oscillating part of the density of states. The panels shows the $|k|$ = 1 terms of $\delta g_{\text{pert}}$ as a function of $E/\hbar \omega$, calculated from (65) with a Gaussian quadrature which is effective for moderate values of $\sigma_\alpha/\hbar$. For the two cases $D = 3$ and $\alpha = 2, 3$, we have in addition confirmed the validity of (67). In those two panels the analytic super-shell nodes given by (68) and (69) predicts the strength of the perturbation to be used in the $\alpha = 2, 3$ rows, for (e.g.) $n_s = 40$, to be $\varepsilon = 1.25 \cdot 10^{-3}$ and $\varepsilon = 1.1 \cdot 10^{-5}$, respectively. For the last ($\alpha = 4$) row we chose $\varepsilon = 1.25 \cdot 10^{-7}$. A local numerical investigation showed that only the two cases $D = 3$ and $\alpha = 2, 3$ have perfect super-shell structure, i.e., where the amplitude of the envelope totally disappears in the super-shell nodes, while in for example the panel $D = 3$ and $\alpha = 4$ a tiny amplitude of the envelope remains (compare mid panel of figure 3). We observe that the amplitudes of the shell oscillations are increasing by approximately a factor of ten when the spatial dimension is increased.
of table 2 to calculate $\text{Re} \left\{ \sum_{k=-\infty}^{\infty} (-1)^k M_k e^{ikS_0/h} \right\}$ from (17), for which we obtain (excluding the $k = 0$ term)

$$
\frac{2\hbar}{\sigma_\alpha a_1} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \left\{ \sin \left( \frac{k}{\hbar} [S_0 - \sigma_\alpha a_0] \right) - \sin \left( \frac{k}{\hbar} [S_0 - \sigma_\alpha (a_0 + a_1)] \right) \right\}.
$$

As first reported in [17] (for $\alpha = 2$ and with a spin-factor of 2), this allows us to use trigonometric identities to write the trace formula for the oscillating part of the DOS on a factorised form

$$
\delta g_{\text{pert}} (E) \simeq \frac{\omega^2 (\alpha - 1)}{\pi \varepsilon a_1 \hbar^2} \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \cos \left( \frac{k}{\hbar} [S_0 - \sigma_\alpha (a_0 + a_1)] \right) \sin \left( \frac{k \omega a_1}{2\hbar} \right).
$$

From (40) and (41) we see that $2a_0 = 3(5)$ and $2a_1 = -1(-3)$ for $\alpha = 2(3)$. In both cases the dimension of (67) is $E^{-1}$ as it should for the DOS. It is clear from the second factor in (67) that we have a perfect super-shell structure here, with so called super-shell nodes (i.e., where the envelope of $\delta g(E)$ is zero) when the argument of the sine is a multiple $s = 1, 2, \ldots$ of $\pi$, i.e., with the super-shell nodes $n_S$ (main HO quantum number) given for $\alpha = 2$ by

$$
n_s = \frac{E}{\hbar \omega} = \sqrt{\frac{2s\omega^3}{|\varepsilon| \hbar}},
$$

and for $\alpha = 3$ by

$$
n_s = \frac{E}{\hbar \omega} = \sqrt{\frac{2s\hbar^3}{3|\varepsilon| \hbar^3}}.
$$

In figure 4 we illustrate the perfect super-shell structure, and in particular the super-shell nodes [68] and [69], for the $(D = 3)$ cases $\alpha = 2, 3$, as opposed to (e.g.) the case $\alpha = 4$. Be aware that using the SPA for small values of $\sigma_\alpha / \hbar$ can also generate false super-shell nodes, e.g., for $D = 4$ and $\alpha = 2$ (compare upper-right panel of figure 4). Let us finally stress that the results presented in the two panels $D = 2, 3$ and $\alpha = 2$ in figure 4 agrees with earlier work published in [20] and [21] respectively. In the latter $D = 3$ case the validity of the analytic result presented here have then implicitly also been checked against the DOS calculated numerically from the corresponding Schrödinger equation [21]. It is important to mention that due to the restriction in the orbits included in the perturbative trace formula, it does not converge to the full semiclassical (EBK) spectrum for spherical systems, i.e., where individual energy levels can be labeled by two quantum numbers. It rather gives the smooth DOS within each energyband of the main HO quantum shells, and it marks the start- ($\ell_{\text{min}}$) and end-point ($\ell_{\text{max}}$) of such a band [24].

5 Summary

As Bohr discovered 100 years ago, one can obtain information about a quantum system by study its classical counterpart. We present a calculation of the gross
structure of the quantum mechanical density of energy states in the form of a perturbative semiclassical trace formula. We have generalised earlier work of S. Creagh \cite{20} and M. Brack et al. \cite{21}, in order to handle a $D$-dimensional harmonic oscillator perturbed by an arbitrary monomial potential. The leading order perturbative classical action was found to be an even polynomial in a scaled angular momentum \cite{39}. These polynomials (table 1) are independent of the spatial dimension, and they have a simple representation \cite{42} by well known Legendre polynomials. Utilizing the equivalence between averaging the classical periodic orbits over a $n = 2D - 1$ dimensional sphere $S^n$, and a complex $n = D - 1$ dimensional projective space $\mathbb{C}P^n$, we obtained the modulation factor for the perturbed trace formula. This high dimensional integral \cite{19} was then reduced to a one-dimensional Fourier integral \cite{52}. For the two lowest orders of perturbative monomial potentials (e.g., coming from the leading order of Taylor expansions of more general potentials) the modulation factor was even calculated exactly \cite{53}. In odd dimensions, this modulation factor may be given in elementary functions (table 2). In any dimension and perturbation, employing the stationary phase approximation, \cite{60} gives the leading order term of the modulation factor (figure 3) which is sufficient for the perturbative periodic orbit theory presented. In particular, this result can explain the occurrence of a perfect super-shell structure (figure 4), seen earlier in the quartic perturbed three-dimensional ($D = 3$) harmonic oscillators \cite{21}. The perfect super-shell structure will occur for quartic- and sextic-perturbations ($\alpha = 2, 3$), when there are only two terms of the same order in $\hbar$ in the modulation factor. In these cases the perturbative trace formula can be written in the form of only one sine-function for the slow envelope modulation, multiplied with one cosine-function for the fast beating modulation \cite{67}.

Our main results are that the classical diameter- and circular-periodic orbits are responsible for the gross quantum-shell structure for radially symmetric polynomial perturbations to the $D$-dimensional harmonic oscillator and that the resulting semiclassical trace formulae have been explicitly derived to leading order in $\hbar^{-1}$.

Acknowledgement

We are grateful to colleagues and friends in Copenhagen for encouragement to publish this timely work, and in particular to J. Gravesen and S. Markvorsen. We also thank N. Temme for expert advice on the end-point correction in \cite{59}, N. Eriksen and P. Brändén for discussions about polynomials, and J. Kvistholm for assistance with figures 1 and 2.

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