Weyl Sums

and Atomic Energy Oscillations

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"...cuando hay vino beben vino
cuando no hay vino, agua fresca."

A. Machado.

Abstract: We extend Van der Corput's method for exponential sums to study an oscillating term appearing in the quantum theory of large atoms. We obtain an interpretation in terms of classical dynamics and we produce sharp asymptotic upper and lower bounds for the oscillations.

Introduction.

The purpose of this paper is to study a certain sum that plays a crucial role in the asymptotic analysis of non–relativistic atomic energies. The sum is given by the expression

$$\Psi_Q(Z) = \sum_{l=1}^{l_{\mathrm{TF}}} \frac{2l+1}{\frac{1}{\pi}\int \left(V_{\mathrm{TF}}^Z(r) - \frac{l(l+1)}{r^2}\right)_+^{-1/2} dr}\, \mu\left(\frac{1}{\pi}\int \left(V_{\mathrm{TF}}^Z(r) - \frac{l(l+1)}{r^2}\right)_+^{1/2} dr\right)$$

where $\mu(x) = \mathrm{dist}\,(x, \mathbf{Z})^2 - \frac{1}{12}$, V_{TF}^Z is the Thomas–Fermi potential with charge Z (see [Li]), which satisfies the perfect scaling condition

$$V_{\mathrm{TF}}^Z(r) = Z^{4/3} V_{\mathrm{TF}}^1\left(Z^{1/3}\cdot r\right) \tag{1a}$$

and we have

$$V_{\mathrm{TF}}^1(r) = \frac{y(a\cdot r)}{r}, \qquad a = \left(\frac{3\pi}{2}\right)^{2/3} \tag{1b}$$

and y is the Thomas–Fermi function, solution of the Thomas–Fermi equation

$$\left.\begin{aligned} y''(r) &= \frac{y^{3/2}(r)}{r^{1/2}} \\ y(0) &= 1 \\ \lim_{r\to\infty} y(r) &= 0 \end{aligned}\right\}$$

and l_{TF} is the greatest integer such that $V_{\mathrm{TF}}^Z(r) - l(l+1)/r^2$ is positive somewhere. Here, and throughout this article, we set

$$(x)_+^{-1/2} = \begin{cases} x^{-1/2} & \text{if } x > 0 \\ 0 & \text{if } x \le 0 \end{cases}$$

The role of the function $\Psi_Q(Z)$ in atomic physics is as follows:
Consider a non–relativistic atom, consisting of a nucleus of charge Z fixed at the origin, and N quantized electrons at positions $x_i \in \mathbf{R}^3$. The hamiltonian of such a system is given by

$$H_{Z,N} = \sum_{i=1}^{N}\left(-\Delta_{x_i} - \frac{Z}{|x_i|}\right) + \frac{1}{2}\sum_{i\neq j}\frac{1}{|x_i - x_j|}$$

acting on

$$\psi \in \mathcal{H} = \bigwedge_{i=1}^{N} L^2\left(\mathbf{R}^3 \otimes \mathbf{Z}_2\right)$$

We define the energy of such an atom as

$$E(Z) = \inf_{N \geq 0} E(Z,N), \qquad E(Z,N) = \inf_{\substack{\phi \in \mathcal{H} \\ \|\phi\|=1}} \langle H_{Z,N}\phi, \phi \rangle$$

The computation of $E(Z)$ can only be done explicitly for $Z = 1$, when it equals $-\frac{1}{4}$. For $Z = 2$ good upper and lower bounds are known, but the situation gets more and more complicated as Z grows. It was observed very early in the history of quantum mechanics, in 1927 (see [Th] and [Fe]), by Thomas and Fermi, that for Z large, $E(Z)$ must approximately equal $c_{\mathrm{TF}} Z^{7/3}$ for c_{TF} a well known explicit constant. This was made rigorous by Lieb and Simon in 1973 ([LS] and ([Li]), a very beautiful result which also holds for molecules.
Comparisons with numerical results showed that the Thomas–Fermi approximation was only good up to a term of size Z^2, and Scott ([Sc]) in 1950 was the first to realize that this Z^2 effect was due to electrons very near the nucleus, which behave as if they were in the exactly solvable model without electronic interaction. His argument was make rigorous in a series of papers by Hughes–Siedentop–Weikard ([Hu], [SW1], [SW2] and [SW3]) in 1985—89. This was proved to be true also for molecules by Ivrii–Sigal [IS].
A smaller effect, of size $Z^{5/3}$ was observed by Dirac, in 1930 ([Di]), which comes from a delicate analysis of electronic correlations. Additional effects were also found by Scott ([Sc]), corrected by March and Plaskett [MP], and then finally established by Schwinger ([Sch]), who argued that the asymptotic energy expansion should then contain the term $c_{DS} Z^{5/3}$, for c_{DS} an explicit constant. The proof of Schwinger's result was announced in [FS1], and is as follows:

$$E(Z) = c_{\mathrm{TF}}\, Z^{7/3} + \tfrac{1}{8}\, Z^2 + c_{DS}\, Z^{5/3} + \mathcal{O}\Big(Z^{\frac{5}{3}-a}\Big), \qquad a > 0.$$

Its complete proof appears in [FS2], [FS3], [FS4], [FS5], [FS6], [FS7] and [FS8].
It has been known for some time that nice asymptotics for atomic energies in powers of $Z^{1/3}$ will stop after the Dirac–Schwinger term. This can most easily be conjectured by looking at simpler, exactly solvable models such as the harmonic oscillator (see [Si]). Comparisons with numerical results also show that the next correction will be oscillatory in nature. We refer the reader to the book of Englert ([En]; see also [ES1] and [ES2]) for a physical discussion of the energy asymptotics up to including oscillatory terms. The exact form of the function Ψ_Q above originates from the proof of the Dirac–Schwinger's term in [FS1], where it is seen that

$$E(Z) = c_{\mathrm{TF}}\, Z^{7/3} + \tfrac{1}{8}\, Z^2 + C_{DS}\, Z^{5/3} + \Psi_Q(Z) + \mathcal{O}\Big(Z^{\frac{5}{3}-a}\Big), \qquad a > 0 \tag{2}$$

although the current estimates for a above do not yet guarantee that Ψ_Q really dominates over the $\mathcal{O}$–term.

Note that in establishing (2) not only do we need estimates for the error terms with a large enough, but also we need lower bounds for the size of the function Ψ_Q, which are not completely obvious. It follows from our results in the present article that one would need $a > \frac{1}{6}$ in order to show that Ψ_Q dominates over the error terms contained in the $\mathcal{O}$–term.

From the abstract mathematical perspective, sums such as Ψ_Q are quite old, the best known going back to Gauss, which is related to estimating the number of integral lattice points inside a convex curve: most notably, a circle, which gave rise to the *circle* problem, and a hyperbola, which comes from the *divisor* problem, two of the most elusive problems in analytic number theory (see [GK] for a general description; [IM] and [Hx] for the latest results). It is worth noting the close similarity between our problem and the circle problem, which comes from a refined analysis of the number of bound states of quantum free particles in a box.
A step higher in sophistication, but still within the same realm of problems, is the Selberg trace formula, which, very loosely speaking, expresses spectral information about the laplacian on an abstract manifold in terms of the closed geodesics on that manifold, which can also be seen as the mathematical version of the Feynmann Path integrals for abstract systems. We refer the reader to [G] and references thereof for a wealth of ideas in the theory of trace formulas, quantum chaos, classical mechanics, and all that.

Our work is organized as follows:
First, after making some trivial modifications to the well known stationary phase lemma (Section 1), we set out (in Section 2) to study sums of the type

$$S(\lambda) = \sum_{l=1}^{\lambda} f\left(\frac{l}{\lambda}\right) \mu\left(\lambda \cdot \phi\left(\frac{l}{\lambda}\right)\right)$$

where $\phi''(x) \geq c_0 > 0$, and μ is a periodic function of average 0. Examples of such sums are

1. If $f \equiv 1$, $\mu(x) = e^{2\pi i x}$, $\phi(x) = x^2$, we have the well–known Gauss sums modulo λ.

2. If $f \equiv 1$, $\mu(x) = x - [x] - \frac{1}{2}$, then S represents the error term in the lattice point problem for a curve ϕ dilated by λ.

While the first item above is well understood, the second remains very hard. In our analysis, we will have to deal only with functions μ whose Fourier coefficients decrease rather rapidly ($\hat{\mu}(n) \sim |n|^{-3/2+\varepsilon}$), and this allows a complete analysis of the sums via the usual method of Van der Corput (Poisson summation followed by stationary phase; see [GK]), since all expressions turn out to be absolutely convergent in this case. A little elementary number theory will be needed here to rule out the possibility of a small denominator problem, which gives rise to an error term whose size depends on whether a certain number is rational or irrational.

In Section 3, we apply the results of Section 2 to Ψ_Q, obtaining a new sum Ψ_0, a leading "dual" version of Ψ_Q, reminiscent of the Jacobi identity for the modular function. Sharp upper bounds for Ψ_Q are an easy consequence of this. However, obtaining the right regularity properties for the curve and amplitude involved in the formula for Ψ_Q turns out to be rather tedious.

In Section 4 we obtain *lower* bounds for Ψ_Q in the form of an Ω–result, by understanding how Ψ_0 behaves on average.

In Section 5 we use the *dual* expression Ψ_0 to give us a dynamical interpretation of the sum Ψ_Q as a sum of classical data extended over all closed trajectories of a classical hamiltonian. This result appears to have similarities also with a recent result of Bleher [B1].

Section 6 is devoted to side issues.

1. Stationary Phase Estimates

We begin with a review of stationary phase. Consider $f \in C_0^\infty(\mathbf{R})$. Then, if $t > 0$,

$$\int_{-\infty}^{\infty} e^{itx^2} f(x)\, dx = e^{\frac{\pi i}{4}} \sqrt{\frac{\pi}{t}} \int_{-\infty}^{\infty} e^{-\pi^2 i\xi^2/t} \hat{f}(\xi)\, d\xi$$

Using the identity

$$e^s = 1 + \int_0^1 e^{su} s\, du$$

we deduce

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{itx^2} f(x)\,dx &= e^{\frac{\pi i}{4}}\sqrt{\frac{\pi}{t}}\left(f(0)+\int_{-\infty}^{\infty}\hat f(\xi)\int_0^1\left(\frac{-\pi^2 i\xi^2}{t}\right)e^{-\pi^2 iu\xi^2/t}\,du\,d\xi\right)\\
&= e^{\frac{\pi i}{4}}\sqrt{\frac{\pi}{t}}\left(f(0)+\frac{i}{4t}\int_{-\infty}^{\infty}\widehat{f''}(\xi)\int_0^1 e^{-\pi^2 iu\xi^2/t}\,du\,d\xi\right)\\
&= e^{\frac{\pi i}{4}}\sqrt{\frac{\pi}{t}}f(0)+\frac{i}{4t}\int_{-\infty}^{\infty} f''(x)\int_0^1 e^{itx^2/u}\,\frac{du}{u^{1/2}}\,dx\\
&= e^{\frac{\pi i}{4}}\sqrt{\frac{\pi}{t}}f(0)+\frac{i}{4t^{3/2}}\int_{-\infty}^{\infty} f''(x)g_t(x)\,dx
\end{aligned}$$

for

$$g_t(x)=\int_0^1 e^{itx^2/u}\left(\frac{t}{u}\right)^{1/2}du$$

Note that $g_t(x)=t^{1/2}g_1\left(t^{1/2}x\right)$, and

$$g_1(x)=i\,e^{ix^2/u}\frac{u^{3/2}}{x^2}\Bigg|_0^1-\frac{3i}{2}\int_0^1 e^{ix^2/u}\frac{u^{1/2}}{x^2}\,du$$

hence $|g_1(x)|\le\frac{2}{|x|^2}$ and thus, g_1 is integrable. Furthermore

$$\|g_t\|_1=\|g_1\|_1=\mathcal{O}(1)$$

and $|g_t(x)|\le 2|x|^{-2}t^{-1/2}$.

We also consider one–sided integrals of the form

$$\int_0^{\infty} e^{itx^2} f(x)\,dx$$

Define

$$f^+(x)=\begin{cases} f(x) & \text{if } x\ge 0\\ f(-x) & \text{if } x\le 0\end{cases}$$

and consider $f_\epsilon = f^+ * \varphi_\epsilon$, for a suitable approximation to the identity φ_ϵ. Using our previous identity, we obtain

$$\begin{aligned}
\int_0^{\infty} e^{itx^2} f(x)\,dx &= \tfrac12\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} e^{itx^2} f_\epsilon(x)\,dx\\
&= \tfrac12 e^{\frac{\pi i}{4}}\sqrt{\frac{\pi}{t}}f(0)+\frac{i}{8t^{3/2}}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} f_\epsilon''(x)g_t(x)\,dx\\
&= \tfrac12 e^{\frac{\pi i}{4}}\sqrt{\frac{\pi}{t}}f(0)+\frac{i}{4t^{3/2}}\int_0^{\infty} f''(x)g_t(x)\,dx
\end{aligned}$$

The last step follows since g_t is integrable and both functions g_t and f^+ are even.

Definition: Let ϕ such that

$$|\phi^{(n)}(x)| \leq C_n, \quad (0 \leq n \leq 5), \qquad\qquad c_0 = \inf |\phi''(x)| > 0$$

for x in a certain interval which will be clear in our applications. We denote by

$$c_0^+ = \min(1, c_0), \qquad B(\phi) = \left(\frac{1 + \|\phi\|_{C^5}}{c_0^+} \right)^{54}.$$

Lemma 1–(Stationary Phase Lemma): *Let $f(x) \in C_0^2(\mathbf{R})$, such that*

$$|f'(x)| \leq \begin{cases} N_1 & \text{if } |x| \leq L \\ N_2 & \text{if } |x| > L \end{cases} \qquad (N_1 \leq N_2)$$

and

$$|f''(x)| \leq \begin{cases} M_1 & \text{if } |x| \leq L \\ M_2 & \text{if } |x| > L \end{cases} \qquad (M_1 \leq M_2)$$

and let $\phi(x)$ such that $\phi(0) = \phi'(0) = 0$, $\left|\phi^{(n)}(x)\right| \leq C_n$ for $0 \leq n \leq 5$, and $\phi''(x) \geq c_0 > 0$ for all x in the support of f.
Then

$$\left| \int_{-\infty}^{\infty} e^{it\phi(x)} f(x)\, dx - \left(\frac{2\pi}{|t|\phi''(0)} \right)^{1/2} e^{\mathrm{sign}\ (t)\ \frac{\pi i}{4}} f(0) \right| \\ \leq A\, B(\phi)\, t^{-3/2} \left(\|f\|_\infty + N_1 + \frac{N_2}{t^{1/2} L} + M_1 + \frac{M_2}{t^{1/2} L} \right) \tag{3a}$$

Similarly,

$$\left| \int_{0}^{\infty} e^{it\phi(x)} f(x)\, dx - \left(\frac{\pi}{2|t|\phi''(0)} \right)^{1/2} e^{\mathrm{sign}\ (t)\ \frac{\pi i}{4}} f(0) \right| \\ \leq A\, B(\phi)\, t^{-3/2} \left(\|f\|_\infty + N_1 + \frac{N_2}{t^{1/2} L} + M_1 + \frac{M_2}{t^{1/2} L} \right) \tag{3b}$$

We also have the usual L–independent estimates

$$\left| \int_{-\infty}^{\infty} e^{it\phi(x)} f(x)\, dx - \left(\frac{2\pi}{|t|\phi''(0)} \right)^{1/2} e^{\mathrm{sign}\ (t)\ \frac{\pi i}{4}} f(0) \right| \\ \leq A\, B(\phi)\, t^{-3/2} \left(\|f\|_\infty + \|f'\|_1 + \|f''\|_1 \right) \tag{3c}$$

and

$$\left| \int_0^\infty e^{it\phi(x)} f(x)\, dx - \left(\frac{\pi}{2|t|\phi''(0)} \right)^{1/2} e^{\mathrm{sign}\ (t)\ \frac{\pi i}{4}} f(0) \right|$$
$$\leq A\, B(\phi)\, t^{-3/2} \left(\|f\|_\infty + \|f'\|_1 + \|f''\|_1 \right) \qquad \text{(3d)}$$

where A is a universal constant, and $B(\phi)$ is as defined above for x in the support of f. Here, sign (t) *stands for the function which equals* 1 *if* $t > 0$ *and* -1 *if* $t < 0$.

Proof: It will obviously be enough to consider the case $t > 0$.
Consider the change of variables given by

$$u(x) = x \sqrt{\frac{\phi(x)}{x^2}}$$

and its inverse $z(u)$. We begin by obtaining regularity properties of u and z.

Let $k \geq 1$. In what follows, A_k will denote a collection of universal constants depending only on k.
First, we consider $|x| \leq 1$ and define

$$\phi_1(x) = x^{-2}\, \phi(x).$$

Since

$$\phi_1(x) = \int_0^1 \int_0^1 \phi''(s\, t\, x)\, s\, dt\, ds$$

we have

$$\|\phi_1\|_{C^k} \leq A_k \, \|\phi\|_{C^{k+2}}.$$

Next, define

$$\phi_2(x) = \sqrt{\phi_1(x)}, \qquad |x| \leq 1$$

and note that

$$\frac{d^k \phi_2(x)}{dx^k} = \frac{\displaystyle\sum_{\substack{1\cdot i_1 + \cdots + p\cdot i_p = k \\ i_j \geq 0}} c^{(k)}_{i_1,\ldots,i_p} \, (\phi_1'(x))^{i_1} \cdot \cdots \cdot \left(\phi_1^{(p)}(x)\right)^{i_p}}{\phi_1^{k-\frac{1}{2}}(x)}$$

which can easily be checked by induction. As a result, we have

$$\|\phi_2\|_{C^k} \leq A_k \frac{(1 + \|\phi_1\|_{C^k})^k}{c_0^{k-\frac{1}{2}}} \leq A_k \frac{(1 + \|\phi\|_{C^{k+2}})^k}{c_0^{k-\frac{1}{2}}}$$

where we have used the fact that $\phi_1(x) \geq \frac{1}{2} c_0$. Therefore, since $u(x) = x \cdot \phi_2(x)$, we conclude that

$$\left| \frac{d^k u(x)}{dx^k} \right| \leq A_k \, \frac{(1 + \|\phi\|_{C^{k+2}})^k}{{c_0^+}^{k-\frac{1}{2}}}, \qquad \text{when } |x| \leq 1.$$

When $|x| > 1$ we obviously have that

$$\frac{d^k u(x)}{dx^k} = \sum_{i=1}^{k} \phi^{\frac{1}{2}-i}(x) \sum_{\substack{1\cdot i_1 + \cdots + p \cdot i_p = k \\ i_j \geq 0}} c^{i,k}_{i_1,\ldots,i_p} \left(\phi'(x)\right)^{i_1} \cdot \cdots \cdot \left(\phi^{(p)}(x)\right)^{i_1}, \qquad |x| > 1$$

hence

$$|u^{(k)}(x)| \leq A_k \, \frac{(1 + \|\phi\|_{C^k})^k}{{c_0^+}^{k-\frac{1}{2}}}, \qquad |x| > 1$$

so altogether we obtain

$$\|u\|_{C^k} \leq A_k \, \frac{(1 + \|\phi\|_{C^{k+2}})^k}{{c_0^+}^{k-\frac{1}{2}}}.$$

Finally, since

$$\begin{aligned} & z'\big(u(x)\big) \cdot u'(x) = 1 \\ & \frac{d^k z}{du^k}\big(u(x)\big) \cdot (u'(x))^k = \sum_{p=1}^{k-1} K_{k,p} \, \frac{d^p z}{du^p}\big(u(x)\big) \\ & \qquad \cdot \sum_{\substack{1\cdot i_1 + \cdots + q \cdot i_q = k+1-p \\ i_j \geq 0}} c^{k,p}_{i_2,\ldots,i_q} \left(u'(x)\right)^{i_1} \cdot \cdots \cdot \left(u^{(q)}(x)\right)^{i_q}, \qquad k \geq 2 \end{aligned}$$

and

$$|u'(x)| = \frac{1}{2} \left| \frac{\phi'(x)}{\sqrt{\phi(x)}} \right| \geq c, \qquad c \ \stackrel{\text{def}}{\equiv} \ \frac{c_0}{\sqrt{C_2/2}}$$

we obtain by induction that

$$\left| \frac{d^k z(u)}{du^k} \right| \leq A_k \, \left(\frac{1 + C_2}{c_0^+} \right)^{k^2} \, (1 + \|u\|_{C^k})^{k^2}.$$

With our previous estimate for $\|u\|_{C^k}$ we then conclude that

$$\left| \frac{d^k z(u)}{du^k} \right| \leq A_k \, \left(\frac{1 + \|\phi\|_{C^{k+2}}}{c_0^+} \right)^{2k^3}.$$

Then

$$\int_{-\infty}^{\infty} e^{it\phi(x)} f(x) \, dx = \int_{-\infty}^{\infty} e^{itu^2} \tilde{f}(u) \, du$$

for

$$\tilde{f}(u) = f(z(u)) \cdot z'(u)$$

Note that $\tilde{f}(0) = f(0) \cdot \sqrt{\frac{2}{\phi''(0)}}$. Since $z'(u) \le c^{-1}$,

$$|f'(z(u))| \le \begin{cases} N_1 & \text{if } |u| \le cL \\ N_2 & \text{otherwise} \end{cases}, \qquad |f''(z(u))| \le \begin{cases} M_1 & \text{if } |u| \le cL \\ M_2 & \text{otherwise} \end{cases}.$$

As a result, using stationary phase, we arrive at

$$\left| \int_{-\infty}^{\infty} e^{it\phi(x)} f(x)\, dx - \left(\frac{2\pi}{t\phi''(0)}\right)^{1/2} e^{\frac{\pi i}{4}} f(0) \right| \le t^{-3/2} \left(|I_1| + |I_2| + |I_3|\right)$$

for

$$\begin{aligned} I_1 &= \int g_t(u)\, f(z(u))\, z'''(u)\, du \\ I_2 &= \int g_t(u)\, f'(z(u))\, z'(u)\, z''(u)\, du \\ I_3 &= \int g_t(u)\, f''(z(u))\, \left(z'(u)\right)^3 du. \end{aligned}$$

Now,

$$|I_1| \le \|z\|_{C^3}\, \|f\|_\infty \int |g_t(u)|\, du \le A \cdot \left(\frac{1 + \|\phi\|_{C^5}}{c_0^+}\right)^{54} \cdot \|f\|_\infty$$

Next,

$$\begin{aligned} |I_2| &\le A \left(\frac{C_0}{\sqrt{c_0}}\right) \cdot \left(\frac{1 + \|\phi\|_{C^4}}{c_0^+}\right)^{16} \cdot \left(N_1 \int_{|u| \le cL} |g_t(u)|\, du + 2\, N_2 \int_{|u| \ge cL} t^{-1/2} u^{-2}\, du \right) \\ &\le A \left(\frac{1 + \|\phi\|_{C^5}}{c_0^+}\right)^{54} \cdot \left(N_1 \|g_1\|_1 + \frac{2\, N_2}{t^{1/2} L} \right) \end{aligned}$$

Finally,

$$\begin{aligned} |I_3| &\le M_1 c^{-3} \int_{|u| \le cL} |g_t(x)|\, dx + 2M_2 c^{-3} \int_{|u| \ge cL} t^{-1/2} u^{-2}\, du \\ &\le M_1 c^{-3} \|g_1\|_1 + \frac{2M_2}{c^3 t^{1/2} L} \end{aligned}$$

which proves the first claim in our lemma. The one–sided integral is estimated in the same way. The L–independent estimates are obtained in a similar manner, except that integrals I_2 and I_3 in this case are estimated directly by

$$|I_2| \le \left(\frac{C_0}{\sqrt{c_0}}\right) \cdot \left(\frac{1 + \|\phi\|_{C^4}}{c_0^+}\right)^{16} \|f'\|_\infty \|g_t\|_1, \qquad |I_3| \le c^{-3} \|f''\|_\infty \|g_t\|_1.$$

The one–sided estimate in this case is also analogous. QED

This lemma will be complemented with the following trivial results:

Lemma 2: *Let $f \in C_0^2(\mathbf{R})$, and ϕ such that $|\phi'(x)| \geq d$ for all x in the support of f. Then*

$$\left|\int_{\mathbf{R}} e^{it\phi(x)}\, f(x)\, dx\right| \leq t^{-1}\left(\frac{\|f'\|_1}{d} + \frac{\|f\cdot\phi''\|_1}{d^2}\right) \tag{4a}$$

$$\left|\int_{\mathbf{R}} e^{it\phi(x)}\, f(x)\, dx\right| \leq t^{-1}\left(\frac{\|f\cdot\phi''\|_1}{d^2}\right) + 4\,t^{-2}\left(\frac{\|f''\|_1}{d^2} + \frac{\|f'\cdot\phi''\|_1}{d^3}\right) \tag{4b}$$

$$\left|\int_{\mathbf{R}} e^{it\phi(x)}\, f(x)\, dx\right| \leq 10\,t^{-2}\left(\frac{\|f''\|_1}{d^2} + \frac{\|f'\cdot\phi''\|_1}{d^3} + \frac{\|f\cdot\phi'''\|_1}{d^3} + \frac{\left\|f'\cdot(\phi'')^2\right\|_1}{d^4}\right) \tag{4c}$$

Proof: Integration by parts yields

$$\begin{aligned}\int_{\mathbf{R}} e^{it\phi(x)}\, f(x)\, dx &= -\frac{1}{it}\int_{\mathbf{R}} e^{it\phi(x)}\frac{d}{dx}\left(\frac{f(x)}{\phi'(x)}\right) dx \\ &= \frac{1}{it}\int_{\mathbf{R}} e^{it\phi(x)}\left(\frac{f'(x)}{\phi'(x)}\right) dx - \frac{1}{it}\int_{\mathbf{R}} e^{it\phi(x)}\left(\frac{f(x)\,\phi''(x)}{\phi'(x)^2}\right) dx\end{aligned} \tag{5}$$

This yields (4a). For (4b) we perform another integration by parts to the first integral above, which equals

$$\frac{1}{t^2}\int_{\mathbf{R}} e^{it\phi(x)}\left(\frac{f''(x)}{(\phi'(x))^2}\right) dx + \frac{2}{t^2}\int_{\mathbf{R}} e^{it\phi(x)}\left(\frac{f'(x)\,\phi''(x)}{(\phi'(x))^3}\right) dx$$

which yields (4b). For (4c), we integrate by parts also the last integral in (5), which gives

$$-t^{-2}\int\left(\frac{f'(x)\,\phi''(x)}{\phi'(x)^3} + \frac{f(x)\,\phi'''(x)}{\phi'(x)^3} - 3\,\frac{f(x)\,\phi''(x)^2}{\phi'(x)^4}\right) e^{it\phi(x)}\, dx$$

as needed. QED

Lemma 3: *Let $f \in C_0^2((a,b))$ and ϕ such that $\phi''(x) \geq c_0 > 0$, and $\phi'(x) \neq 0$ for $x \in [a,b]$. Then,*

$$\left|\int_a^b e^{it\phi(x)}\, f(x)\, dx\right| \leq t^{-1}\cdot|b-a|\cdot\left(\frac{\|f''\|_\infty}{c_0} + \frac{\|f\|_\infty\cdot\|\phi''\|_\infty}{c_0^2}\right)$$

Remark: The point in this result is that the estimate is independent of $\inf |\phi'(x)|$.

Proof: f vanishes at a at order 2, which implies

$$|f(x)| \le \|f''\|_\infty \cdot |x-a|^2, \qquad |f'(x)| \le \|f''\|_\infty \cdot |x-a|.$$

So,

$$\phi'(x) \ge c_0 \cdot (x-a).$$

The lemma follows trivially by integration by parts, since

$$\int_a^b e^{it\phi(x)}\, f(x)\, dx = \frac{i}{t} \int_a^b \left(\frac{f'(x)}{\phi'(x)} - \frac{f(x)\cdot \phi''(x)}{\phi'(x)^2} \right) e^{it\phi(x)}\, dx. \qquad \text{QED}$$

The following is a trivial variant of the usual Van der Corput lemmas.

Lemma 4: *Let f be differentiable in $[a,b]$, and ϕ such that $\phi''(x) \ge c_0 > 0$ for $x \in [a,b]$ Then,*

$$\left| \int_a^b e^{it\phi(x)}\, f(x)\, dx \right| \le 8\, t^{-1/2} c_0^{-1/2} \left(1 + \|f\|_\infty + \|f'\|_1\right)$$

Proof: Let $R = t^{-1/2} c_0^{1/2}$, and consider

$$E_1 = \{x \,:\, |\phi'(x)| \ge R\}, \qquad E_2 = \{x \,:\, |\phi'(x)| < R\}.$$

It is obvious that E_1 has at most two components, and $|E_2| \le R/c_0$. The contribution of the integral over E_2 is thus trivial. The integral over E_1, after integration by parts, equals

$$\left. \frac{f(x)}{it\phi'(x)} \right|_{\partial E_1} + i(I_1 - I_2)$$

for

$$I_1 = \int_{E_1} e^{it\phi(x)} \frac{f'(x)}{t\phi'(x)}\, dx, \qquad I_2 = \int_{E_1} e^{it\phi(x)} \frac{f(x)\phi''(x)}{t\,(\phi'(x))^2}\, dx.$$

The boundary terms contribute with at most $4\|f\|_\infty/(Rt)$, which is fine, and the I_i are trivially estimated by

$$|I_1| \le \frac{\|f'\|_1}{t \cdot R}$$

and

$$|I_2| \le \|f\|_\infty \int_{E_1} \frac{\phi''(x)}{t\,(\phi'(x))^2}\, dx \le \frac{4\|f\|_\infty}{t \cdot R}$$

which gives us the bound in the claim of the lemma. QED

2. The Heart of the Matter

In this Section we consider a function μ periodic with period 1, average 0, and Fourier coefficients satisfying

$$|\hat{\mu}(n)| \leq M\,|n|^{-\sigma}, \qquad \sigma \geq 1.$$

We also assume that

$$\sum_{n\neq 0} \sqrt{|n|} \cdot |\hat{\mu}(n)| < \infty \tag{6}$$

Our estimates will depend on M in a trivial way, but since for the applications we will be satisfied with $M = 10$, we will not bother to keep track of the dependence on M. In fact, we will be mostly interested in $\hat{\mu}(n) = |n|^{-s}$, with $s = \sigma + it$ and $\sigma \geq 1$, and for the applications to the energy asymptotics we will be dealing with

$$\mu(x) = \mathrm{dist}(x, \mathbf{Z})^2 - \tfrac{1}{12}, \qquad \hat{\mu}(n) = \frac{e^{-\pi i n}}{2\pi^2 n^2}.$$

However, our estimates will be independent of the value of the sum in (6), which could even be λ–dependent.

Consider also ϕ smooth, defined on $[\,a\,, b\,]$, and satisfying the crucial nondegeneracy condition $-\phi''(x) \geq c_0 > 0$: of course, the same argument will work if we assumed $\phi''(x) > c_0$, with only a few signs being flipped, but we choose this sign in our non–degeneracy condition because it is exactly the one satisfied by the function ϕ in our application to the sum $\Psi_Q(Z)$.
We also assume the bounds

$$\left|\phi^{(n)}(x)\right| \leq C_n, \qquad 0 \leq n \leq 5, \qquad \text{for } x \in [\,a\,, b\,]$$

where $|b - a|$ is bounded by a universal constant, and define

$$S(\lambda) = \sum_{l \in (\mathbf{Z}+\gamma)\cap[\,a\cdot\lambda\,,\, b\cdot\lambda\,]} f\left(\frac{l}{\lambda}\right) \mu\left(\lambda\phi(\frac{l}{\lambda})\right)$$

where γ is a real number.

In our applications, we will be concerned with the following two situations:
on the one hand, we will have functions f and ϕ independent of λ; this simplifies some estimates, but the amplitude function f does not vanish at the endpoint b, which gives origin to a certain diophantine analysis of the phase ϕ.

On the other hand, we will have to deal with functions f and ϕ which depend on λ, which will force us to keep track of error terms in a careful way: furthermore, there is no obvious multiscale analysis in the problem and we thus have to analyze blow up manually. However, in this case the amplitude function is supported inside $[a,b]$ which avoids diophantine discussions.

We summarize both cases as follows.

Case I: $f \in C_0^\infty((a,b])$. In this case, we shall impose that the bounds satisfied by ϕ and f are universal, i.e, independent of λ. The obvious singularity in the sum appearing around $l = b\lambda$ will give rise to a purely arithmetic behavior of the sum.

Case II: $f \in C_0^\infty((a,b))$. In this case, the functions ϕ and f will depend on λ in the sense that the bounds satisfied by ϕ will grow (slowly) as a function of λ. We will thus keep track carefully of the dependence of our error bounds in terms of the regularity assumptions of f and ϕ. The absence of singularities in this case will make the study of the sums purely analytical.

We wish to understand the behavior of $S(\lambda)$ for large λ in both cases.

Case I

As mentioned above, f and ϕ will satisfy universal bounds for its derivatives of the type

$$\|\phi'(x)\|_{C^5} \leq C, \qquad -\phi''(x) \geq c_0, \qquad \|f\|_{C^2} \leq C$$

for constants C and c_0 independent of λ. As a consequence, we will not keep track of the dependence of constants on the regularity properties of either f or ϕ, and the constant C will be ubiquitously used to denote a universal constant depending on the regularity properties of f and ϕ as stated above. Another constant will play a role, though, which is $\phi'(b)$ in the case that it is a rational number $\frac{p}{q}$: in this case, some constants will depend on q, and this dependence will be made explicit.

Let $\varphi(x)$ supported on $(-\infty,b)$, identically equal to 1 on $[a,b-\lambda^{-\frac{1}{2}-\epsilon}]$, for

$$\epsilon = \tfrac{1}{20}$$

φ as smooth as possible. We denote by

$$I_\lambda = [\, b - \lambda^{-\frac{1}{2}-\epsilon}, b\,]$$

the set where φ' is supported.
It is clear that

$$S(\lambda) = \sum_{l \in \mathbf{Z}+\gamma} f\left(\frac{l}{\lambda}\right) \mu\left(\lambda\phi(\frac{l}{\lambda})\right) \varphi(\lambda^{-1} l) + \mathcal{O}\Big(\|f\|_\infty \lambda^{\frac{1}{2}-\epsilon}\Big)$$

and that in the new sum above, only finitely many terms are non–zero. Moreover, $\mu\left(\lambda\phi(x/\lambda)\right)(f\cdot\varphi)(\lambda^{-1}x)$ is a piecewise smooth function of compact support. We set

$$\varphi_f(x) = (f\cdot\varphi)(x)$$

which satisfies $\|\varphi_f\|_\infty \leq \|f\|_\infty$, and

$$\left|\varphi_f'(x)\right| \leq \begin{cases} C & \text{if } x \notin I_\lambda \\ \lambda^{\frac{1}{2}+\epsilon} & \text{if } x \in I_\lambda \end{cases} \qquad \left|\varphi_f''(x)\right| \leq \begin{cases} C & \text{if } x \notin I_\lambda \\ \lambda^{1+2\epsilon} & \text{if } x \in I_\lambda \end{cases} \tag{7}$$

The Poisson summation formula yields

$$\begin{aligned} \sum_{l\in\mathbf{Z}+\gamma} \mu\left(\lambda\phi(\frac{l}{\lambda})\right)\varphi_f(\lambda^{-1}l) &= \sum_l e^{2\pi i l\gamma}\int_{-\infty}^{\infty} \mu\left(\lambda\phi(\frac{x}{\lambda})\right)\varphi_f(\lambda^{-1}x)e^{-2\pi i x l}\,dx \\ &= \sum_l e^{2\pi i l\gamma}\int_{\lambda a}^{\lambda b} \mu\left(\lambda\phi(\frac{x}{\lambda})\right)\varphi_f(\lambda^{-1}x)e^{-2\pi i x l}\,dx \\ &= \sum_{\substack{l\in\mathbf{Z}\\ n\neq 0}} \hat{\mu}(n)e^{2\pi i l\gamma}\int_{\lambda a}^{\lambda b} e^{2\pi i(\lambda n\phi(x/\lambda)-xl)}\varphi_f(\lambda^{-1}x)\,dx \\ &= \lambda\sum_{\substack{l\in\mathbf{Z}\\ n\neq 0}} \hat{\mu}(n)e^{2\pi i l\gamma}\int_a^b e^{2\pi i\lambda\left(n\phi(x)-xl\right)}\varphi_f(x)\,dx. \end{aligned}$$

We will show below that the sum is absolutely convergent, due to the fast decrease of $\hat{\mu}$ assumed in (6), and the fast decrease of the integrals; therefore, the infinite sum can be taken in any order we like.

Define

$$I(n,l) = e^{2\pi i l\gamma}\int_a^b e^{2\pi i\lambda\left(n\phi(x)-xl\right)}\varphi_f(x)\,dx$$

For integers n and l, define $x_{n,l}$ as the unique point (when it exists) satisfying $\phi'(x_{n,l}) = \frac{l}{n}$. Note that

$$c_0^{-1}\left|\frac{l}{n}-\frac{l'}{n'}\right| \geq |x_{n,l}-x_{n',l'}| \geq \|\phi''\|_\infty^{-1}\left|\frac{l}{n}-\frac{l'}{n'}\right|$$

Define also

$$\theta(n,l) = n\cdot\phi(x_{n,l}) - l\cdot x_{n,l}$$

and

$$\sigma_\phi(n,l) = \lambda^{1/2}\frac{1}{|n\cdot\phi''(x_{n,l})|^{1/2}}\, e^{-\text{sign }(n)\,\frac{\pi i}{4}+2\pi i\left(\lambda\theta(n,l)+\gamma\cdot l\right)}$$

We write σ_ϕ to point out that σ depends only on ϕ: the amplitude f does not appear. We begin with the following crude estimate, which is a trivial consequence of Lemma 4.

Lemma 5:

$$|I(n,l)| \leq C\,\lambda^{-1/2}\cdot|n|^{-1/2}.$$

This already implies that only the terms appearing for small n play a role in our sum.

Theorem 6: *With the previous notation, we have*

$$S(\lambda) = \left(\sum_{\substack{n\neq 0\\ l\in\mathbf{Z}\\ x_{n,l}\in(a,b]}} \hat{\mu}(n)\cdot\varepsilon_{n,l}\cdot f(x_{n,l})\cdot\sigma(n,l)\right) + A(\lambda)$$

where $\varepsilon_{n,l}=1$, unless $\phi'(b)=\frac{l}{n}$ when $\varepsilon_{n,l}=\frac{1}{2}$, and

$$A(\lambda) = o\left(\lambda^{1/2}\right)$$

If $\phi'(b)=\frac{p}{q}$, then we have

$$A(\lambda) = \mathcal{O}\left(C_q\lambda^{\frac{1}{2}-\gamma}\right), \qquad \gamma > 0.$$

If, however, $\phi'(b)$ is irrational, the o–term depends on the diophantine properties of $\phi'(b)$. In any case, $|A(\lambda)| \leq C\sqrt{\lambda}$ for C which only depends on $\|f\|_{C^2}$ and $B(\phi)$.

Proof: Note that there are three types of pairs (n,l): those for which $\phi'(x) = \frac{l}{n}$ for some $x = x_{n,l} \in [a,b)$, those such that $\phi'(x)$ never equals $\frac{l}{n}$ for any $x \in [a,b)$, and those (if any) for which $\frac{l}{n}$ equals $\phi'(b)$ ($\phi'(a)$ will play no role here since f vanishes to infinite order at a). We need to deal with these cases separately, and we thus write

$$S(\lambda) = S_1(\lambda) + S_2(\lambda) + S_3(\lambda)$$

where

$$\begin{aligned} S_1(\lambda) &= \lambda \sum_{\phi'(a) \le \frac{l}{n} < \phi'(b)} \hat{\mu}(n) \cdot I(n,l) \\ S_2(\lambda) &= \lambda \sum_{\frac{l}{n} = \phi'(b)} \hat{\mu}(n) \cdot I(n,l) \\ S_3(\lambda) &= \lambda \sum_{\frac{l}{n} \notin [\phi'(a), \phi'(b)]} \hat{\mu}(n) \cdot I(n,l). \end{aligned}$$

Sum S_1: For every term in this sum, the integrand in $I(n,l)$ has a stationary point $x_{n,l}$. Our stationary phase analysis then shows, using (7), that

$$|\lambda \cdot I(n,l) - f(x_{n,l}) \cdot \sigma_{n,l}| \le \lambda \cdot E_{n,l},$$

$$E_{n,l} = C \cdot (\lambda |n|)^{-3/2} \left(1 + \min \left(\lambda^{1+2\epsilon} \, , \, \frac{\lambda^{\frac{1}{2}+2\epsilon}}{|n|^{1/2} \cdot \text{dist } (x_{n,l} \, , \, I_\lambda)} \right) \right) \tag{8}$$

where the min appears as the best of estimates (3a) and (3c) above.

The terms in S_1 will be grouped into three categories. First, those for which $x_{n,l}$ falls far from b, and second, those for which $x_{n,l}$ falls near b. Within the second class, we will have to consider separately those that appear only when n is large, and those with n small.

Fix n in the sum above. For each n, the number of terms in the sum in l is at most $C|n|$. And of those terms, the number of l for which $x_{n,l}$ falls within d of I_λ is bounded by at most $1 + C|n|(d + \lambda^{-\frac{1}{2}-\epsilon})$. If, say, $\phi'(b) = \frac{p}{q}$ is rational, and we take $d > \lambda^{-1/2}$, we have

$$d \ge |b - x_{n,l}| \ge C_2^{-1} \left| \tfrac{l}{n} - \tfrac{p}{q} \right| \ge \frac{C_2^{-1}}{|n\, q|}$$

which means that, if

$$|n| < \|\phi\|_{C^2}^{-1} q^{-1} d^{-1}$$

then there are no l such that $x_{n,l}$ falls within d if I_λ. Similarly, if $\phi'(b)$ is irrational, the number of such l is at most 1 for

$$|n| < {\|\phi\|_{C^2}}^{-1} d^{-1}$$

if $d > \lambda^{-\frac{1}{2}-\epsilon}$. We denote this unique l (when it exists) by $l_0(n,d,\lambda)$, and we denote by $n_0(d,\lambda)$ the smallest $|n|$ for which n has such an l_0.

After all this, we choose

$$d = \lambda^{-7\epsilon}, \qquad c^\sharp = \begin{cases} \|\phi\|_{C^2}^{-1} & \text{if } \phi'(b) \text{ is irrational} \\ \|\phi\|_{C^2}^{-1}\, q^{-1} & \text{if } \phi'(b) = \frac{p}{q} \end{cases}$$

and break up

$$\lambda^{-1} S_1(\lambda) = \sum_{\substack{|n| \le c^\sharp d^{-1} \\ d(x_{n,l}, I_\lambda) \ge d}} \hat{\mu}(n) I(n,l) + \sum_{\substack{|n| > c^\sharp d^{-1} \\ \text{all } l}} \hat{\mu}(n) I(n,l) + \sum_{c^\sharp d^{-1} > |n| \ge n_0(d,\lambda)} \hat{\mu}(n) I\left(n, l_0(n,d,\lambda)\right) \tag{9}$$

where it is understood that if $\phi'(b)$ is rational, the sum in the third term above is null, and the sum in n also in the third term is extended only to those n with a corresponding $l_0(n,d,\lambda)$.

For the first term we use (3a) to obtain

$$E_{n,l} \le C \cdot (\lambda |n|)^{-3/2} \left(1 + |n|^{-1/2} \lambda^{\frac{1}{2}+9\epsilon}\right)$$

Since $|n| \le c^\sharp \lambda^{7\epsilon}$, we obtain (recall $\varepsilon = \frac{1}{20}$),

$$E_{n,l} \le C |n|^{-2} \lambda^{-1+9\epsilon}$$

and, using again $\epsilon = \frac{1}{20}$, we obtain

$$\sum_{\substack{|n| \le c^\sharp d^{-1} \\ d(x_{n,l}, I_\lambda) \ge d}} \lambda \cdot \hat{\mu}(n) \cdot I(n,l) = \sum_{\substack{|n| \le c^\sharp d^{-1} \\ d(x_{n,l}, I_\lambda) \ge d}} \hat{\mu}(n) \cdot f(x_{n,l}) \cdot \sigma_{n,l} + \mathcal{O}\left(\lambda^{\frac{1}{2}-\epsilon} \sum_{n \ne 0} \left|\frac{\hat{\mu}(n)}{n}\right|\right)$$

For the second term in (9), we use the trivial estimate (3b) in (8) to conclude that

$$E_{n,l} = \mathcal{O}\left(\lambda^{-\frac{1}{2}+2\epsilon} |n|^{-3/2}\right)$$

and since $|n| \geq c^\sharp \lambda^{7\epsilon}$,

$$E_{n,l} = \mathcal{O}_q\left(\lambda^{-\frac{1}{2}-\epsilon}|n|^{-{}^{15}\!/_{14}}\right)$$

and we obtain

$$\sum_{|n|>c^\sharp d^{-1}} \lambda \cdot \hat{\mu}(n) I(n,l) = \sum_{|n|>c^\sharp d^{-1}} \hat{\mu}(n) \cdot f(x_{n,l}) \cdot \sigma_{n,l} + \mathcal{O}_q\left(\lambda^{\frac{1}{2}-\epsilon} \sum_{n \neq 0} \frac{|\hat{\mu}(n)|}{|n|^{{}^{15}\!/_{14}}}\right).$$

Note that, here, we could simply have used Lemma 4 to conclude that both $I(n,l)$ and $\sigma_{n,l}$ give a negligible contribution, but this would have required, either, to use the stronger assumption that $\sigma > \frac{3}{2}$, or to obtain an error estimate which depends on the value of the sum (6).

Finally, for the third term, it is clear that

$$\lim_{\lambda \to \infty} n_0\left(\lambda^{-7\epsilon}, \lambda\right) = \infty$$

which, using Lemma 5, implies that

$$\begin{aligned}\left|\sum_{|n|\geq n_0(d,\lambda)} \hat{\mu}(n) I\left(n, l_0(n,d,\lambda)\right)\right| &\leq C \sum_{|n|\geq n_0(d,\lambda)} |\hat{\mu}(n)| \left(\lambda |n|\right)^{-{}^{1}\!/_{2}} \\ &\leq C \lambda^{-{}^{1}\!/_{2}} \left|n_0(d,\lambda)\right|^{-\sigma+\frac{1}{2}} \\ &= o\left(\lambda^{-{}^{1}\!/_{2}}\right)\end{aligned}$$

Similarly, observe that

$$\begin{aligned}\left|\sum_{|n|\geq n_0(d,\lambda)} \hat{\mu}(n) \cdot f(x_{n,l}) \cdot \sigma_{n,l_0(n,d,\lambda)}\right| &\leq C \lambda^{{}^{1}\!/_{2}} \left|n_0(d,\lambda)\right|^{-\sigma+\frac{1}{2}} \\ &= o\left(\lambda^{{}^{1}\!/_{2}}\right)\end{aligned}$$

Therefore, we can conclude that

$$S_1(\lambda) = \sum_{\frac{l}{n} \in [\,\phi'(a)\,,\,\phi'(b)\,)} \hat{\mu}(n) \cdot f(x_{n,l}) \cdot \sigma_{n,l} + o\left(\lambda^{{}^{1}\!/_{2}}\right)$$

Sum S_2: If $\phi'(b)$ is irrational, this sum is empty. We thus assume that $\phi'(b)$ is rational. If we tried to proceed as we did for S_1, we find that $E_{n,l}$ is too big, and this has no remedy. This is so because we would be comparing $I(n,l)$ with the wrong thing: it is not $f(x_{n,l}) \cdot \sigma_{n,l}$ what we should look at, but $\frac{1}{2} f(x_{n,l})\sigma_{n,l}$ instead. We proceed as follows: Say $\phi'(b) = \frac{l}{n}$. We have, by (3d), that

$$\begin{aligned} e^{2\pi i l\gamma} \int_0^1 e^{2\pi i\lambda(n\phi(x)-lx)} \varphi_f(x)\, dx &= e^{2\pi i l\gamma} \int_0^1 e^{2\pi i\lambda(n\phi(x)-lx)} f(x)\, dx + \mathcal{O}\Big(\lambda^{-\frac{1}{2}-\epsilon}\Big) \\ &= \frac{1}{2\lambda} f(x_{n,l}) \cdot \sigma_{n,l} + \mathcal{O}\Big((|n|\lambda)^{-3/2}\Big) + \mathcal{O}\Big(\lambda^{-\frac{1}{2}-\epsilon}\Big) \end{aligned}$$

which yields

$$S_2(\lambda) = \tfrac{1}{2} \sum_{\frac{l}{n}=\phi'(b)} \hat{\mu}(n) \cdot f(x_{n,l}) \cdot \sigma_{n,l} + \mathcal{O}\Big(\lambda^{\frac{1}{2}-\epsilon}\Big)\,.$$

Sum S_3: As for S_1, we deal separately with those l and n for which $\phi'(x) - \frac{l}{n}$ is small or large, and for those for which it is small, we distinguish between small and large n.

When $|\phi'(x) - \frac{l}{n}| > d$ for all $x \in [a,b]$, we use (4c) to obtain

$$I(n,l) = \mathcal{O}\left(\frac{\lambda^{-\frac{3}{2}+\epsilon}}{|n|^2 d^2} + \frac{\lambda^{-2}}{|n|^2 d^3} + \frac{\lambda^{-2}}{|n|^2 d^4} \right)$$

which implies

$$\left| \sum_{(n,l):|\phi'(x)-\frac{l}{n}|>d} \hat{\mu}(n) \cdot I(n,l) \right| \leq C\lambda^{-3/2} \sum_{\text{all } n\neq 0} \left| \frac{\hat{\mu}(n)}{n} \right| \left(\frac{\lambda^{\epsilon}}{d} + \frac{1}{\lambda^{1/2} d^2} + \frac{1}{\lambda^{1/2} d^3} \right)$$

If we now set $d = \lambda^{-7\epsilon}$ we obtain

$$\sum_{(n,l):|\phi'(x)-\frac{l}{n}|>d} \hat{\mu}(n) \cdot I(n,l) = \mathcal{O}\Big(\lambda^{-\frac{1}{2}-\epsilon}\Big)$$

When $0 < |\phi'(b) - \frac{l}{n}| \leq d$, for a fixed n there are at most $1 + |n|\ d$ terms in the sum. And, as before, if $\phi'(b)$ is rational and $|n| < d^{-1}$, then there are no l, and if $\phi'(b)$ is irrational, there is at most one such l, which, if it really existed, we would denote by $l_0(n,d,\lambda)$; we denote by $n_0(d,\lambda)$ the first $|n|$ for which n has such an l. Therefore we break up the remaining part of S_3 given by $0 < |\phi'(b) - \frac{l}{n}| \leq d$, into

$$\sum_{\substack{(n,l):|\phi'(x)-\frac{l}{n}|\leq d \\ |n|>d^{-1}}} \hat{\mu}(n) \cdot I(n,l) \qquad \text{and} \qquad \sum_{|n|\geq n_0(d,\lambda)} \hat{\mu}(n) \cdot I\left(n, l_0(n,d,\lambda)\right).$$

The first sum above is trivially controlled by (4c), which implies

$$I(n,l) = \mathcal{O}\left(\lambda^{-2+\frac{7}{5}}|n|^{-2}\right)$$

hence

$$\sum_{\substack{(n,l):|\phi'(x)-\frac{l}{n}|>d \\ |n|>d^{-1}}} \hat{\mu}(n) I(n,l) = \mathcal{O}\left(\lambda^{-\frac{1}{2}-\epsilon}\right)$$

For the second term, note as before that $\lim_{\lambda\to\infty} n_0(d,\lambda) = \infty$, and therefore, using Lemma 4, we get

$$\begin{aligned}\left|\sum_{|n|\geq n_0(d,\lambda)} \hat{\mu}(n)\cdot I\left(n, l_0(n,d,\lambda)\right)\right| &\leq C \sum_{|n|\geq n_0(d,\lambda)} |\hat{\mu}(n)|\cdot(\lambda|n|)^{-1/2} \\ &\leq C\lambda^{-1/2} n_0^{-\sigma+\frac{1}{2}} \\ &= o\left(\lambda^{-1/2}\right)\end{aligned}$$

All this implies that

$$S_3(\lambda) = o\left(\lambda^{1/2}\right)$$

and the theorem follows. QED

Case II

In this case we will not need $\varphi(x)$ since f is compactly supported and smooth. In fact, $\mu\left(\lambda\phi(x/\lambda)\right) f(\lambda^{-1}x)$ is a piecewise smooth function of compact support, and by the Poisson summation formula, as before,

$$\sum_{l\in\mathbf{Z}+\gamma} \mu\left(\lambda\phi(\frac{l}{\lambda})\right) f(\lambda^{-1}l) = \lambda \sum_{\substack{l\in\mathbf{Z} \\ n\neq 0}} \hat{\mu}(n)\cdot e^{2\pi i l\gamma}\int_a^b e^{2\pi i\lambda\left(n\phi(x)-xl\right)} f(x)\,dx$$

Define, as before,

$$I(n,l) = e^{2\pi i l\gamma}\int_a^b e^{2\pi i\lambda\left(n\phi(x)-xl\right)} f(x)\,dx$$

and $x_{n,l}$ as the unique point (if it did exit) satisfying $\phi'(x_{n,l}) = \frac{l}{n}$. Also as before, we have

$$c_0^{-1}\left|\frac{l}{n}-\frac{l'}{n'}\right| \geq |x_{n,l}-x_{n',l'}| \geq \|\phi''\|_\infty^{-1}\left|\frac{l}{n}-\frac{l'}{n'}\right|$$

Define also $\theta(n,l)$ and $\sigma(n,l)$ exactly as in Case I.

Theorem 7: *With the previous notation, we have*

$$S(\lambda) = \sum_{\substack{n\neq 0\\ l\in\mathbf{Z}}} \hat{\mu}(n)\cdot\sigma(n,l) + \mathcal{O}(B(\phi)\cdot\|f\|_{C^2}\cdot(1+\|f'\|_\infty))$$

Proof: In this case now there are only two types of pairs (n,l): those for which $\phi'(x) = \frac{l}{n}$ for some $x = x_{n,l} \in [a,b]$, and those such that $\phi'(x)$ never equals $\frac{l}{n}$, and thus we write

$$S(\lambda) = S_1(\lambda) + S_2(\lambda)$$

where

$$S_1(\lambda) = \lambda \sum_{\frac{l}{n}\in[\phi'(a),\phi'(b)]} \hat{\mu}(n)\cdot I(n,l)$$
$$S_2(\lambda) = \lambda \sum_{\frac{l}{n}\notin[\phi'(a),\phi'(b)]} \hat{\mu}(n)\cdot I(n,l).$$

Sum S_1: We proceed as in the previous section,

$$|\lambda\cdot I(n,l) - f(x_{n,l})\cdot\sigma_{n,l}| \leq \lambda\cdot E_{n,l}$$

where, by (3c), $E_{n,l}$ is given now by

$$E_{n,l} = C\cdot B(\phi)\cdot\|f\|_{C^2}\cdot(\lambda|n|)^{-3/2}$$

For each n, the number of terms in the sum is at most $(3+C_1)|n|$. Therefore, we can conclude that

$$S_1(\lambda) = \lambda \sum_{\frac{l}{n}\in[\phi'(a),\phi'(b)]} \hat{\mu}(n)\cdot f(x_{n,l})\cdot\sigma_{n,l} + \mathcal{O}\left(C_1^+\cdot B(\phi)\cdot\|f\|_{C^2}\cdot\lambda^{-1/2}\right)$$

for

$$C_1^+ = \max(1, C_1)$$

Sum S_2: By Lemma 3, we have

$$|I(n,l)| \leq C\,\|f\|_{C^2}\,B(\phi)\,\big(\lambda|n|\big)^{-1}$$

which we use when $|l| \leq 2C_1^+|n|^{1-\delta}$, for $\delta > 0$, to obtain

$$\sum_{\{(n,l):\,|l|\leq 2C_1^+|n|^{1-\delta}\}} |\hat{\mu}(n)\cdot I(n,l)| \leq C\lambda^{-1}\,\|f\|_{C^2}\,B(\phi)\cdot C_1^+\sum_{n\neq 0}\frac{|\hat{\mu}(n)|}{|n|^{\delta}}$$

Outside of this range, we have

$$\left|\phi'(x) - \tfrac{l}{n}\right| \geq \tfrac{1}{2}\left|\frac{l}{n}\right| \qquad \text{for all } x\in[a,b].$$

Therefore, (4b) implies

$$|I(n,l)| \leq \frac{C\,\|f\|_{C^2}\,B(\phi)}{\lambda^2\,|n|^2}\,\left(\frac{n^2}{l^2} + + \frac{|n|^3}{|l|^3} + \frac{n^4}{l^4}\right)$$

Therefore,

$$\sum_{\{(n,l):\,|l|>2C_1^+|n|^{1-\delta}\}} |\hat{\mu}(n)\cdot I(n,l)| \leq C\lambda^{-2}\,\|f\|_{C^2}\,B(\phi)\sum_{n\neq 0}\frac{|\hat{\mu}(n)|}{|n|^{1-4\delta}}$$ QED

3. Energy Asymptotics

We plan to apply our previous estimates to the function

$$\Psi_C(Z) = 2\pi\cdot Z^{4/3}\cdot\sum_{l\in(\mathbf{Z}+\frac{1}{2})\cap[1\,,\,a^{-1/2}\cdot Z^{1/3}\cdot\Omega_c]} \eta\left(l\cdot Z^{-1/3}\right)\;\cdot\;\mu\Big(Z^{1/3}\phi\big(l\cdot Z^{-1/3}\big)\Big)$$

where

$$\mu(x) = \operatorname{dist}(x,\mathbf{Z})^2 - \tfrac{1}{12}$$

$$\phi(\Omega) = \frac{1}{\pi}\int\left(V^1_{\mathrm{TF}}(r) - \frac{\Omega^2}{r^2}\right)_+^{1/2} dr = \frac{a^{-1/2}}{\pi}\int\left(\frac{y(r)}{r} - \frac{a\cdot\Omega^2}{r^2}\right)_+^{1/2} dr$$

$$\eta(\Omega) = \frac{\Omega}{P(\Omega)}$$

$$P(\Omega) = \int\left(V^1_{\mathrm{TF}}(r) - \frac{\Omega^2}{r^2}\right)_+^{-1/2} dr = a^{-3/2}\int_{r_1(a^{1/2}\,\Omega)}^{r_2(a^{1/2}\,\Omega)}\left(\frac{y(r)}{r} - \frac{a\cdot\Omega^2}{r^2}\right)^{-\frac{1}{2}} dr$$

Here, $r_i(\Omega)$ are the two points where $y(r)/r$ equals Ω^2/r^2 (see below) and Ω_c is the supremum of the Ω for which

$$\frac{y(r)}{r} - \frac{\Omega^2}{r^2}$$

is positive somewhere.

The crucial result we need is the non–vanishing of the second derivative of ϕ. This was proved in [FS8]. Because of its vital importance, we display it explicitly:

Theorem 8: *There exists a number c_0 such that*

$$-\phi''(\Omega) \geq c_0 > 0 \qquad \text{for all } \Omega \in (0, \Omega_c)$$

We will first recall some known results (which appear, for example, in [FS8], [Hi] and [Hu]) which we will need here. After that, we will complement them with further properties of ϕ and P, some of which are taking from similar estimates appearing in [FS2—8].

Review of earlier results. If we set $u(r) = r \cdot y(r)$, then u has a unique maximum at $r = r_c$, where $r_c \sim 2.1$. We set $\Omega_c^2 = u(r_c)$. Then, u is increasing on $[0, r_c]$ and decreasing on (r_c, ∞). This is a crucial fact whose proof goes back to Sommerfeld, and can be found in [Hu].

Around 0, u satisfies the expansions

$$u(x) = \sum_{n=2}^{\infty} u_n \, x^{n/2}, \qquad u_2 = 1, \quad u_3 = 0, \quad u_4, \sim -1.588.$$

Rigorous numerical bounds for u_4 can be found in [FS8]. However, it is easy to see analytically that $u_4 < 0$. We also have

$$\sum_{n=2}^{\infty} |u_n| \cdot \rho_0^n < \infty, \qquad \rho_0 > 0,$$

therefore, the function

$$f(z) = \sum_{n=2}^{\infty} u_n z^n$$

is analytic in a small neighborhood around 0.

Around ∞, we have the expansion

$$u(x) = \frac{144}{x^2} \sum_{n=0}^{\infty} b_n \, x^{-\frac{n\alpha}{2}}, \qquad b_0 = 1, \quad b_1 \sim -13, \qquad \alpha = \frac{\sqrt{73} - 7}{2} \sim 0.772.$$

Again, rigorous numerical bounds for b_1 are found in [FS8], and it can be seen analytically that $b_1 < 0$. We also have that

$$\sum_{n=0}^{\infty} |b_n|\,\rho_1^n < \infty, \qquad \rho_1 > 0,$$

and, as a result, we have

$$u(x) = \frac{144}{x^2}\, f\left(x^{-\alpha/2}\right) \tag{10}$$

for a function f analytic in a neighborhood of 0.

Given any $\Omega \in (0, \Omega_c)$, there exist two numbers, $r_1(\Omega) \le r_2(\Omega)$ where u equals Ω^2. We then have

Lemma 9: *The following formulas hold:*

$$\phi(\Omega) = \frac{a^{-1/2}}{\pi} \cdot F\left(a^{1/2}\Omega\right)$$

where

$$F(\Omega) = \int \left(u(x) - \Omega^2\right)_+^{1/2} \frac{dx}{x}$$

$$F'(\Omega) = -\Omega \int \left(u(x) - \Omega^2\right)_+^{-1/2} \frac{dx}{x}$$

$$F''(\Omega) = -\lim_{\delta\to 0}\left(\int_{r_1(\Omega)+\delta}^{r_2(\Omega)-\delta} \left(u(x) - \Omega^2\right)^{-3/2} y(x)\,dx + c(\Omega)\delta^{-1/2}\right)$$

where $c(\Omega)$ is uniquely specified by requiring the finiteness of the limit.

Moreover, if b is any number less than $r_2(\Omega)$, then

$$\frac{d^2}{d\Omega^2}\int_{r_1(\Omega)}^{b} \left(u(x) - \Omega^2\right)_+^{1/2} \frac{dx}{x}$$

equals

$$-\lim_{\delta\to 0}\left(\int_{r_1(\Omega)+\delta}^{b} \left(u(x) - \Omega^2\right)^{-3/2} y(x)\,dx + c_1(\Omega)\delta^{-1/2}\right)$$

again, for a constant c_1 that makes the limit finite. The corresponding symmetric case also holds.

Furthermore, F can be extended as an analytic function to a complex neighborhood of $(0, \Omega_c]$. However, 0 is an essential singularity of ϕ (or F), and, moreover,

$$\lim_{\Omega\to 0} \phi''(\Omega)\cdot\Omega^{\gamma} = \kappa, \qquad \gamma = \frac{9-\sqrt{73}}{2} > 0,$$

where κ is a strictly negative real number.

A consequence of this which is of importance to us is that although ϕ and ϕ' remain bounded as we approach 0, the second derivative blows up slowly, and third will blow up much faster. In other words, ϕ does not satisfy sensible non–degenerate multiscale analysis bounds.

Further background results. Here we will obtain growth and regularity properties of the functions ϕ and P above. We define

$$g_\gamma(x) = \int_1^{x^{-2}} (t-1)^{-1/2}\, t^\gamma\, dt, \qquad \text{for } 0 < x \le \tfrac{1}{2}.$$

We begin listing several elementary results of calculus:

Lemma 10: *For $\gamma \in \mathbf{R}$, we have*

$$g_\gamma^{(k)}(x) \le C_k \left(|\gamma| + 1\right)^{k-1} x^{-2\gamma-1-k}, \qquad \text{for } k \ge 1 \tag{11a}$$

Furthermore, if $\gamma < -\frac{1}{2}$, then

$$\frac{1 - 2^{\gamma+\frac{1}{2}}}{|\gamma + \frac{1}{2}|} \le g_\gamma(x) \le 100 + \frac{100}{|\gamma + \frac{1}{2}|} \tag{11b}$$

and if $\gamma > -\frac{1}{2}$, then

$$\frac{x^{-2\gamma-1} - 1}{|\gamma + \frac{1}{2}|} \le g_\gamma(x) \le \left(100 + \frac{100}{|\gamma + \frac{1}{2}|}\right) x^{-2\gamma-1} \tag{11c}$$

where $0 < x \le \frac{1}{2}$.

Proof: Estimate (11a) is completely trivial. For (11b), we use

$$\int_1^2 t^{-\frac{1}{2}+\gamma}\, dt \le g_\gamma(x) \le 4 + \int_2^\infty (t-1)^{-\frac{1}{2}+\gamma}\, dt$$

For (11c), we use the fact that $t - 1 > \frac{1}{2}t$ for $t > 2$ to write

$$\int_1^{x^{-2}} t^{\gamma-\frac{1}{2}}\, dt \le g_\gamma(x) \le 2^{|\gamma|+3} + 2\int_2^{x^{-2}} t^{\gamma-\frac{1}{2}}\, dt$$

which implies (11c) after using the fact that $2^{|\gamma|+\frac{1}{2}} \le 4\, x^{-2\gamma-1}$. QED

Lemma 11: *Define*

$$f(\Omega) = \left(\Omega_\varepsilon^2 - \Omega^2\right)^{-1/2}$$

Then, $|f^{(k)}(\Omega)| \leq C_k\, \Omega_\varepsilon^{-1-k}$ *for* $\Omega \leq \frac{1}{2}\Omega_\varepsilon$ *and* $k \geq 0$.

Proof:

$$f(\Omega) = \Omega_\varepsilon^{-1} g\left(\frac{\Omega}{\Omega_\varepsilon}\right), \qquad \text{for } g(x) = \left(1 - x^2\right)^{-1/2}. \tag{12}$$

Done. QED

Lemma 12: *Given* $\beta > 0$, $\delta > 0$, $\Omega_\varepsilon > 0$, τ, d *and* w_n *for* $n = 0, 1, 2, \ldots$, *let*

$$f(\Omega) = \sum_{n=0}^{\infty} w_n\, m_n(\Omega), \qquad m_n(\Omega) = \Omega^{2\gamma_n + d} g_{\gamma_n}\left(\frac{\Omega}{\Omega_\varepsilon}\right)$$

where $\gamma_n = \tau + \beta \cdot n$ *and* $|\gamma_n + \frac{1}{2}| > \delta$ *for all* $n \geq 0$.
Assume that $\sum w_n z^n$ *has a radius of convergence* ρ *and* $\Omega_\varepsilon^{2\beta} \leq \frac{1}{2}\rho$.
Then,

$$\left|\frac{d^k f}{d\Omega^k}(\Omega)\right| \leq \begin{cases} C\,\Omega^{2\tau + d - k} & \text{if } \tau < -\frac{1}{2} \\ C\,\Omega^{d-1-k} & \text{if } \tau > -\frac{1}{2} \end{cases} \qquad \text{when } \Omega \leq \tfrac{1}{2}\Omega_\varepsilon$$

for a certain constant C *which depends on everything except* Ω.

Proof: Let's consider first those n such that $\gamma_n > -\frac{1}{2}$. In this case, using Lemma 10 we obtain

$$\begin{aligned} \left|\frac{d^k m_n}{d\Omega^k}(\Omega)\right| &\leq \sum_{l=0}^{k} C(k;\delta) \cdot (n+1)^{k-l} \cdot \Omega^{2\gamma_n + d - (k-l)} \cdot \Omega_\varepsilon^{-l} \cdot \left|\frac{d^l g_{\gamma_n}(\Omega)}{d\Omega^l}\left(\frac{\Omega}{\Omega_\varepsilon}\right)\right| \\ &\leq C(k;\delta) \cdot (n+1)^k \cdot \Omega_\varepsilon^{2\gamma_n+1} \cdot \Omega^{d-1-k} \end{aligned}$$

If, on the other hand, $\gamma_n < -\frac{1}{2}$, the $l = 0$ term above has to be estimated by

$$C(k;\delta) \cdot (n+1)^k \cdot \Omega^{2\gamma_n + d - k}$$

and we obtain

$$\begin{aligned} \left|\frac{d^k m_n}{d\Omega^k}(\Omega)\right| &\leq C(k;\delta) \cdot (n+1)^k \cdot \left(\Omega_\varepsilon^{2\gamma_n+1} \cdot \Omega^{d-1-k} + \Omega^{2\gamma_n+d-k}\right) \\ &\leq 2\,C(k;\delta) \cdot (n+1)^k \cdot \Omega^{2\gamma_n+d-k} \end{aligned}$$

because $\Omega \leq \Omega_\varepsilon$. Since we can only have $\gamma_n < -\frac{1}{2}$ for finitely many n, we conclude that

$$\sum_{n=0}^{\infty} w_n \, m_n^{(k)}(\Omega) = \frac{d^k f}{d\Omega^k}(\Omega)$$

where the sum converges absolutely, and we obtain the required estimate. QED

This ends our presentation of calculus results. In what follows we will develop the regularity bounds for ϕ first and then P.

Lemma 13: *For constants C_n and $c > 0$ we have*

$$|\phi(t)| \leq C_0, \qquad |\phi'(t)| \leq C_1, \qquad \left|\frac{d^n \phi}{d\Omega^n}\right| \leq C_n \, \Omega^{-n+1+\alpha} \quad (n \geq 2)$$

and

$$-\phi''(\Omega) \geq c \cdot \Omega^{-1+\alpha}.$$

Proof: As in Lemma 9, in order not to bother with the presence of the constant a, we will prove this result for the function F instead.
The inequalities for ϕ and ϕ' are obvious. For the higher derivatives, the bounds outside a neighborhood of 0 are a direct consequence of the analytic extension of F to a complex neighborhood of $(0, \Omega_c]$, which is Corollary 1.3 in [FS8]. We are thus only left with proving the bounds in an arbitrarily small neighborhood to the right of 0, given by $(0, \bar{\Omega}_\varepsilon)$, for a small universal number $\bar{\Omega}_\varepsilon$ to be picked up later in the proof.
Arguing as in formula (4.1abc) [FS8], using Lemma 9, we write

$$-F''(t) = I_1 + I_2 + I_3$$

for

$$I_1 = \int_a^b \left(u(r) - \Omega^2\right)^{-3/2} y(r)\, dr$$

$$I_2 = \lim_{\delta \to 0} \left(\int_{r_1(\Omega)+\delta}^{a} \left(u(r) - \Omega^2\right)^{-3/2} y(r)\, dr - G_1(\Omega)\delta^{-1/2} \right)$$

$$I_3 = \lim_{\delta \to 0} \left(\int_{b}^{r_2(\Omega)-\delta} \left(u(r) - \Omega^2\right)^{-3/2} y(r)\, dr - G_2(\Omega)\delta^{-1/2} \right)$$

with G_i such that the limit is finite, and a and b any numbers such that $r_1(\Omega) < a < b < r_2(\Omega)$. In practice, we will take a and b such that

$$u(a) = u(b) = \Omega_\varepsilon^2$$

for Ω_ε a small number, and later, we will take $\bar{\Omega}_\varepsilon \ll \Omega_\varepsilon$.

First, $I_1(\Omega)$ is C^∞ in a neighborhood of 0, and therefore satisfies

$$\left| \frac{d^k I_1}{d\Omega^k}(\Omega) \right| \le C_k(\Omega_\varepsilon) \qquad \text{for } \Omega \in (0, \Omega_\varepsilon)$$

no matter which Ω_ε we will end up choosing.

For I_2, we write $I_2 = \frac{d}{d\Omega}\tilde{I}_2$, where, by Lemma 9,

$$\tilde{I}_2(\Omega) = \Omega \int_{r_1(\Omega)}^{a} \left(u(r) - \Omega^2\right)^{-1/2} \frac{dr}{r}$$

Let $r(t)$ be the inverse of u near 0, $u(r(t)) = t$, and set $w(t) = r'(t)/r(t)$. Changing variables above we obtain,

$$\begin{aligned} \tilde{I}_2(\Omega) &= \Omega \int_{\Omega^2}^{\Omega_\varepsilon^2} \left(t - \Omega^2\right)^{-1/2} w(t)\, dt \\ &= \Omega^2 \int_1^{\Omega^{-2}\Omega_\varepsilon^2} (t-1)^{-1/2}\, w\left(t \cdot \Omega^2\right)\, dt \end{aligned}$$

which implies, after differentiation,

$$I_2(\Omega) = 2\Omega \int_1^{\Omega^{-2}\Omega_\varepsilon^2} (t-1)^{-1/2}\, h\left(t \cdot \Omega^2\right)\, dt - 2\left(\Omega_\varepsilon^2 - \Omega^2\right)^{-1/2} w(\Omega_\varepsilon^2) \cdot \Omega_\varepsilon^2$$

for

$$h(t) = t w'(t) + w(t)$$

Next, we recall that $u(r) = r \cdot f(r^{1/2})$ for f analytic around 0 and $f(0) = 1$. Therefore, $u^{1/2}(r) = r^{1/2}\tilde{f}(r^{1/2})$, for $\tilde{f}$ also analytic around 0, or $u^{1/2}(r) = \tilde{\tilde{f}}(r^{1/2})$, for $\tilde{\tilde{f}}$ also analytic around 0, $\tilde{\tilde{f}}(0) = 0$ and $\tilde{\tilde{f}}\,'(0) = 1$. Therefore, $\tilde{\tilde{f}}$ has an analytic inverse g, with $g(0) = 0$ and $g'(0) = 1$, and therefore, $r^{1/2} = u^{1/2}\tilde{g}(u^{1/2})$, for $\tilde{g}$ analytic and $\tilde{g}(0) = 1$. Squaring both sides, we obtain

$$r(t) = t \cdot \tilde{\tilde{g}}(t^{1/2})$$

for $\tilde{\tilde{g}}$ analytic around 0, $\tilde{\tilde{g}}(0) = 1$. As a consequence of this, we also have

$$w(t) = t^{-1} \cdot W(t^{1/2})$$

for W analytic around 0 and

$$h(t) = t^{-1} \cdot H(t^{1/2})$$

It was shown in [FS8] that $H(0) = H'(0) = 0$, and $H''(0) = -2y'(0)$, which implies that in fact

$$h(t) = f_h(t^{1/2}), \qquad f_h(0) = -y'(0).$$

Therefore,

$$f_h(z) = \sum_{n=0}^{\infty} h_n z^n, \qquad \sum_{n=0}^{\infty} |h_n| \rho_2^n < \infty$$

for ρ_2 a small universal constant.

We break up $I_2(\Omega) = f_1(\Omega) + f_2(\Omega)$ for

$$f_1(\Omega) = 2\Omega \int_1^{\Omega^{-2}\Omega_\varepsilon^2} (t-1)^{-1/2} \, h\left(t \cdot \Omega^2\right) \, dt = \sum_{n=0}^{\infty} 2 h_n \Omega^{1+n} \cdot g_{n/2}\left(\frac{\Omega}{\Omega_\varepsilon}\right)$$

$$f_2(\Omega) = -2\left(\Omega_\varepsilon^2 - \Omega^2\right)^{-1/2} w(\Omega_\varepsilon^2) \cdot \Omega_\varepsilon^2$$

Lemma 11 shows that $f_2^{(k)}(\Omega)$ is bounded for all $k \geq 0$ and $\Omega \leq \frac{1}{2}\Omega_\varepsilon$ by a constant that may depend on Ω_ε. For f_2, we apply Lemma 12 with $d = 1$, $\tau = 0$ and $\beta = \frac{1}{2}$ to obtain

$$\left| \frac{d^k f_2}{d\Omega^k}(\Omega) \right| \leq C(k, \Omega_\varepsilon) \cdot \Omega^{-k}.$$

We conclude the analysis of I_2 by observing that all the bounds we obtained are in agreement with the statement of the lemma.

We continue now with I_3. Denote by $r(t)$ the inverse function of $u(r)$, such that $u(r(t)) = t$. We proceed as in Section 4 in [FS8] to construct $w(t) = -\frac{r'(t)}{r(t)}$ and then set $h(t) = tw'(t) + w(t)$ which allows us to argue as before to obtain (equation (4.21a) in [FS8])

$$I_3 = 2\Omega \int_1^{\Omega^{-2}\Omega_\varepsilon^2} (t-1)^{-1/2} h\left(t\Omega^2\right) \, dt - 2\left(\Omega_\varepsilon^2 - \Omega^2\right)^{-1/2} w(\Omega_\varepsilon^2) \cdot \Omega_\varepsilon^2$$

By (10) we have that $r^2 u(r) = g(r^{-\alpha})$ for g analytic in a neighborhood of 0, with $g(0) = \frac{1}{144}$. Therefore, setting $z = r^{-\alpha}$ and $u(r) = t$ we have $t = z^{2/\alpha} g(z)$, or $t^{\alpha/2} = \tilde{g}(z)$ for a new $\tilde{g}$ analytic in a small neighborhood of 0, with $\tilde{g}(0) = 0$ and $\tilde{g}'(0) \neq 0$. Thus, $\tilde{g}$ has an analytic inverse, f, with $f(0)=0$, $f'(0)\neq 0$, and we have $z=f(t^{\alpha/2})$, or $z=t^{\alpha/2}\tilde f(t^{\alpha/2})$ for $\tilde f$ analytic around 0 and $\tilde f(0)\neq 0$. Therefore, $r(t)=z^{-1/\alpha}=t^{-1/2}v(t^{\alpha/2})$ for a new function v analytic around 0 which also satisfies $v(0)\neq 0$. Hence,

$$r'(t)=t^{-3/2}v_p(t^{\alpha/2}),\qquad r''(t)=t^{-5/2}v_{pp}(t^{\alpha/2}) \tag{13}$$

for functions v_p and v_{pp} analytic in a small neighborhood around 0. Therefore,

$$h(t)=\frac{1}{4t}f_h(t^{\alpha/2})$$

where, by (13), $f_h(z)$ is analytic in a small neighborhood around 0, $|z|<\rho_h$. It is observed in [FS8] that $f_h(0)=0$ and $f_h'(0)>0$ (Equation (4.20) in [FS8]). This allows us to put

$$I_3(\Omega)=f_1(\Omega)+f_2(\Omega)$$

where

$$f_1(\Omega)=\sum_{n=1}^{\infty}2\,h_n\,m_n(\Omega),\quad m_n(\Omega)=\Omega^{-1+n\alpha}\int_1^{\Omega^{-2}\Omega_\varepsilon^2}(t-1)^{-1/2}t^{-1+\frac{n\alpha}{2}}\,dt \tag{14}$$

$$f_2(\Omega)=-2\left(\Omega_\varepsilon^2-\Omega^2\right)^{-1/2}w(\Omega_\varepsilon^2)\cdot\Omega_\varepsilon^2.$$

If we make sure that

$$\Omega_\varepsilon^\alpha\leq\tfrac12\,\rho_h \tag{15}$$

we can invoke Lemma 12, with $\tau=-1+\frac{\alpha}{2}$, which is less than $-\frac12$, $\beta=\frac{\alpha}{2}$ and $d=1$ to obtain

$$\left|\frac{d^kf_1}{d\Omega^k}(\Omega)\right|\leq C(\Omega_\varepsilon;k)\cdot\Omega^{-1+\alpha-k}.$$

This ends the proof of all upper bounds in the statement of the lemma. For the lower bound for $-\phi''$, we use the notation in (14) to write

$$f_1(\Omega)=2h_1\cdot m_1(\Omega)+\tilde f_1(\Omega),\qquad \tilde f_1(\Omega)=\sum_{n=2}^{\infty}2\,h_n\,m_n(\Omega)$$

Applying Lemma 10 to the first term above with $\gamma=-1+\frac{\alpha}{2}<-\frac12$, and Lemma 12 applied to $\tilde f_1(\Omega)$ with $\tau=-1+\alpha>-\frac12$, we obtain

$$f_1(\Omega)\geq c\,h_1\Omega^{-1+\alpha},\qquad |\tilde f_1(\Omega)|\leq C(\Omega_\varepsilon).$$

Since all other terms in the break–up of $-\phi''$ remain bounded as $\Omega\to 0$, we conclude that

$$-\phi''(\Omega)\geq c\Omega^{-1+\alpha},\qquad \Omega\leq\bar\Omega_\varepsilon$$

for $\bar\Omega_\varepsilon\ll\Omega_\varepsilon$, as required. QED

We now turn our attention to P. In this case, rather than introducing a new function that allows us to do without the bothersome constant a, we will simply proceed as if a did not appear in the definition of P. This simplification clearly does not change the result, except of course, that the details of the proof will not contain the a dependence.
The following result is a trivial adaptation of Lemma 1.2 in [FS8] for P instead of ϕ.

Lemma 14: *We have $P \in C^\infty(0, \Omega_c)$. Furthermore, P admits an analytic extension to a neighborhood of Ω_c.*

Proof: Let
$$H(\delta, \Omega) = \Omega \int_{r_1(\Omega)+\delta}^{r_2(\Omega)-\delta} \left(u(r) - \Omega^2\right)^{-1/2} \, r\,dr$$
Consider the analytic change of variables given by
$$t(r) = \begin{cases} \left(\Omega_c^2 - u(r)\right)^{1/2} & \text{if } r \geq r_c \\ -\left(\Omega_c^2 - u(r)\right)^{1/2} & \text{if } r \leq r_c \end{cases} \tag{16}$$
Note that t is smooth and strictly increasing in the range $(0, \infty)$. We can therefore consider its inverse, $r(t)$, and use it to rewrite
$$H(\delta, \Omega) = \Omega \int_{t_1(\delta,\Omega)}^{t_2(\delta,\Omega)} \left(D^2 - t^2\right)^{-1/2} w(t)\,dt$$
where
$$t_1 = t(r_1 + \delta), \qquad t_2 = t(r_2 - \delta), \qquad D^2 = \Omega_c^2 - \Omega^2, \qquad w(t) = r'(t) \cdot r(t).$$
Note that w is smooth on $(-\Omega_c, \Omega_c)$, and that
$$t_1 = -D\left(1 + \tau_1(\delta)\right), \qquad t_2 = D\left(1 + \tau_2(\delta)\right), \qquad c\delta \leq |\tau_i| \leq C\delta \quad \text{for } i = 1, 2 \tag{17}$$
uniformly on compact subsets of $(-\Omega_c, \Omega_c)$, which implies that
$$H(\delta, \Omega) = \Omega \int_{D^{-1}t_1}^{D^{-1}t_2} \left(1 - t^2\right)^{-1/2} w(tD)\,dt$$
converges as $\delta \to 0$ uniformly to the C^1 function
$$H(0, \Omega) = \Omega \int_{-1}^{1} \left(1 - t^2\right)^{-1/2} w(tD)\,dt = P(\Omega). \tag{18}$$

To show analyticity around Ω_c, note that $w(t)$ is analytic around 0; thus, it admits a convergent power series expansion given by

$$w(t) = \sum_{n=0}^{\infty} w_n t^n, \qquad |t| \le \rho$$

which implies

$$P(\Omega) = \Omega \sum_{n=0}^{\infty} w_n \cdot D^n \int_{-1}^{1} \left(1 - t^2\right)^{-1/2} t^n \, dt.$$

The integral corresponding to the odd terms in the sum is 0, which implies that in fact

$$P(\Omega) = \Omega \sum_{n=0}^{\infty} w_{2n} \cdot D^{2n} \int_{-1}^{1} \left(1 - t^2\right)^{-1/2} t^{2n} \, dt$$

which defines an analytic function of Ω around Ω_c, since D^2 now is analytic in Ω. QED

Lemma 15: *For constants C_n and $c > 0$ we have*

$$\left| \frac{d^k P}{d\Omega^k}(\Omega) \right| \le C_k \cdot \Omega^{-3-k}, \qquad |P(\Omega)| \ge c \cdot \Omega^{-3}.$$

Proof: Lemma 14 establishes our inequalities outside an arbitrarily small neighborhood of 0. For a neighborhood to the right of 0 given by $(0, \bar{\Omega}_\varepsilon)$ we proceed as before, setting

$$f(\Omega) = I_1 + I_2 + I_3$$

for

$$I_1 = \int_a^b \left(u(r) - \Omega^2\right)^{-1/2} r \, dr$$

$$I_2 = \int_{r_1(\Omega)}^{a} \left(u(r) - \Omega^2\right)^{-1/2} r \, dr$$

$$I_3 = \int_b^{r_2(\Omega)} \left(u(r) - \Omega^2\right)^{-1/2} r \, dr$$

with a and b any numbers such that $r_1(\Omega) < a < b < r_2(\Omega)$. We will take a and b such that $u(a) = u(b) = \Omega_\varepsilon^2$ for Ω_ε a small number to be picked later.

I_1 is C^∞ around 0, and thus satisfies all the required upper bounds.

For I_2, denote by $r(t)$ the inverse function of $u(r)$ around 0, such that $u(r(t)) = t$, $r(t) \leq r_c$, and set $w(t) = r'(t)r(t)$. By the same argument as before, we can see that

$$w(t) = t \cdot f_0\left(t^{1/2}\right)$$

for

$$f_0(z) = \sum_{n=0}^{\infty} w_n z^n$$

analytic for $|z| \leq \rho_3$, ρ_3 a small universal number, and $f_0(0) \neq 0$.

Then,

$$\begin{aligned} I_2 &= \int_{\Omega^2}^{\Omega_\varepsilon^2} \left(t - \Omega^2\right)^{-1/2} w(t)\, dt \\ &= \Omega \int_1^{\Omega^{-2}\Omega_\varepsilon^2} (t-1)^{-1/2}\, w(t\Omega^2)\, dt \\ &= \sum_{n=0}^{\infty} w_n\, \Omega^{3+n}\, g_{1+\frac{n}{2}}\left(\frac{\Omega}{\Omega_\varepsilon}\right). \end{aligned}$$

Thus, Lemma 12, for $\Omega_\varepsilon \leq \frac{1}{2}\rho_3$, $\tau = 1$, $\beta = \frac{1}{2}$, $d = 1$, yields

$$\left|\frac{d^k I_2}{d\Omega^k}(\Omega)\right| \leq C(k;\Omega_\varepsilon) \cdot \Omega^{-k}, \qquad \text{for } \Omega \leq \tfrac{1}{2}\Omega_\varepsilon.$$

For I_3, denote by $r(t)$ the inverse function of $u(r)$ around ∞, such that $u(r(t)) = t$, $r(t) \geq r_c$, and set $w(t) = -r'(t)r(t)$. By the same argument as before, we can see that

$$w(t) = t^{-2} f_1\left(t^{\alpha/2}\right)$$

for

$$f_1(z) = \sum_{n=0}^{\infty} w_n\, z^n$$

analytic for $|z| \leq \rho_4$, ρ_4 a small universal number, and $f_1(0) \neq 0$.

Then,

$$I_3 = \int_{\Omega^2}^{\Omega_\varepsilon^2} \left(t - \Omega^2\right)^{-1/2} w(t)\, dt$$

$$= \Omega \int_1^{\Omega^{-2}\Omega_\varepsilon^2} (t-1)^{-1/2}\, w(t\Omega^2)\, dt$$

$$= \Omega^{-3} \sum_{n=0}^{\infty} w_n \Omega^{\alpha n} \int_1^{\Omega^{-2}\Omega_\varepsilon^2} (t-1)^{-1/2}\, t^{-2+\frac{\alpha n}{2}}\, dt$$

$$= \sum_{n=0}^{\infty} w_n\, m_n(\Omega), \qquad m_n(\Omega) = \Omega^{-3+\alpha n} g_{-2+\frac{\alpha n}{2}}\left(\frac{\Omega}{\Omega_\varepsilon}\right).$$

Thus, Lemma 12, for $\Omega_\varepsilon \leq \frac{1}{2}\rho_4$, $\tau = -2$, $\beta = \frac{\alpha}{2}$, $d = 1$, yields

$$\left|\frac{d^k I_3}{d\Omega^k}(\Omega)\right| \leq C(k;\Omega_\varepsilon) \cdot \Omega^{-3-k}, \qquad \text{for } \Omega \leq \tfrac{1}{2}\Omega_\varepsilon.$$

For the lower bound, we write

$$I_3(\Omega) = w_n m_0(\Omega) + \tilde{I}_3(\Omega), \qquad \tilde{I}_3(\Omega) = \sum_{n=1}^{\infty} w_n m_n(\Omega).$$

Lemma 10 applied to m_0 and Lemma 12 applied to $\tilde{I}_3$ with $\tau = -2 + \frac{\alpha}{2} < -\frac{1}{2}$, $\beta = \alpha/2$, $d = 1$, yield that

$$|m_0(\Omega)| \geq c\,\Omega^{-3}, \qquad \left|\tilde{I}_3(\Omega)\right| \leq C(\Omega_\varepsilon)\,\Omega^{-3+\alpha}, \qquad \text{for } \Omega \leq \tfrac{1}{2}\Omega_\varepsilon.$$

Therefore, for Ω small enough, we obtain

$$I_3(\Omega) \geq c\,\Omega^{-3}, \qquad \Omega \leq \bar{\Omega}_\varepsilon$$

for a number $\bar{\Omega}_\varepsilon \ll \Omega_\varepsilon$. Since I_1 and I_2 remain bounded as $\Omega \to 0$, the lemma is proved. QED

Corollary 16: *For constants C_k and c_0 we have*

$$\eta(\Omega) \geq c_0 \Omega^4, \qquad \left|\frac{d^k \eta}{d\Omega^k}(\Omega)\right| \leq C_k\, \Omega^{4-k}, \qquad k \geq 0.$$

We apply now our growth estimates for ϕ and η to show that Ψ_C is very much like Ψ_Q in the introduction.

Lemma 17:

$$|\Psi_Q(Z) - \Psi_C(Z)| \leq C \cdot Z^{4/3}$$

Proof: Set

$$\tilde{l} = \frac{l+\frac{1}{2}}{\lambda}, \qquad \lambda = Z^{1/3},$$

and note that

$$l(l+1) \cdot \lambda^{-2} = \tilde{l}^2 - \frac{1}{4\lambda^2}.$$

We then use (1a,b) to conclude that

$$\Psi_Q = 2\pi \cdot Z^{4/3} \cdot \sum_{l=1}^{l_{\mathrm{TF}}} \frac{\tilde{l}}{P\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)} \cdot \mu\left(Z^{1/3} \cdot \phi\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)\right).$$

Define $l_{\max}$ as the largest l appearing in the sum defining Ψ_C. Note:

1. Each term appearing in the definition of either Ψ_Q above, or in Ψ_C, is bounded by a constant independent of Z;

2. The sum in Ψ_Q is taken over integers, while the sum in Ψ_Q is taken over half–integers.

3. The number of terms in either sum (l_{TF} for Ψ_Q and $l_{\max} - \frac{1}{2}$ for Ψ_C) may differ slightly because in general, $l_{\mathrm{TF}} + \frac{1}{2} \neq l_{\max}$.

We show now that the number of terms in both sums differ by at most 1. $l_{\max}$ is the greatest element in $\mathbf{Z} + \frac{1}{2}$ which is less than or equal to $a^{-1/2} Z^{1/3} \cdot \Omega_c$. Similarly, l_{TF} is the largest integer that satisfies

$$l_{\mathrm{TF}}\ (l_{\mathrm{TF}}+1) = \left(l_{\mathrm{TF}} + \tfrac{1}{2}\right) \cdot \sqrt{1 - \frac{1}{(2 \cdot l_{\mathrm{TF}} + 1)^2}} \leq a^{-1/2} Z^{1/3} \cdot \Omega_c.$$

An immediate consequence of this is that

$$c \cdot Z^{1/3} \leq l_{\mathrm{TF}}\ , \ l_{\max} \leq C \cdot Z^{1/3}$$

Then, for Z large enough, $l_{\mathrm{TF}} + \frac{1}{2} \leq a^{-1/2} Z^{1/3} \Omega_c + 1$ which implies

$$l_{\mathrm{TF}} + \tfrac{1}{2} \leq l_{\max} + 1. \tag{19}$$

On the other hand,

$$l_{\max} - l_{\mathrm{TF}} \leq a^{-1/2} \cdot Z^{1/3} \cdot \Omega_c - l_{\mathrm{TF}}.$$

Since we must have

$$l_{\mathrm{TF}} + \tfrac{3}{2} > \frac{a^{-1/2} \cdot Z^{1/3} \cdot \Omega_c}{\sqrt{1 - (2l_{\mathrm{TF}} + 3)^{-2}}}$$

which implies

$$a^{-1/2} \cdot Z^{1/3} \cdot \Omega_c - l_{\mathrm{TF}} - \tfrac{1}{2} \leq \tfrac{3}{2}.$$

we conclude that $l_{\max} - \frac{1}{2} - l_{\mathrm{TF}} < 1$, or

$$l_{\max} - \tfrac{1}{2} \leq l_{\mathrm{TF}} \tag{20}$$

Thus, using (19),

$$\left| l_{\max} - \tfrac{1}{2} - l_{\mathrm{TF}} \right| \leq 1 \tag{21}$$

for Z large enough.

As a consequence of this, if we rewrite

$$\Psi_C(Z) = 2\pi \cdot Z^{4/3} \cdot \sum_{l=1}^{l_{\max}-\frac{1}{2}} \eta\left((l+\tfrac{1}{2}) \cdot Z^{-1/3}\right) \cdot \mu\left(Z^{1/3} \cdot \phi\left((l+\tfrac{1}{2}) \cdot Z^{-1/3}\right)\right)$$

$$\tilde{\Psi}_Q(Z) = 2\pi \cdot Z^{4/3} \cdot \sum_{l=1}^{l_{\max}-\frac{1}{2}} \frac{\tilde{l}}{P\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)} \cdot \mu\left(Z^{1/3} \cdot \phi\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)\right)$$

which makes sense by (20), and by noting that $l_{\max}$ in fact refers to a half–integer, we see that

$$\left| \Psi_Q(Z) - \tilde{\Psi}_Q(Z) \right| \leq C \cdot Z^{4/3}$$

since, after all, the difference is at most one term of size at most $Z^{4/3}$. Next, we compare Ψ_C and $\tilde{\Psi}_Q$ term by term. To this end, we observe that, since $\tilde{l} \geq Z^{-1/3}$, we have

$$\left| \frac{1}{P(\tilde{l})} - \frac{1}{P\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)} \right| \leq \frac{\left| P(\tilde{l}) - P\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right) \right|}{P(\tilde{l}) \cdot P\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)}$$

$$\leq C \cdot \tilde{l}^{\,6} \cdot \tilde{x}^{-4} \cdot \tilde{l} \cdot \left(1 - \sqrt{1 - \frac{1}{4\tilde{l}^2\lambda^2}}\right)$$

for $\tilde{x} \in [\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}, \tilde{l}]$

$$\leq C \cdot \tilde{l} \cdot \lambda^{-2}$$

which implies

$$\left|\eta\left(\frac{l+\frac{1}{2}}{\lambda}\right) - \frac{\tilde{l}}{P\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)}\right| \leq \tilde{l} \cdot \left|\frac{1}{P\left(\tilde{l}\right)} - \frac{1}{P\left(\tilde{l}^{\,2} - \frac{1}{4\lambda^2}\right)}\right|$$
$$\leq C \cdot \tilde{l}^{\,2} \cdot \lambda^{-2}$$

Similarly, since ϕ' is bounded,

$$\left|\phi\left(\tilde{l}\right) - \phi\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)\right| \leq C \cdot \tilde{l} \cdot \left(1 - \sqrt{1 - \frac{1}{4\tilde{l}^2\lambda^{-2}}}\right)$$
$$\leq C \cdot \tilde{l}^{-1} \cdot \lambda^{-2}$$

and since μ is Lipschitz, we conclude that

$$\left|\mu\left(\lambda \cdot \phi\left(\frac{l+\frac{1}{2}}{\lambda}\right)\right) - \mu\left(\lambda\phi\left(\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}\right)\right)\right| \leq C \cdot \tilde{l}^{-1} \cdot \lambda^{-1}$$

Therefore, the terms indexed by l in $\tilde{\Psi}_Q$ and Ψ_C differ by at most

$$C \cdot \left(\lambda^{-2} \cdot \tilde{l}^2 + \sup_{x \in [\sqrt{\tilde{l}^{\,2} - \frac{1}{4\lambda^2}}, \tilde{l}]} |\eta(x)| \cdot \lambda^{-1} \cdot \tilde{l}^{-1}\right)$$

which implies

$$\left|\Psi_Q(Z) - \tilde{\Psi}_C(Z)\right| \leq C \cdot Z^{4/3} \sum_{l=1}^{l_{\mathrm{TF}}} \left(Z^{-4/3} \cdot l^2 + Z^{-4/3} \cdot l^3\right)$$
$$\leq C \cdot Z^{4/3}$$

as required. QED

In what follows, we will denote either of the sums Ψ_C or Ψ_Q simply by Ψ, since we now know that both are the same modulo errors of order $Z^{4/3}$.

Define $\Omega_{n,l}$ such that $\phi'(\Omega_{n,l}) = \frac{l}{n}$, and

$$\theta(n,l) = n \cdot \phi(\Omega_{n,l}) - l \cdot \Omega_{n,l}$$

Theorem 18:

$$\Psi(Z) = \Psi_0(Z) + o\Big(Z^{\frac{3}{2}}\Big)$$

where

$$\Psi_0(Z) = 2\pi \cdot Z^{3/2} \sum_{n,l} \frac{\eta(\Omega_{n,l}) \cdot \hat{\mu}(n)}{\left|n \cdot \phi''(\Omega_{n,l})\right|^{1/2}} \cdot e^{2\pi i \cdot Z^{1/3} \cdot \theta(n,l) + \pi i \left(l - \frac{\text{sign }(n)}{4}\right)}$$

Also, Ψ_0 satisfies the bound

$$|\Psi_0(Z)| \le C\, Z^{\frac{3}{2}}$$

for a constant C.

Proof: Construct now a partition of unity given by $\{U_\nu, \theta_\nu\}$ for $\nu = 0, 1, \cdots$, such that

$$\begin{aligned}
&U_\nu = [a_\nu, b_\nu], \qquad a_\nu = 2^{-\nu-2} \cdot a^{-1/2} \cdot \Omega_c, \quad b_\nu = 2^{-\nu} \cdot a^{-1/2} \cdot \Omega_c,\\
&d_\nu \stackrel{\text{def}}{\equiv} b_\nu - a_\nu, \quad d_\nu \sim a_\nu \sim b_\nu,\\
&\sum_\nu \theta(x) = \begin{cases} 1 & \text{if } 0 < x \le \Omega_c \\ 0 & \text{otherswise,} \end{cases}\\
&\theta_\nu \in C_0^\infty \qquad \text{and} \qquad \text{supp } \theta_\nu \subset U_\nu, \qquad \text{for } \nu \ge 1,\\
&\theta_0(x) \equiv 0 \quad \text{for } x \notin [a_0, b_0],\\
&\left|\frac{d^k \theta_\nu}{dx^k}(x)\right| \le C_k \cdot d_\nu^{-k},
\end{aligned}$$

for universal constants C_k independent of ν. Clearly, we have

$$\Psi_C(Z) = 2\pi\, Z^{4/3} \sum_{\nu=0}^{\infty} S_\nu(Z^{1/3}) \tag{22}$$

for

$$S_\nu = \sum_{l \in \mathbf{Z}+\frac{1}{2}} (\eta \cdot \theta_\nu)\left(\frac{l}{\lambda}\right) \cdot \mu\left(\lambda\phi\big(\frac{l}{\lambda}\big)\right), \qquad \lambda = Z^{1/3}.$$

Note that we have

$$\left.\begin{aligned}
&|\phi(x) \le C, \qquad |\phi'(x)| \le C,\\
&c\, d_\nu^{-1+\alpha} \le |\phi''(x)| \le C\, d_\nu^{-1+\alpha},\\
&\left|\frac{d^k\phi}{d\Omega^k}(x)\right| \le C d_\nu^{1-k+\alpha} \qquad (k \ge 2),\\
&\left|\frac{d^k(\theta_\nu \cdot \eta)}{d\Omega^k}(x)\right| \le C d_\nu^{4-k} \qquad (k \ge 0),
\end{aligned}\right\} \qquad \text{for } x \in U_\nu \tag{23a}$$

which implies that, in each S_ν, we have

$$B(\phi) \le C\, a_{\nu_1}^{-400} \le C\, 2^{400\nu} \tag{23b}$$

We consider

$$\nu_1 = \varepsilon_1 \cdot |\log_2 \lambda|, \qquad \varepsilon_1 = 10^{-3}.$$

For $\nu = 0$, we apply Theorem 6 to obtain

$$S_0 = \sum_{\substack{n\neq 0\\ l\in \mathbf{Z}}} \varepsilon_{n,l}\, \hat{\mu}(n) \cdot \theta_0(\Omega_{n,l}) \cdot \eta\,(\Omega_{n,l}) \cdot \sigma(n,l) + o\Big(Z^{1/6}\Big) \tag{24}$$

For $0 < \nu \le \nu_1$, we use (23) and Theorem 7 to obtain

$$S_\nu = \sum_{\substack{n\neq 0\\ l\in \mathbf{Z}}} \hat{\mu}(n) \cdot (\theta_\nu \cdot \eta)\,(\Omega_{n,l}) \cdot \sigma(n,l) + \mathcal{O}\big(2^{400\cdot\nu}\big) \tag{25}$$

If $\nu > \nu_1$, we argue directly as we did before before Theorem 6 to obtain that

$$S_\nu = \lambda \sum_{\substack{n\neq 0\\ l\in \mathbf{Z}}} \hat{\mu}(n) \cdot I(n,l), \qquad I(n,l) = \int (\theta_\nu \cdot \eta)\,(x)\, e^{2\pi i\lambda\big(n\phi(x) - lx\big)}\, dx.$$

In order to analyze $I(n,l)$, we use lemma 4 to obtain

$$|I(n,l)| \le C\,\big(\lambda|n|\big)^{-1/2}\,\left(d_\nu^{-1+\alpha}\right)^{-1/2} \cdot d_\nu^{3+\alpha}$$

which we will use when $|l| \le 4\,\|\phi'\|_\infty\,|n|$, to obtain

$$\left|\sum_{|l|\le 4\,\|\phi'\|_\infty\,|n|} \hat{\mu}(n) \cdot I(n,l)\right| \le C\,\lambda^{-1/2} \cdot d_\nu^{4+\frac{\alpha}{2}} \tag{26a}$$

When $|l| \ge 4\,\|\phi'\|_\infty\,|n|$, we have $|\phi'(x) - \frac{l}{n}| \ge \frac{|l|}{4|n|}$; thus, we apply (4b) directly to $I(n,l)$ to obtain

$$|I(n,l)| \le \big(\lambda|n|\big)^{-1}\, \frac{d_\nu^{4+\alpha}}{\left(\frac{|l|}{4|n|}\right)^2} + 4\,\big(\lambda|n|\big)^{-2}\, \left(\frac{d_\nu^3}{\left(\frac{|l|}{4|n|}\right)^2} + \frac{d_\nu^{3+\alpha}}{\left(\frac{|l|}{4|n|}\right)^3}\right)$$

which implies that, for n fixed,

$$\left|\sum_{\{l\,:\,|l|\ge 4\,\|\phi'\|_\infty\,|n|\}} I(n,l)\right| \le C\,\left(\lambda^{-1} \cdot d_\nu^{4+\alpha} + \frac{\lambda^{-2} \cdot d_\nu^3}{|n|} + \frac{\lambda^{-2} \cdot d_\nu^{3+\alpha}}{|n|}\right)$$

which finally implies

$$\left|\sum_{|l|>4\,\|\phi'\|_\infty\,|n|} \hat{\mu}(n)\cdot I(n,l)\right| \le \lambda^{-1}\cdot d_\nu^3 \tag{26b}$$

Putting (26a) and (26b) together, we obtain

$$|S_\nu| \le \lambda^{1/2}\cdot d_\nu^3$$

which implies

$$\left|\sum_{\nu>\nu_1} S_\nu\right| \le \lambda^{1/2}\cdot 2^{-3\,\nu_1} = \lambda^{\frac{1}{2}-3\,\varepsilon_1}. \tag{27}$$

Also,

$$\left|\sum_{\nu>\nu_1}\ \sum_{(n,l):\,\Omega_{n,l}\in U_\nu} \frac{\hat{\mu}(n)\,(\eta\cdot\theta_\nu)(\Omega_{n,l})}{|n\cdot\phi''(\Omega_{n,l})|^{1/2}}\, e^{2\pi i\lambda\theta(n,l)+\pi i\left(l-\frac{\text{sign }(n)}{4}\right)}\right| \le C \sup_{x\in\cup_{\nu=\nu_1+1}^{\infty}U_\nu} |\eta(x)|$$
$$= \mathcal{O}\left(d_{\nu_1}^4\right) = \mathcal{O}\left(\lambda^{-4\,\varepsilon_1}\right).$$

and, putting (22), (24), (25) and (27) together, we obtain

$$\Psi(Z) = \Psi_0(Z) + o\left(Z^{3/2}\right)$$

QED

4. Lower Bounds

Theorem 18 told us two things: that Ψ has a leading expression as a trigonometric sum, and that the size of this trigonometric sum, and therefore of Ψ, is *at most* of order $Z^{3/2}$. The question remains whether this bound is sharp or not. In related problems, such as the lattice point problem, sharp upper and lower bounds *on average* have been known for over fifty years (see [B2] and [HB] for recent developments). This, in our context, would translate into the statement that indeed $Z^{3/2}$ is best possible.

The aim of this section is to derive such estimates *on average* for the function Ψ_0. Classical ideas will work effortlessly after we show that a certain number is not 0. This number can be viewed as a certain (analytic, not necessarily arithmetic) L–function evaluated at the point $s = 2$. Thus, it is not surprising that such a condition appears if one thinks, for example, about the lattice point problem for parabola.

First, we will consider real values for Z, and then use this to study the case of interest, integer Z, as it relates to our original goal to understand the ground state energy of an atom of nuclear charge Z.

We begin by defining

$$a_{n,l} = \frac{\hat{\mu}(n) \cdot \eta(\Omega_{n,l})}{|\phi''(x_{n,l}) \cdot n|^{1/2}} e^{\pi i (l - \frac{\text{sign } n}{4})}.$$

Let $\{\theta_\nu\}$ the set of all possible values of $\theta(n,l)$, selected such that $\theta_\nu \neq \theta_{\nu'}$ for $\nu \neq \nu'$. Define

$$L \stackrel{\text{def}}{\equiv} L_{\eta,\phi} = \sum_\nu \left| \sum_{\theta(n,l)=\theta_\nu} a_{n,l} \right|^2$$

which Lemma 20 will prove it to be non–zero; if, however, L were equal to 0, then it is easy to see that in fact we would have that

$$\Psi_0(Z) \equiv 0 \qquad \text{all } Z.$$

In the meantime, we will simply assume $L \neq 0$.

Define also

$$C^* = 1 + \left(\frac{48 \cdot \|\eta\|_\infty \cdot \|\phi'\|_\infty}{c_0 \cdot L} \right)^{2/3}$$
$$c^\sharp = \inf \left\{ |\theta(n,l) - \theta(n',l')| \ : \ \theta(n,l) \neq \theta(n',l') \text{ and } |n|, |n'| \leq C^* \right\}.$$

Therefore, setting as usual $\lambda = Z^{1/3}$,

$$\begin{aligned} Z^{-3} |\Psi_0(Z)|^2 &= \sum_{n,n',l,l'} a_{n,l} \cdot \overline{a_{n',l'}} \cdot e^{2\pi i \lambda \left(\theta(n,l) - \theta(n',l')\right)} \\ &\geq \sum_{\substack{n,n',l,l' \\ \theta(n,l)=\theta(n',l')}} a_{n,l} \cdot \overline{a_{n',l'}} \\ &\quad + \sum_{\theta(n,l) \neq \theta(n',l')} a_{n,l} \cdot \overline{a_{n',l'}} \cdot e^{2\pi i \lambda \left(\theta(n,l) - \theta(n',l')\right)} \end{aligned}$$

The first term above is our L defined above. In the second term, we separate the terms for small $|n|, |n'|$, which we keep untouched, and the ones for which *either* n or n' are large, which we estimate using the fact that $|l| \leq \|\phi'\|_\infty \cdot |n|$ and $|l'| \leq \|\phi'\|_\infty \cdot |n'|$, to obtain

$$
\begin{aligned}
&\geq L - \sum_{\substack{\left|\theta(n,l)-\theta(n',l')\right|>0 \\ |n|,|n'|\leq C^*}} a_{n,l}\cdot\overline{a_{n',l'}}\cdot e^{2\pi i\lambda\left(\theta(n,l)-\theta(n',l')\right)} \\
&\qquad - 2c_0^{-1}\cdot\|\eta\|_\infty^2\cdot\|\phi'\|_\infty^2\cdot\sum_{\substack{|n|\geq C^* \\ \text{all } n'}} |n\cdot n'|^{-5/2} \\
&\geq L - \sum_{\substack{\left|\theta(n,l)-\theta(n',l')\right|>0 \\ |n|,|n'|\leq C^*}} a_{n,l}\cdot\overline{a_{n',l'}}\cdot e^{2\pi i\lambda\left(\theta(n,l)-\theta(n',l')\right)} \\
&\qquad - 24\cdot c_0^{-1}\cdot\|\eta\|_\infty^2\cdot\|\phi'\|_\infty^2\cdot(C^*-1)^{-3/2}
\end{aligned}
$$

which, by our choice of C^*, implies

$$
Z^{-3}\,|\Psi_0(Z)|^2 \geq \tfrac{1}{2}L - \sum_{\substack{\left|\theta(n,l)-\theta(n',l')\right|>0 \\ |n|,|n'|\leq C^*}} a_{n,l}\cdot\overline{a_{n',l'}}\cdot e^{2\pi i\lambda\left(\theta(n,l)-\theta(n',l')\right)}.
$$

Now we consider $Z_0 \geq 1$ and $Z \leq \frac{1}{2}Z_0$ and prepare to integrate both sides from Z_0 to Z_0+Z. For that, note that $dZ = 3\lambda^2\,d\lambda$ and, if we set $\lambda_0 = Z_0^{1/3}$, then

$$
(Z_0+Z)^{1/3} = \lambda_0 + \Lambda, \qquad \Lambda \leq Z/Z_0^{2/3}.
$$

Also,

$$
\left|\int_a^b \lambda^2 e^{i\lambda\theta}\,d\lambda\right| \leq \frac{3b^2}{\theta}, \qquad a,b>0.
$$

Therefore,

$$
\begin{aligned}
&\int_{Z_0}^{Z_0+Z} |\Psi_0(z)|^2\,\frac{dz}{z^3} \\
&\qquad \geq \frac{Z}{2}L - 36\,Z_0^{2/3}c_0^{-1}\cdot\|\eta\|_\infty^2\cdot\|\phi'\|_\infty^2\cdot\sum_{\substack{\left|\theta(n,l)-\theta(n',l')\right|>0 \\ |n|,|n'|\leq C^*}} \frac{|n\cdot n'|^{-5/2}}{2\pi\,|\theta(n,l)-\theta(n',l')|} \\
&\qquad \geq \frac{Z}{2}L - 36\,Z_0^{2/3}\,\frac{\|\eta\|_\infty^2\cdot\|\phi'\|_\infty^2}{c_0\cdot c^\sharp}\sum_{|n|,|n'|\leq C^*} |n\cdot n'|^{-5/2} \\
&\qquad \geq \frac{Z}{2}L - Z_0^{2/3}\,\frac{18000\cdot\|\eta\|_\infty^2\cdot\|\phi'\|_\infty^2}{c_0\cdot c^\sharp}.
\end{aligned}
$$

As a consequence, taking $Z/Z_0^{2/3}$ large depending on L, c_0, $c^\sharp$, $\|\eta\|_\infty$ and $\|\phi'\|_\infty$, but still Z not larger than $\frac{1}{2}\,Z_0$, we have

$$
\int_{Z_0}^{Z_0+Z} |\Psi_0(z)|^2\,\frac{dz}{z^3} \geq \frac{Z}{4}L.
$$

Next, we turn to the non–vanishing of L. In preparation for the proof, set

$$\alpha_1 = \phi'(0), \qquad \alpha_2 = \phi'\left(a^{-1/2} \cdot \Omega_c\right)$$

and note that $0 > \alpha_1 > \alpha_2$. Clearly, the (n, l) that enter in the sum for Ψ_0 are determined by the lattice points in $\mathbf{Z}^2$ which fall in the double–cone

$$\Gamma = \{(u, v) : \quad \alpha_2 \cdot |u| \leq -|v| < \alpha_1 \cdot |u|, \qquad u \cdot v < 0\}$$

Define $x_{u,v}$, for $(u, v) \in \Gamma$, as the unique point satisfying

$$\phi'(x_{u,v}) = \frac{v}{n}.$$

Note that $x_{u,v}$ is strictly positive.
Then, we define

$$\theta(u, v) = u \cdot \phi(x_{u,v}) - v \cdot x_{u,v}, \qquad (u, v) \in \Gamma.$$

The following is a trivial fact

Lemma 19: *On Γ we have*

$$\nabla\theta(u, v) = (\phi(x_{u,v}), -x_{u,v})$$

A consequence of this trivial fact is the result we mentioned above.

Lemma 20: $L \neq 0$.

Proof: We will show that there is one θ_ν which only has one $(n, l) \in \Gamma$ such that $\theta(n, l) = \theta_\nu$. This clearly shows that L is not 0.

Let n_0 be the smallest positive integer such that $(n, l) \in \Gamma$ for some l. In our case, this l is negative. Choose the largest (negative) such l, which we denote by l_0. That is, l_0 is the largest negative integer that satisfies $l < \alpha_1 \cdot n_0$. Then we claim that there is no other pair $(n', l') \in \Gamma$ such that $\theta(n_0, l_0) = \theta(n', l')$. Indeed, since $\theta(n, l)$ is strictly positive for $n > 0$, and strictly negative for $n < 0$, such n' would also have to be positive. It cannot equal n_0 because, since we should have $l' < l_0$, by the previous lemma we have

$$\theta(n_0, l') > \theta(n_0, l_0)$$

We must then have $n' > n_0$, which also implies

$$l' < \alpha_1 \cdot n' < \alpha_1 \cdot n_0 \quad (< 0)$$

thus showing that $l' \leq l$. But this is also impossible because, also by the previous lemma, there exists a pair (ξ, η) on the segment joining (n_0, l_0) to (n', l'), such that

$$\theta(n', l') - \theta(n_0, l_0) = \phi(x_{\xi,\eta}) \cdot (n' - n_0) - x_{\xi,\eta} \cdot (l' - l_0)$$

and this last expression is then strictly positive. QED

We summarize all this in the following lemma

Lemma 21: *There is a small constant κ_0 and a large constant K such that*

$$\int_{Z_0}^{Z_0+Z} z^{-3} \left|\Psi_0(z)\right|^2 \, dz \geq \kappa_0 \cdot Z$$

whenever $Z \geq K \cdot Z_0^{2/3}$, and $Z_0 \geq K$.

Proof: Our previous calculations show this result in the case that $Z \geq C\, Z_0^{2/3}$ but $Z \leq \frac{1}{2}\, Z$, for a certain large constant C. For the general case, break up

$$\int_{Z_0}^{Z_0+Z} z^{-3} \left|\Psi_0(z)\right|^2 \, dz = \sum_{n=0}^{N} \int_{Z_n}^{Z_{n+1}} z^{-3} \left|\Psi_0(z)\right|^2 \, dz$$

where

$$Z_{n+1} = 1.01\, Z_n \quad \text{when } n = 0, \ldots, N-1; \qquad Z_{N+1} = Z_0 + Z$$

and N is chosen so that $1.01^{N+1}\, Z_0 \leq Z_0 + Z < 1.01^{N+2}\, Z_0$. Our previous calculations would apply to each of the integrals in the sum provided

$$Z_n - Z_{n-1} \geq C\, Z_{n-1}^{2/3}, \quad (n = 1, \ldots, N); \qquad Z + Z_0 \geq Z_N^{2/3}$$

which amounts to requiring $Z_0 \geq 10^6$. QED

This mean value information can be used to obtain information about the oscillating behavior of Ψ_0, as follows:
Let

$$I = [\, Z_0, Z_0 + \hat{C} Z_0^{2/3} \,] = \bigcup I_j$$

for

$$I_j = [\, Z_0 + \hat{c} \cdot j \cdot Z_0^{2/3}, Z_0 + \hat{c} \cdot (j+1) \cdot Z_0^{2/3} \,]$$

where $\hat{C}$ is large depending on K and $\hat{c}$ is small depending on κ_0.

Denote also, for any function f,

$$m_j(f) = \inf_{x \in I_j} \left| x^{-3/2} f(x) \right| .$$

Corollary 22: *Given any $\varepsilon > 0$ small depending on k_0, any $\hat{C}$ and $\hat{c}$ as above, with the extra requirement that $\hat{c}$ is small depending on ε, and Z_0 also large enough, there exists a constant $0 < \alpha < 1$ such that $m_j(\Psi_0) > \varepsilon$ for at most $\alpha \hat{C}/\hat{c}$ of the I_j .*

Proof: Put

$$Z^{-3/2} \Psi_0(Z) = F(Z) + E(Z)$$

such that $F(Z)$ contains only finitely many terms in the sum, and $|E(Z)|$ is always less than ε. In particular, we have that in order that $m_j(\Psi_0) < \varepsilon$ we must have $m_j(F) < 2\varepsilon$. It will therefore be enough to count how many of the $m_j(F)$ stay below 2ε to obtain the conclusion of the lemma.

Since both ϕ and ϕ' are bounded, we have the trivial bound

$$|F'(Z)| \leq C_\varepsilon \, Z^{-2/3}$$

for some constant C_ε which depends on ε. Thus, if $m_j(\Psi_0) \leq \varepsilon$, we have $F(Z) \leq 2\varepsilon + \hat{c} \cdot C_\varepsilon$ which implies

$$\int_{I_j} |F(z)|^2 \, dz \leq 16 \, |I_j| \cdot \left(\varepsilon^2 + \hat{c}^2 \cdot C_\varepsilon^2 \right) .$$

Therefore, if we denote by

$$M = \text{number of } j \text{ such that } m_j(\Psi_0) < \varepsilon$$

we use the trivial bound $|F(z)| \leq C$ for all z, for a universal constant C, to get

$$\begin{aligned}\kappa_0 \cdot \hat{C} \cdot Z_0^{2/3} &\leq \int_I |F(z)|^2 \, dz \\ &\leq \left(\frac{\hat{C}}{\hat{c}} - M\right) \cdot C \cdot \hat{c} \cdot Z_0^{2/3} + 16\, M\, \hat{c} \cdot Z_0^{2/3} \cdot \left(\varepsilon^2 + \hat{c}^2 \cdot C_\varepsilon^2\right)\end{aligned}$$

This implies that

$$M \leq \alpha \frac{\hat{C}}{\hat{c}} \quad \text{for } \alpha = \frac{C - \kappa_0}{C - 16(\varepsilon^2 + \hat{c}^2 \cdot C_\varepsilon^2)}$$

By adjusting $\hat{c}$ depending on ε it is easy to make $\alpha < 1$. QED

A consequence of this corollary is another which shows that the size of $\Psi_0(Z)$ is at most $cZ^{3/2}$, for a small constant c, even when we restrict our attention to integer values of Z.

Corollary 23:

$$\liminf_{\substack{Z \to \infty \\ Z = 1,2,3,\ldots}} \left| Z^{-2/3} \cdot \Psi_0(Z) \right| \neq 0$$

Proof: Apply the previous corollary to any $\varepsilon > 0$ small as required, and to any $\hat{C}$ large and $\hat{c}$ small also as needed, and then to infinitely Z_0 to conclude that there are infinitely many intervals of lengths going to infinity where $|x^{-3/2} \cdot \Psi_0(x)|$ is never smaller than ε. QED

5. The Classical Picture

In this Section we identify all quantities appearing in the expression for Ψ_0 in terms of data coming from the classical dynamics of a particle in the field created by the Thomas–Fermi potential. We begin with a brief review of elementary classical mechanics, which can be found, among many other places, in [Ar].

Consider a particle with mass $\frac{1}{2}$, in $\mathbf{R}^3$, moving in a negative radial potential $-V(r)$, which for us, will equal $-V^1_{\mathrm{TF}}(r)$. The motion is planar, and can be described by the distance to the origin $r(t)$ and the angle φ, which satisfy the relations

$$\dot{\varphi} = \frac{2M}{r^2}, \qquad \tfrac{1}{4}\left(\dot{r}^2 + r^2\dot{\varphi}^2\right) - V(r) = E$$

where M is the angular momentum, and E is the energy of the orbit. We begin assuming that the particle travels counter–clockwise in our frame of reference (r, φ). The motion takes place between radii $r_{\min}$ and $r_{\max}$ given by the two solutions of the equation

$$-V(r) + \frac{M^2}{r^2} = E.$$

This implies that all trajectories for a fixed energy and angular momentum can be obtained by rotation of a fixed one.

At energy 0, we denote by $t_{\min}$ and $t_{\max}$ the times at which the particle passes through $r_{\min}$ and $r_{\max}$ respectively. The angle of motion φ and the distance to the origin r satisfy the equations

$$\frac{dr}{dt} = 2\sqrt{V(r) - \frac{M^2}{r^2}}, \qquad \frac{d\varphi}{dr} = \frac{M/r^2}{\sqrt{V(r) - \frac{M^2}{r^2}}}.$$

As a consequence, the particle going from $r_{\min}$ to $r_{\max}$ sweeps out an angle given by

$$M\int_{r_{\min}}^{r_{\max}} \left(V(r) - \frac{M^2}{r^2}\right)^{-1/2} \frac{dr}{r^2} = -\pi\phi'(M).$$

and the trajectory is clearly symmetric with respect to either $r_{\min}$ (or $r_{\max}$). Therefore, the angular momentum M will give rise to a closed orbit if and only if

$$-\phi'(M) = \tfrac{l}{n} \tag{28}$$

and in this case, n represents the number of times the particle oscillates between successive $r_{\min}$ (or $r_{\max}$) before closing, and l represents the winding number of the orbit around 0. Our initial assumption that the particle travels counter–clockwise means that $n, l \geq 0$. In our previous notation, we also have

$$M = \Omega_{n,-l}$$

If $(l, n) = 1$ (where $(,)$ denotes greatest common divisor), the orbit is usually called *primitive.*

The period is given by

$$\begin{aligned} T(M) &= 2n \cdot \int_{t_{\min}}^{t_{\max}} dt \\ &= n \int_{r_{\min}}^{r_{\max}} \frac{dr}{\sqrt{V(r) - \frac{M^2}{r^2}}} \\ &= n \cdot P\,(M)\,. \end{aligned}$$

In order to find the action S along this closed trajectory,

$$S = 2n \cdot \int_{t_{\min}}^{t_{\max}} (\text{Kinetic Energy } + V)\ dt,$$

we note that, since we are at energy 0, Kinetic Energy $= V(r)$, which implies

$$\begin{aligned} S &= 4n \int_{r_{\min}}^{r_{\max}} \frac{V(r)}{2\sqrt{V(r) - \frac{M^2}{r^2}}}\, dr \\ &= 2n \left(\int_{r_{\min}}^{r_{\max}} \sqrt{V - \frac{M^2}{r^2}}\, dr + \int_{r_{\min}}^{r_{\max}} \frac{M^2/r^2}{\sqrt{V - \frac{M^2}{r^2}}}\, dr \right) \\ &= 2\pi\,(n\phi\,(M) + l \cdot M) \\ &= 2\pi\,(n\phi(\Omega_{n,-l}) + l \cdot \Omega_{n,-l})\,. \end{aligned}$$

As a consequence, denoting by $S(M)$ as the action along a closed counter–clockwise trajectory at energy 0 with angular momentum M, we have

$$2\pi\theta(n,-l) = S\,(\Omega_{n,-l})$$

When the particle travels clockwise, we agree that S, T, n and l change sign, but we keep $M \geq 0$.

We have so far identified all terms in the definition of Ψ_0 except $n \cdot \phi''(\Omega_{n,l})$. For this one, consider a closed trajectory arising from angular momentum M, which gives rise to n oscillations between successive $r_{\max}(M)$; for ε small, consider a trajectory with angular momentum $M+\varepsilon$ which begins at $r_{\max}(M+\varepsilon)$ and denote by $2\pi\alpha_M(\varepsilon)$ the absolute value of the angle the particle forms between the initial position at $r_{\max}(M+\varepsilon)$ and the position after n oscillations also at $r_{\max}(M+\varepsilon)$, where we take α between 0 and 1/2. Then

$$D(M) \overset{\text{def}}{\equiv} \lim_{\varepsilon \to 0} \varepsilon^{-1} \alpha_M(\varepsilon) = |n \cdot \phi''(M)|$$

It is clear now that the nonvanishing of the second derivative of ϕ translates into the fact that closed trajectories are isolated modulo the trivial symmetry given by the rotation group.

The motion degenerates for the one circular orbit arising from $M_{\max} = a^{-1/2}\,\Omega_c$, the maximum angular momentum allowed in our system. In this case, we define the above classical variables simply in terms of ϕ' using the formulas we derived for the other trajectories.

Theorem 24:

$$\Psi_0(Z) = 2\pi \cdot Z^{3/2} \cdot \sum_{\text{closed trajectories}} \delta\,\frac{n\,\hat{\mu}(n)\,M}{T} \cdot |D(M)|^{-1/2} \cdot e^{i\left(Z^{1/3} S - \pi\cdot(l + \frac{\text{sign } n}{4})\right)}$$

where circular trajectories appear in the sum only when they has associated a finite number of oscillations n. We have $\delta = 1$ except for the circular trajectories, when $\delta = \frac{1}{2}$. The sum is absolutely convergent.

Remark: Note that the contribution of each trajectory depends on the particular frame of reference we take to compute n and l, but the sum is independent of it.

Remark: One might think of the different values for δ as follows: non–circular trajectories contribute fully to eigenvalues, while the circular ones, being right at the outskirts of the classically allowed region, contribute half as eigenvalues, half as resonances.

6. Further Considerations

In this section we will compute the derivatives of ϕ at the ends of our interval of interest $[0, a^{-1/2} \cdot \Omega_c]$. The derivative at $a^{-1/2} \cdot \Omega_c$ plays a role in the sense described on **The Heart of the Matter**, since its rationality or irrationality translates in the appearance or absence of a certain contribution to Ψ or size $Z^{3/2}$. The derivative at 0 does not play such a role since the amplitude vanishes there.

Lemma 25:

$$-\frac{1}{\pi}F'(\Omega_c) = \left(1 - \tfrac{1}{2}r_c^{3/2} \cdot y_c^{1/2}\right)^{-1/2} = \frac{1}{\sqrt{1 - \frac{1}{2}r_c \cdot \Omega_c}} \sim 1.9376783$$

Proof: We use the change of variables $t(r)$ given by (16), and its inverse $r(t)$, to write

$$-F'(\Omega_c) = \Omega_c \cdot \int_{-1}^{1} (1-t^2)^{-1/2} \cdot w(0)\, dt,$$

with

$$w(0) = \frac{r'(0)}{r_c} = \frac{1}{r_c \cdot t'(r_c)} = \frac{\sqrt{2}}{r_c \cdot |u''(r_c)|^{1/2}}.$$

Thus,

$$-\frac{1}{\pi}F'(\Omega_c) = \frac{\Omega_c}{r_c \cdot \left|\frac{1}{2}u''(r_c)\right|^{1/2}} = \left|\frac{2y(r_c)}{r_c \cdot u''(r_c)}\right|^{1/2}$$

since

$$\frac{1}{\pi}\int_{-1}^{1}(1-t^2)^{-1/2}\, dt = 1.$$

Manipulations using the identities

$$u(x) = xy(x), \quad u'(x) = xy'(x) + y(x), \quad u''(x) = xy''(x) + 2y'(x) = x^{1/2}y^{3/2}(x) + 2y'(x)$$

and

$$r_c\, y'(r_c) = -y(r_c)$$

yield our result. QED

Lemma 26:

$$-\lim_{\Omega\to 0} F'(\Omega) = \tfrac{3}{2}\pi$$

Proof: Let $r_0(\Omega)$ and $r_1(\Omega)$ be the two solutions of $u(r) = \Omega^2$. We study first the asymptotics of r_0 and r_1.
For r_0, put $z = r_0^{1/2}$; then, for

$$f(z) = u(z^2) = z^2 - wz^4 + \mathcal{O}(z^5)$$

we have that $f(z) = \Omega^2$. This implies that $z = \Omega + \mathcal{O}(\Omega^2)$ and thus

$$r_0(\Omega) = \Omega^2 + \mathcal{O}(\Omega^3)\,.$$

For r_1, since $u(r)$ decreases monotonically to 0, $r_1(\Omega) \to \infty$. Since we have that $u(r) = 144r^{-2} + \mathcal{O}(r^{-2-\alpha})$, for $\alpha > 0$, we get that

$$r_1(\Omega) = \frac{12}{\Omega} + o(\Omega^{-1})\,.$$

In order now to analyze $F'(\Omega)$, take ϵ be a small enough constant to be picked up later and rewrite

$$\begin{aligned} g(\Omega) &= \int_{r_0(\Omega)}^{\epsilon} \left(u(r) - \Omega^2\right)^{-1/2} \frac{dr}{r} + \int_{\epsilon}^{r_1(\Omega)} \left(u(r) - \Omega^2\right)^{-1/2} \frac{dr}{r} \\ &= \int_{r_0(\Omega)}^{\epsilon} \left(u'(r_0)(r - r_0)\right)^{-1/2} \frac{dr}{r} + \int_{\epsilon}^{r_1(\Omega)} \left(u(r) - \Omega^2\right)^{-1/2} \frac{dr}{r} \\ &\quad + R_0(\Omega) \end{aligned} \tag{29}$$

for

$$R_0 = \int_{r_0}^{\epsilon} \left(\left(u(r) - \Omega^2\right)^{-1/2} - \left(u'(r_0)(r - r_0)\right)^{-1/2}\right) \frac{dr}{r}$$

We show first that $R_0 = \mathcal{O}(1)$.
Fix Ω:

$$\begin{aligned} &\left(u(r) - \Omega^2\right)^{-1/2} - \left(u'(r_0)(r - r_0)\right)^{-1/2} = \\ &\qquad = \sum_{n=1}^{\infty} c_n \left(u'(r_0)(r - r_0)\right)^{-n-1/2} \cdot \Big(\left(u(r) - u(r_0)\right) - u'(r_0)\,(r - r_0)\Big)^n \end{aligned}$$

Throughout this analysis, c_n will denote a generic sequence of bounded constants.
Note that

$$\begin{aligned} |u(r) - u(r_0) - u'(r_0)(r - r_0)| &\le \tfrac{1}{2} \sup_{0 \le r \le \epsilon} |u''(r)| \cdot (r - r_0)^2 \\ &\le \left(y'(0) + \tfrac{1}{2}\epsilon^{1/2}\right) \cdot (r - r_0)^2 \\ &\le C_0\,(r - r_0)^2 \end{aligned}$$

since $u''(r) = 2y'(r) + ry''(r)$, $|y'(r)| \leq |y'(0)|$ and $y''(r) \leq r^{-1/2}$. Therefore, the sum converges uniformly for $|r - r_0| < \frac{1}{2}C_0$ and integrating with respect to dr/r on (r_0, ϵ), for $\epsilon < \frac{1}{2}C_0$, we obtain

$$\begin{aligned}
R_0 &\leq \sum_{n=1}^{\infty} |c_n| \cdot |u'(r_0)|^{-n-1/2} \int_{r_0}^{\epsilon} C_0^n \, |r - r_0|^{n-1/2} \, \frac{dr}{r} \\
&\leq \sum_{n=1}^{\infty} |c_n| \cdot |u'(r_0)|^{-n-1/2} C_0^n r_0^{n-1/2} \int_1^{\epsilon/r_0} (y-1)^{n-1/2} \, \frac{dy}{y} \\
&\leq \sum_{n=1}^{\infty} |c_n| \cdot |u'(r_0)|^{-n-1/2} C_0^n r_0^{n-1/2} \cdot (y-1)^{n-1/2} \Big|_1^{r_0^{-1}\epsilon} \\
&\leq \sum_{n=1}^{\infty} |c_n| \cdot |u'(r_0)|^{-n-1/2} C_0^n \epsilon^{n-1/2}
\end{aligned}$$

For Ω small enough, we can make $|u'(r_0)| < 2$, and this will make the previous sum converge to $\mathcal{O}(1)$ for ϵ small, thus proving that R_0 is bounded.
Recall now that $\Omega r_0(\Omega)^{-1/2} \to 1$, what implies

$$\begin{aligned}
\Omega \cdot \int_{r_0}^{\epsilon} (r - r_0)_+^{-1/2} \, \frac{dr}{r} &= \Omega \cdot r_0^{-1/2} \int_1^{r_0^{-1}\epsilon} y^{-1}(y-1)^{-1/2} \, dy \\
&\to \int_1^{\infty} y^{-1}(y-1)^{-1/2} \, dy \\
&= \pi
\end{aligned}$$

which, with the fact that $u'\left(r_0(\Omega)\right) \to 1$, implies that

$$\begin{aligned}
\lim_{\Omega \to 1} \Omega \int_{r_0}^{\epsilon} \left(u(r) - \Omega^2\right)^{-1/2} \, \frac{dr}{r} &= \lim_{\Omega \to 1} \Omega u'(r_0)^{-1/2} \int_{r_0(\Omega)}^{\epsilon} \left(r - r_0(\Omega)\right)^{-1/2} \, \frac{dr}{r} \\
&= \pi
\end{aligned}$$

which completes the analysis of the first integral in (29).

As for the other integral, we break it up into 5 pieces as follows:

$$\begin{aligned}
\int_{\epsilon}^{r_1} (u(r) - \Omega)^{-1/2} \, \frac{dr}{r} &= \int_{\epsilon}^{M} + \int_{M}^{r_1^{\frac{99}{100}}} + \int_{r_1^{\frac{99}{100}}}^{r_1/2} + \int_{r_1/2}^{r_1 - r_1^{\frac{2}{3}}} + \int_{r_1 - r_1^{\frac{2}{3}}}^{r_1} \\
&= I_1 + I_2 + I_3 + I_4 + I_5
\end{aligned}$$

It is clear that $I_1 = \mathcal{O}(1)$, so we don't worry about it.

For I_2, note that, if M is large enough so that u is decreasing from M on, we have on its domain that

$$\begin{aligned}\left|u(r)-\Omega^2\right| &\geq \left|u\left(r_1^{\frac{99}{100}}\right)-u(r_1)\right| \\ &\geq C\left(r_1^{\frac{99}{100}}\right)^{-2}-cr_1^{-2} \\ &\geq cr_1^{-\frac{99}{50}}\end{aligned}$$

and thus

$$\begin{aligned}|I_2| &\leq C\int_M^{r_1^{\frac{99}{100}}}\left|r_1^{\frac{99}{50}}\right|^{1/2}\frac{dr}{r} \\ &\leq Cr_1^{\frac{99}{100}}\log r_1\end{aligned}$$

which does not contribute to the result.
Similarly, for I_5, note that

$$\begin{aligned}\left|u(r)-\Omega^2\right| &\geq \left(\inf_{|r-r_1|\leq r_1^{2/3}}|u'(r)|\right)\cdot|r-r_1| \\ &\geq Cr_1^{-3}|r-r_1|\end{aligned}$$

thus

$$\begin{aligned}|I_5| &\leq C\int_{r_1-r_1^{2/3}}^{r_1} r_1^{3/2}(r_1-r)^{-1/2}\frac{dr}{r} \\ &\leq Cr_1^{1/2}\int_{r_1-r_1^{2/3}}^{r_1}(r_1-r)^{-1/2}\,dr \\ &\leq Cr_1^{1/2}\cdot r_1^{1/3} \\ &\leq Cr_1^{5/6}\end{aligned}$$

and again, it does not contribute to the total outcome.
For I_4, note that

$$\begin{aligned}|u(r)-\Omega^2| &\geq \left(\inf_{r\sim r_1}|u'(r)|\right)\cdot r_1^{2/3} \\ &\geq Cr_1^{-3}r_1^{2/3}\end{aligned}$$

This implies two things:

First, since $|u(r) - 144r^{-2}| \le Cr^{-2-\alpha} \le Cr_1^{-2-\alpha}$, for $\alpha = \frac{1}{2}(\sqrt{73}-7) > 1 - \frac{2}{3}$, we have that $144r^{-2} - \Omega^2 > 0$ on this range, for Ω small enough.
And second,

$$\begin{aligned}\left|\left(u(r)-\Omega^2\right)^{-1/2} - \left(\frac{144}{r^2}-\Omega^2\right)^{-1/2}\right| &\le \sum_{n=1}^{\infty} c_n |u(r)-\Omega^2|^{-n-\frac{1}{2}} \left(Cr^{-2-\alpha}\right)^n \\ &\le \sum_{n=1}^{\infty} c_n \left(Cr_1^{3-\frac{2}{3}}\right)^{n+\frac{1}{2}} r^{-n(2+\alpha)}\end{aligned}$$

and thus

$$\begin{aligned}\int_{r_1/2}^{r_1 - r_1^{\frac{19}{30}}} \left|\left(u(r)-\Omega^2\right)^{-1/2} - \left(\frac{144}{r^2}-\Omega^2\right)^{-1/2}\right| \frac{dr}{r} &\le \sum_{n=1}^{\infty} c_n \left(Cr_1^{3-\frac{2}{3}}\right)^{n+\frac{1}{2}} r_1^{-n(2+\alpha)} \\ &\le Cr_1^{\frac{7}{3}\cdot\frac{3}{2}-(2+\alpha)} \\ &= o(r_1(\Omega))\end{aligned}$$

Finally, for I_3,

$$\begin{aligned}\int_{r_1^{\frac{99}{100}}}^{r_1/2} \left|\left(u(r)-\Omega^2\right)^{-1/2} - \left(\frac{144}{r^2}-\Omega^2\right)^{-1/2}\right| \frac{dr}{r} \le & \\ &\le \int_{r_1^{\frac{99}{100}}}^{r_1/2} \sum_{n=1}^{\infty} c_n \left(u(\tfrac{r_1}{2})-\Omega^2\right)^{-n-\frac{1}{2}} (cr)^{-n(2+\alpha)} \frac{dr}{r} \\ &\le \int_{r_1^{\frac{99}{100}}}^{r_1/2} \sum_{n=1}^{\infty} c_n \left|Cr_1^{-2}\right|^{-n-\frac{1}{2}} \cdot r^{-n(2+\alpha)} \frac{dr}{r} \\ &\le \sum_{n=1}^{\infty} c_n \left|Cr_1^{2}\right|^{n+\frac{1}{2}} \cdot r_1^{-\frac{99}{100}n(2+\alpha)} \\ &\le Cr_1^3 \cdot r_1^{-\frac{99}{100}(2+\alpha)} \\ &= o(r_1(\Omega))\end{aligned}$$

Therefore, the second integral in (29) agrees modulo $o\left(\Omega^{-1}\right)$ with

$$\begin{aligned}\int_{r_1^{\frac{99}{100}}}^{r_1 - r_1^{2/3}} \left(\frac{144}{r^2}-\Omega^2\right)^{-1/2} \frac{dr}{r} &= \int_{r_1^{\frac{99}{100}}}^{r_1 - r_1^{2/3}} \left(\frac{144}{r^2}\right)^{-1/2} \left(1-\frac{\Omega^2 r^2}{144}\right)^{-1/2} \frac{dr}{r} \\ &= \Omega^{-1} \int_{\frac{\Omega}{12} r_1^{\frac{99}{100}}}^{\frac{\Omega}{12}(r_1 - r_1^{\frac{19}{30}})} (1-y^2)^{-1/2}\, dy\end{aligned}$$

and therefore

$$\lim_{\Omega\to 0}\Omega\int_{\epsilon}^{r_1(\Omega)}\left(u(r)-\Omega^2\right)^{-1/2} = \int_0^1 (1-y^2)^{-1/2}\,dy$$
$$= \frac{\pi}{2}$$

which proves the lemma. QED

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