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Derivation of the Strutinsky method from the least squares principle

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The main purpose of this paper is to rigorously establish the Strutinsky method from the least squares principle. Thus, it is the mathematical basis of this method (aspect often neglected) which is revisited in an extensive way. Some formulas previously given without demonstration or in a simplified way are set out here with all the details. In this respect, the most important mathematical properties of the averaging functions are also established in this paper.

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I. MAIN GOAL OF THE METHOD

In quantum physics, the density of states $g(\epsilon)$ is defined as the number of states per energy unit. These states are deduced from the solution of the time-independent Schrodinger equation. One can distinguish the discrete states in the well and a continuum of scattering states above. For a finite well, there is a finite number of bound states within the well and a continuum above. The level density is then defined as:

$$g(\epsilon) = \sum_{i=0}^{\nu} \delta(\epsilon - \epsilon_i) + g_{\text{cont}}(\epsilon)$$  

For an infinite potential there are only discrete (bound) states.

$$g(\epsilon) = \sum_{i=0}^{\infty} \delta(\epsilon - \epsilon_i)$$

In this respect, it is useful to make the following remarks. From a practical point of view, the continuum is rather difficult to solve. In most of cases, the resolution of the Schrodinger equation is done through a discrete harmonic oscillator basis and all the spectrum is obtained under a discrete form. In principle in this way, only bound states are to be considered and the continuum, obtained thus under a discrete form, is not valid and must be solved in other ways. This makes things difficult. Fortunately, there is a method [1] which avoid that, solving the level density by using also unbound states in their discrete form. In this way Eq. (1) can reduces to the more simple form given by Eq. (2).

Regardless on how this function is solved, in the following, we only will assume that the function $g(\epsilon)$ is known, and that, it is not necessary to specify its explicit form.

It is also assumed that this density of states results from the superposition of a smooth monotonous function $g_0(\epsilon)$ and a fluctuating or oscillating part $\delta g(\epsilon)$. This can be written as:

$$g(\epsilon) = g_0(\epsilon) + \delta g(\epsilon)$$

It is known that $g_0(\epsilon)$ is monotonously increasing function for infinite wells whereas for finite wells it is monotonously increasing and then monotonously decreasing [1]. It will be assumed that, $g(\epsilon)$ and $g_0(\epsilon)$ have the same asymptotic behavior for the increasing part. This is conditioned by the so called asymptotic limit [2, 3]:

$$g(\epsilon) \sim g_0(\epsilon) \text{ as } \epsilon \gg \hbar \omega$$

where $\hbar \omega$ represents one quantum of the energy of the system.

The aim of the proposed method is only to determine the smooth part $g_0(\epsilon)$ which does not contain oscillations. This quantity has already been identified to the semi classical level density $g_{\text{sc}}(\lambda)$ [2]. As we will see, the mathematical process we are going to use, leads to the Strutinsky method. In this context, it is only the mathematical framework of the Strutinsky method that is developed here, especially the derivation from the least squares principle. The physical part of this method has been described at length in the references [2, 3] and the references quoted therein. One therefore limits ourselves to determining the smooth part $g_0(\epsilon)$ without calculating the shell correction itself, insisting only on the mathematical aspect.

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II. DERIVATION OF THE STRUTINSKY PROCEDURE AS A POLYNOMIAL APPROXIMATION FROM A LOCAL LEAST SQUARES PRINCIPLE

The proof will be established in two successive steps.

A. Step 1: Local least squares polynomial fit

In a first step, we want to average or to smooth \( g(\epsilon) \) by a polynomial \( P_M(\epsilon) \) of degree \( M \), in the vicinity of some point \( \epsilon = \lambda \) over a finite range, by means of a Gaussian weight of effective width \( \gamma \). The least squares principle will be applied by minimizing the following integral:

\[
I(M, \gamma, \lambda) = \int_{-\infty}^{+\infty} \{g(\epsilon) - P_M(\epsilon)\}^2 e^{-\left(\frac{\epsilon - \lambda}{\gamma}\right)^2} d\epsilon
\] (5)

Thus polynomial \( P_M(\epsilon) \) averages the function \( g(\epsilon) \) locally over a range defined by the parameter \( \gamma \) around \( \lambda \). By construction, the coefficients of that polynomial depends on the order \( M \) (arbitrarily fixed) and because of the Gaussian, it depends also on \( \gamma \) and \( \lambda \). For this reason, it will be more correct to write this polynomial as follows:

\[
P_{M,\gamma,\lambda}(\epsilon) = \sum_{m=0}^{M} a_m(M, \gamma, \lambda) \epsilon^m
\] (6)

Knowing coefficients \( a_m \), it is always possible to write this polynomial under the following form:

\[
P_{M,\gamma,\lambda}(\epsilon) = \sum_{m=0}^{M} c_m(M, \gamma, \lambda) (\epsilon - \lambda)^m
\] (7)

Expanding the sum of Eq. (7) and indentifying coefficients of power of \( \epsilon \) with those of Eq. (6) it is then possible to solve coefficients \( c_m \) as a linear combination of coefficients \( a_m \). Now, it is convenient to introduce the parameter \( \gamma \) seen before as follows:

\[
P_{M,\gamma,\lambda}(\epsilon) = \sum_{m=0}^{M} c_m(M, \gamma, \lambda) \gamma^m \left(\frac{\epsilon - \lambda}{\gamma}\right)^m
\] (8)

Finally, due to the Gaussian weight, the most interesting form is to write this polynomial as a combination of Hermite’s polynomials of degree \( m \):

\[
P_{M,\gamma,\lambda}(\epsilon) = \sum_{m=0}^{M} d_m(M, \gamma, \lambda) H_m \left(\frac{\epsilon - \lambda}{\gamma}\right)
\] (9)

Consequently, the integral to be minimized can be rewritten in the form:

\[
I = \int_{-\infty}^{+\infty} \left\{g(\epsilon) - \sum_{m=0}^{M} d_m(M, \gamma, \lambda) H_m \left(\frac{\epsilon - \lambda}{\gamma}\right)\right\}^2 e^{-\left(\frac{\epsilon - \lambda}{\gamma}\right)^2} d\epsilon
\] (10)

The coefficients ensuring the least squares principle will be resolved by minimization:

\[
\frac{\partial I}{\partial d_k} = 0
\] (11)

This gives:

\[
\int_{-\infty}^{+\infty} 2 \left\{g(\epsilon) - \sum_{m=0}^{M} d_m(M, \gamma, \lambda) H_m \left(\frac{\epsilon - \lambda}{\gamma}\right)\right\} \left(-H_k \left(\frac{\epsilon - \lambda}{\gamma}\right)\right) e^{-\left(\frac{\epsilon - \lambda}{\gamma}\right)^2} d\epsilon = 0
\] (12)
Using the orthogonality property of Hermite polynomials, one finds:

\[ d_k(M, \gamma, \lambda) = \frac{1}{2^k k! \sqrt{\pi} \gamma} \int_{-\infty}^{+\infty} g(\epsilon) H_k \left( \frac{\epsilon - \lambda}{\gamma} \right) e^{-\left( \frac{\epsilon^2}{\gamma^2} \right)} d\epsilon \]  

(13)

As it can be easily seen coefficient \( d_k(\gamma, \lambda, M) \) does not depend on \( M \), but Polynomial \( P_{M,\lambda,\gamma}(\epsilon) \) does. Consequently, omitting \( M \) in coefficient \( d_m \), this polynomial will be written under the form:

\[ P_{M,\lambda,\gamma}(\epsilon) = \sum_{m=0}^{M} d_m(\gamma, \lambda) H_m \left( \frac{\epsilon - \lambda}{\gamma} \right) \]  

(14)

Note: In the relationship [5], a Gaussian weight function was used. In fact any weight function tending towards the Dirac delta function can be used. For example, it is perfectly possible to replace the Gaussian weight function with a Lorentzian function in order to apply the least squares principle in the same way. In this case, Eq. [5] must be replaced by:

\[ I = \int_{-\infty}^{+\infty} \{ g(\epsilon) - P_{M,\gamma,\lambda}(\epsilon) \}^2 \left( \frac{1}{1 + \left( \frac{\epsilon - \lambda}{\gamma} \right)^2} \right) d\epsilon \]  

(15)

In that respect, references [4, 5] can be consulted. In the present work, for convenience and simplicity, a Gaussian weight function has been chosen. This is mainly due to the ease of use of Hermite polynomials (which are associated to the Gaussian weight).

**B. Step 2: Definition of the Strutinsky level density as a least squares moving average**

Due to the Gaussian factor in Eq. [5], the averaging defined in the above subsection is by definition local and thereby depends essentially on the region near \( \lambda \) centered on an interval of a length about \( \gamma \). Thus, the values that influence the polynomial approximation are the ones which are the closest to \( \lambda \) on either side around \( \lambda \). The latter being fixed in the least squares principle. This means that if \( \epsilon \) is far from \( \lambda \), this averaging becomes erroneous since the neighboring points of \( \epsilon \) play a negligible role whereas the points that are close to \( \lambda \) have the main role. To remedy to this problem, one proposes to move the average in a such way that the points in the neighborhood of \( \epsilon \) take the major role. This amounts to “move” the effective interval of averaging with \( \lambda \). Mathematically, this is simply obtained by making \( \epsilon = \lambda \), namely by replacing \( P_{M,\gamma,\lambda}(\epsilon) \) by \( P_{M,\gamma,\lambda}(\lambda) \) or in equivalent way by \( P_{M,\gamma,\epsilon}(\epsilon) \). In the following, we will choose \( \lambda \) as the new variable.

Thus, in simpler terms, Strutinsky’s density \( g(\lambda) \) is approached by a local polynomial for any value of \( \lambda \). In each point \( \lambda \), polynomial \( P_{M,\gamma,\lambda}(\lambda) \) is the result of the smoothing of \( g(\lambda) \) in the neighborhood of \( \lambda \). However, the coefficients of this polynomial (see Eq. [14]) depend also on \( \lambda \) so that in general \( P_{M,\gamma,\lambda}(\lambda) \) is not really a polynomial. Finally, the approximation of \( g(\lambda) \) is defined by making \( \epsilon = \lambda \) in Eq. (14):

\[ g(\lambda) \approx P_{M,\gamma,\lambda}(\epsilon) \big|_{\epsilon=\lambda} = \sum_{k=0}^{M} d_k(\gamma, \lambda) H_k(0) \]  

(16)

In order to emphasize that \( P_{M,\gamma,\lambda}(\lambda) \) is in general not a polynomial, it is convenient to change the notation as follows:

\[ P_{M,\gamma,\lambda}(\lambda) = \Pi_{M,\gamma}(\lambda) \]  

(17)

Although \( \lambda \) is constant in the least squares procedure, in this definition it must be considered as a variable. Thus, due to the Gaussian weight, \( \Pi_{M,\gamma}(\lambda) \) can be considered as an average in an interval about \( [\lambda - \gamma, \lambda + \gamma] \) whereas \( \Pi_{M,\gamma}(\lambda + \Delta \lambda) \) is obtained from the “moved interval” \( [(\lambda + \Delta \lambda) - \gamma, (\lambda + \Delta \lambda) + \gamma] \). Thus, in the latter, “one moves” the whole averaging region with \( \lambda \) by a quantity equal to \( \Delta \lambda \). For this reason, \( \Pi_{M,\gamma}(\lambda) \) is in fact, obtained from a moving average.

From Eq. (16) one can see that \( \Pi_{M,\gamma}(\lambda) \) is a linear combination of functions \( d_k(\gamma, \lambda) \). In this respect, as noted just above, one can show that in general, this procedure does not necessarily lead to a polynomial. Indeed, making \( x = \frac{\epsilon - \lambda}{\gamma} \), Eq. (13) can be re-written as:

\[ d_k(\gamma, \lambda) = \frac{1}{2^k k! \sqrt{\pi}} \int_{-\infty}^{+\infty} g(\lambda + \gamma x) H_k(x) e^{-x^2} dx \]  

(18)
By Taylor expansion, we obtain:

\[ g(\lambda + \gamma x) = \sum_{j=0}^{\infty} \frac{g^{(j)}(\lambda)}{j!} (\gamma x)^j \]  

(19)

Now, if one assumes that \( g(\lambda) \) is a polynomial in \( \lambda \) of degree \( n \), the previous sum goes only up to \( n \). Replacing that quantity in the above formula, one obtains:

\[ d_k(\gamma, \lambda) = \frac{1}{2^k k! \sqrt{\pi}} \sum_{j=0}^{n} \frac{g^{(j)}(\lambda)}{j!} \gamma^j \int_{-\infty}^{+\infty} x^j H_k(x) e^{-x^2} dx \quad k = 0, 1, \ldots, M \]  

(20)

Since we assume that \( g(\lambda) \) is a polynomial its derivative are also polynomials and hence, \( d_k(\gamma, \lambda, M) \) and therefore \( \Pi_{M, \gamma}(\lambda) \) are also polynomials. Conversely if \( g(\lambda) \) is not a polynomials, Taylor series becomes infinite and \( \Pi_{M, \gamma}(\lambda) \) is no more a polynomial.

### III. DERIVATION OF THE INTEGRAL FORM OF THE MOVING AVERAGE. AVERAGING FUNCTIONS

Coefficient \( d_k \) is given by Eq. (13). Replacing its expression in formula (16) and inverting sum and integral signs, one gets:

\[ \Pi_{M, \gamma}(\lambda) = \int_{-\infty}^{+\infty} g(\epsilon) \left\{ \sum_{m=0}^{M} \frac{H_m(0)}{2^m m!} H_m \left( \frac{\epsilon - \lambda}{\gamma} \right) \right\} e^{-\left( \frac{\epsilon - \lambda}{\gamma} \right)^2} \gamma \sqrt{\pi} d\epsilon \]  

(21)

with:

\[ H_m(0) = (-1)^{m/2} \frac{m!}{(m/2)!}, \quad m = \text{even} ; \quad H_m(0) = 0, \quad m = \text{odd} ; \]  

(22)

for convenience, we define the following constant:

\[ B_m = \frac{H_m(0)}{2^m m!} = (-1)^{m/2} \frac{2^m (m/2)!}{2^m (m/2)!}, \quad m = \text{even} ; \quad B_m = 0, \quad m = \text{odd} \]  

(23)

Making

\[ x = \frac{\epsilon - \lambda}{\gamma} \]  

(24)

One obtains:

\[ \Pi_{M, \gamma}(\lambda) = \int_{-\infty}^{+\infty} g(\lambda + \gamma x) \left\{ \sum_{m=0}^{M} B_m H_m(x) \right\} e^{-x^2} \gamma \sqrt{\pi} dx \]  

(25)

We define the averaging (or smoothing) functions by:

\[ F_M(x) = \left\{ \sum_{m=0}^{M} B_m H_m(x) \right\} \frac{e^{-x^2}}{\sqrt{\pi}} \]  

(26)

Using the Darboux-Christoffel formula (see appendix [B]), function \( F_M(x) \) can also be written in a second form:

\[ F_M(x) = \left\{ B_M \frac{H_{M+1}(x)}{2x} \right\} \frac{e^{-x^2}}{\sqrt{\pi}} \]  

(27)
We thus obtain an equivalent form of the smoothing average cited above (Eq. (16)) as follows:

$$\Pi_{M,\gamma}(\lambda) = \int_{-\infty}^{+\infty} g(\lambda + \gamma x) F_M(x) \, dx$$  \hspace{1cm} (28)$$

Making in the above equation \(x = (\epsilon - \lambda)/\gamma\), i.e. \(\epsilon = \lambda + \gamma x\), an other form for this result is:

$$\Pi_{M,\gamma}(\lambda) = \int_{-\infty}^{+\infty} g(\epsilon) \frac{1}{\gamma} F_M(\frac{\epsilon - \lambda}{\gamma}) \, d\epsilon$$  \hspace{1cm} (29)$$

In the following, we will see that if \(g(\epsilon)\) reduces to a polynomial of degree \(M\) or less, Eq. (29) gives the exact result, i.e., \(g(\lambda) = \Pi_{M,\gamma}(\lambda)\) rigorously. This is logical since the polynomial approximation for another polynomial (of an equal or greater degree) must be exact. In mathematics, Eq. (28) is known as a convolution product of two functions, which are, \(g\) and \(F_M\). It is well known that there is a close relationship between the convolution product and the moving average.

### IV. GENERAL PROPERTIES OF THE AVERAGING (OR SMOOTHING) FUNCTIONS

The main properties of the averaging (or smoothing) functions are given in the following table:

| Property | Condition |
|----------|-----------|
| 1        | \(F_M(x) = 0\)            | \(M\) odd due to the def. of \(B_M\) |
| 2        | \(F_M(-x) = F_M(x)\)      | \(M\) even |
| 3        | \(\int_{-\infty}^{+\infty} G(x)F_M(x) \, dx = 0\) | \(G(x)\) odd function for parity reason |
| 4        | \(\int_{-\infty}^{+\infty} F_M(x) \, dx = 1\) | see appendix C |
| 5        | \(\int_{-\infty}^{+\infty} \frac{1}{\gamma} F_M(\frac{x-\lambda}{\gamma}) \, dx = 1\) | variable change in 4 |
| 6        | \(\int_{-\infty}^{+\infty} x^k F_M(x) \, dx = 0\) | \(1 \leq k \leq M\) |
| 7        | \(\int_{-\infty}^{+\infty} x^k F_M(x-x_0) \, dx = x_0^k\) | \(1 \leq k \leq M\) |
| 8        | \(\int_{-\infty}^{+\infty} \frac{1}{\gamma} F_M(\frac{x-\lambda}{\gamma}) \, dx = \lambda^k\) | \(1 \leq k \leq M\) |
| 9        | \(\int_{-\infty}^{+\infty} x^k F_M(x) \, dx = C_{k,M}\) | \(k \geq M + 2\), \(k\) even see appendix C |

| Property | Condition |
|----------|-----------|
| 10       | \(\int_{-\infty}^{+\infty} (\epsilon - \lambda)^k \frac{1}{\gamma} F_M(\frac{\epsilon - \lambda}{\gamma}) \, d\epsilon = C_{k,M} \gamma^k\) | \(k \geq M + 2\), \(k\) even variable change in 9 |

**TABLE I.** Main properties of the averaging functions.

### V. THE WIDTH OF THE AVERAGING FUNCTION

#### A. Two extreme cases in which the averaging function reduces to Dirac delta distribution

(i) If we make \(\gamma = 0\) in Eq. (25) and use the property number 4 of the table, we obtain rigorously \(\Pi_{M,\gamma}(\lambda) = g(\lambda)\). Because Eq. (29) is equivalent to Eq. (28), we can conclude that for \(\gamma \to 0\), \(\frac{1}{\gamma} F_M(\frac{\epsilon - \lambda}{\gamma}) \to \delta(\epsilon - \lambda)\) where \(\delta\) represents the Dirac distribution.

(ii) For \(M \to +\infty\), the constant \(B_M\) defined in Eq. (23) tends to \(0^+\) or \(0^-\). From the definition (27) of the averaging function \(F_M(x)\), we should distinguish two cases. For \(x \neq 0\), the function given by Eq. (26) is finite everywhere so that for a fixed \(x\), the corresponding amplitude tends towards zero when \(M\) tends towards infinity. For \(x = 0\), in Eq. (27) the quotient \(H_{M+1}(x)/2x\) becomes indefinite because the numerator and the denominator cancel simultaneously. Applying L’Hospital’s rule, this quotient becomes \(2(M + 1)H_M(x)/2\). Multiplying by \(B_M e^{-x^2/\sqrt{\pi}}\), for \(x = 0\) in Eq. (27), we get \(F_M(0) = B_M(M + 1)H_M(0)\). Using Eq. (22) and (23), we find for \(M \to \infty\) that \(F_M(0) \to 1\). Thus, when \(M\) tends towards infinity the function \(F_M(x)\) tends towards zero everywhere except at the point \(x = 0\) where it becomes infinite. Moreover its area is equal to 1 so this function tends towards the Dirac delta distribution. we can write: \(F_M(x) \to \delta(x)\) when \(M \to \infty\).
FIG. 1. Averaging functions Eq. (27) for three values of the order $M$. It is to be noted that these functions practically cancel as soon as $M \gtrsim 2$.

B. The width of the averaging function for finite values of $M$ and $\gamma$

In the title of this subsection, the expression "finite values" means neither infinity nor zero. In these cases the curve $F_M(x)$ does not reduce to delta function as seen in the previous subsection.

So, contrarily to what one might think, the actual width of the function $F_M(x)$ is not due to the sole $\gamma$ parameter but is governed by the both parameters $\gamma$ and $M$. In fact, the parameter $\gamma$ ($\gamma \neq 0$) is proportional to the width of the Gaussian contained in the function $F_M(x)$, $M$ even. However, as seen in the equation (27), this Gaussian is modulated by the polynomial $B_M H_{M+1}(x)/(2x)$. The Hermite polynomial $H_{M+1}(x)$ has $M+1$ real symmetrical roots with respect to the axis $x=0$. The value $x=0$ is itself a root of the numerator. However, in $x=0$, the denominator also cancels and the function $F_M(x)$ has actually no root for this value. So, this function has $M$ symmetrical roots with respect to the $x=0$ axis. $(M/2)$ positive and $(M/2)$ negative with $M$ even. The function has a main maximum in $x=0$ and successive oscillations with an amplitude that decreases rapidly (see Fig. 1). The area of this curve is normalized to the unit. The main contribution of this area comes from the central part because these oscillations decrease rapidly in amplitude when one walks away from the center and also because they have successive areas that are of opposite signs and thereby, approximately compensate each other. The larger $M$ is, the smaller the width of the curve ($\gamma$ being constant). This means that the larger $M$ is, the more the entire surface of the curve is located near $x=0$. To get an idea of the “convergence” of the surface of this curve, let us say that if an integration is performed over a finite interval $[-2, 2]$ for $M = 4$, we could see that this integral is already quite close to the unit (in fact numerical test gave 0.99). Since the width decreases with $M$, this result is a fortiori valid for any value of the order $M$. Thus, we can say that the averaging function $F_M(x)$ practically cancels as soon as $x \gg 1$ so that one can
write:

\[ \int_{-X}^{+X} F_M(x) dx \approx 1 \quad \text{if} \quad X \gg 1 \quad (30) \]

VI. APPROACH OF THE SMOOTH PART OF THE FUNCTION. THE REMAINDER OF THE AVERAGING

A. Absolute and relative remainders

In Eq. (28), let’s expand \( g(\lambda + \gamma x) \) by Taylor’s theorem in the vicinity of \( \lambda \) to the order \((M + 1)\) with a rest. There is then a number such as \( \vartheta \) with \(-1 < \vartheta < 1\), so that:

\[
\Pi_{M,\gamma}(\lambda) = \int_{-\infty}^{\infty} \left( g(\lambda) + \sum_{m=1}^{M} \frac{g^{(m)}(\lambda)}{m!}(\gamma x)^m + \frac{g^{(M+1)}(\lambda)}{M+1!}(\gamma x)^{M+1} + \frac{g^{(M+2)}(\lambda + \vartheta \gamma x)}{(M+2)!}(\gamma x)^{M+2} \right) F_M(x) dx
\]

The first term gives back \( g(\lambda) \), the second has no contribution since \( m \leq M \) (see property number 6 in the table given above), the third also cancels since the power of \( x \) is odd (see property number 3 of the table). Finally this gives:

\[
\Pi_{M,\gamma}(\lambda) = g(\lambda) + r_{M+2,\gamma}(\lambda)
\]

(32)

where the absolute remainder contains the \((M + 2)th\) power of \( \gamma \):

\[
r_{M+2,\gamma}(\lambda) = \frac{\gamma^{M+2}}{(M+2)!} \int_{-\infty}^{\infty} g^{(M+2)}(\lambda + \vartheta \gamma x) x^{M+2} F_M(x) dx
\]

(33)

Thus, we can see that the averaging yields \( g(\lambda) \) itself but with some noise (remainder). In fact, since all terms corresponding to \( 1 \leq m \leq M \) cancel, \( g(\lambda) \) is simply the first term of this expansion plus a remainder. For reasons we will explain just below, we first define the relative remainder by:

\[
R_{M+2,\gamma}(\lambda) = \frac{r_{M+2,\gamma}(\lambda)}{g(\lambda)} = \frac{\gamma^{M+2}}{(M+2)!} \int_{-\infty}^{\infty} \frac{1}{g(\lambda)} g^{(M+2)}(\lambda + \vartheta \gamma x) x^{M+2} F_M(x) dx
\]

(34)

So Eq. (32) can be written under the form:

\[
\Pi_{M,\gamma}(\lambda) = g(\lambda) \left( 1 + R_{M+2,\gamma}(\lambda) \right)
\]

(35)

B. The relative remainder in the asymptotic limit

In Eq. (34), since \( |\vartheta| < 1 \) and since the surface of curve \( F_M(x) \) is practically confined between \( x = -1 \) and \( x = +1 \) (see Eq. (30)), the condition \( \lambda \gg |\vartheta \gamma x| \) turns to be simply \( \lambda \gg \gamma \) and it is then legitimate to neglect the quantity \( \vartheta \gamma x \) with respect to \( \lambda \). Consequently, we will have in Eq. Eq. (34) \( g^{(M+2)}(\lambda + \vartheta \gamma x) \approx g^{(M+2)}(\lambda) \) and the relative remainder will be about:

\[
R_{M+2,\gamma}(\lambda) \approx \frac{\gamma^{M+2}}{(M+2)!} \frac{g^{(M+2)}(\lambda)}{g(\lambda)} \int_{-\infty}^{\infty} \frac{x^{M+2}}{g(\lambda)} F_M(x) dx
\]

(36)

Taking into account property number 9 in the table given previously, we obtain:

\[
R_{M+2,\gamma}(\lambda) \approx \frac{C_{M+2,M}}{(M+2)!} \frac{\gamma^{M+2}}{g(\lambda)/g^{(M+2)}(\lambda)}
\]

(37)
replacing coefficient $C_{M+2,M}$ by its expression, we explicitly obtain:

$$R_{M+2,\gamma}(\lambda) \approx \frac{(-1)^{M/2}}{(M/2)!2^{M+1}(M+2)} \frac{\gamma^{M+2}}{[g(\lambda)/g^{(M+2)}(\lambda)]}$$

This result is valid only if the following condition holds:

$$\lambda \gg \gamma$$

In fact $\gamma$ is of the order of $\hbar \omega$ (see the next subsection) and the above condition is also called the asymptotic limit and is equivalent to Eq. (4). Usually, for finite wells, the bound states are characterized by negatives levels, in this case the quantity $\lambda$ must be counted from the bottom of the well [2].

**C. “Absolute remainder” vs “Relative remainder”**

We suppose $M$ fixed, if we make $\gamma = 0$ in Eq. (33), the absolute remainder cancels rigorously and from Eq. (32) we will have exactly:

$$\Pi_{M,\gamma}(\lambda) = g(\lambda)$$

This limit corresponds to an averaging (or smoothing) over a zero interval ($\gamma = 0$), the polynomial reduces simply to the oscillating function $g(\lambda)$ and actually does not constitute a true averaging. In fact, the goal of the present work is to remove the oscillations contained in $g(\lambda)$ in order to recover the smooth part $g_0(\lambda)$ (see section I). This is why it is not interessant to take a too small value of $\gamma$ which makes the smoothing inefficient and the absolute remainder close to zero. To find the smooth function $g_0(\lambda)$, it will rather be necessary to increase gradually the parameter $\gamma$ (which defines the averaging interval) until these oscillations stop, i.e., until the curve becomes strictly increasing. This amounts to average the function over a range which is at least as large as the “wavelength” of the oscillations. Let $\gamma_0$ be this “optimal value” of the smoothing. We define the “smoothing condition” by the following relation:

$$\gamma = \gamma_0 \gtrsim \hbar \omega$$

Where $\hbar \omega$ is the mean spacing between shells (which is of the same order of the one quantum of energy). Thus, in the sense of least squares fit, we have $g(\lambda) \approx g_0(\lambda)$ and Eq. (35) becomes:

$$\Pi_{M,\gamma}(\lambda) \approx g_0(\lambda) (1 + R_{M+2,\gamma}^0(\lambda))$$

In which the relative remainder is:

$$R_{M+2,\gamma}^0(\lambda) \approx \frac{C_{M+2,M}}{(M+2)!} \frac{\gamma_0^{M+2}}{[g_0^{(M)}(\lambda)/g_0^{(M+2)}(\lambda)]}$$

Naturally for this value ($\gamma_0$), the absolute remainder in Eq. (33) is not very small. But in this method it is the relative remainder which plays the main role. For reason of accuracy, it is essential that this relative remainder be very small compared to the unit (see equation 42). Once again, the relative remainder becomes small in Eq. (42) if the condition $\lambda \gg \gamma_0$ is satisfied. The condition of the asymptotic limit and the smoothing condition can be summarized in one double equation:

$$\lambda \gg \gamma_0 \gtrsim \hbar \omega$$

As noted in section I, the smoothed level density has been identified as an approximation of the semi classical level density [2]:

$$g_0(\lambda) \approx g_{sc}(\lambda)$$
VII. PARTICLE IN A CUBIC BOX WITH REFLECTING WALLS. ASYMPTOTIC EXPANSION OF THE LEVEL DENSITY:

In order to test the accuracy of the Strutinsky method, it is possible to obtain an asymptotic approximation by combining Eq. (28) with the Euler-Maclaurin formula. Let us apply this method to a particle in a cubic box with equal sides a for which the level density is:

\[ g(\epsilon) = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \frac{1}{\gamma} \delta \left( \frac{\epsilon - \epsilon_{n_x n_y n_z}}{\gamma} \right) \]  

(46)

where the \( n^{th} \) energy level is given by:

\[ \epsilon_{n_x n_y n_z} = (n_x^2 + n_y^2 + n_z^2)E_0 \]  

(47)

\[ E_0 = \frac{\pi^2 \hbar^2}{2ma^2} \]  

(48)

herein \( n_x \) or \( n_y \) or \( n_z = 1, 2, \ldots, \infty \) are quantum numbers (the value 0 is forbidden because the wave function cancels in this case). \( \hbar \) is the Planck constant and \( m \) is the mass of the particle.

To obtain the asymptotic form of \( g(\epsilon) \), i.e. \( g_0(\epsilon) \) (which is hidden in \( g(\epsilon) \)), we replace this quantity from Eq. (46) into Eq. (28), getting:

\[ \Pi_{M,\gamma}(\lambda) = \int_{-\infty}^{\infty} \frac{1}{\gamma} \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \delta \left( \frac{\lambda + \gamma x - (n_x^2 + n_y^2 + n_z^2)E_0}{\gamma} \right) F_M(x) dx \]  

(49)

Interverting discrete sum and integral symbol and using Dirac \( \delta \) property, we find:

\[ \Pi_{M,\gamma}(\lambda) = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \frac{1}{\gamma} F_M \left( \frac{(n_x^2 + n_y^2 + n_z^2)E_0}{\gamma} - \frac{\lambda}{\gamma} \right) \]  

(50)

Making:

\[ G(n_x, n_y, n_z) = \frac{1}{\gamma} F_M \left( \frac{(n_x^2 + n_y^2 + n_z^2)E_0}{\gamma} - \frac{\lambda}{\gamma} \right) \]  

(51)

and using the three dimensional Euler-MacLaurin formula with the first terms (neglecting the derivatives):

\[ \Pi_{M,\gamma}(\lambda) = \int_{-\infty}^{\infty} G(n_x, n_y, n_z) dn_x dn_y dn_z - \frac{3}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(n_x, n_y, 1) dn_x dn_y + \frac{3}{4} \int_{-\infty}^{\infty} G(n_x, 1, 1) dn_x \]  

(52)

After some algebra (see details in the appendix [9]), one gets an asymptotic expansion.

\[ \Pi_{M,\gamma}(\lambda) \approx \frac{\pi \lambda^{1/2}}{4E_0^{3/2}} \left( 1 + a_{M+2} C_{M+2,M} \left( \frac{\gamma}{\lambda} \right)^{M+2} + a_{M+4} C_{M+4,M} \left( \frac{\gamma}{\lambda} \right)^{M+4} + \ldots \right) \]

\[ - \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2} \lambda^{1/2}} \left( 1 + b_{M+2} C_{M+2,M} \left( \frac{\gamma}{\lambda} \right)^{M+2} + b_{M+4} C_{M+4,M} \left( \frac{\gamma}{\lambda} \right)^{M+4} + \ldots \right) \]  

(53)

Coefficient \( C_{k,M} \) is given in the table above.

This asymptotic series has been obtained from the Euler MacLaurin formula. It is a divergent series. To obtain an approximation of the triple integral given above (Eq. (50)), we have to take a finite number of terms. To this end, we can ignore for example the powers which are higher than \( (M + 2) \).

\[ \Pi_{M,\gamma}(\lambda) \approx \frac{\pi \lambda^{1/2}}{4E_0^{3/2}} \left( 1 + a_{M+2} C_{M+2,M} \left( \frac{\gamma}{\lambda} \right)^{M+2} \right) - \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2} \lambda^{1/2}} \left( 1 + b_{M+2} C_{M+2,M} \left( \frac{\gamma}{\lambda} \right)^{M+2} \right) \]  

(54)
From Ref. [2], it turns out that the expression for \( \gamma = 0 \) is the semi classical level density and is the exact result and the one obtained by the Strutinsky is only an approximation to it, i.e. to:

\[
g_{sc}(\lambda) = \frac{\pi \lambda^{1/2}}{4E_0^{3/2}} - \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2}\lambda^{1/2}}
\]  

(55)

This is not surprising because the Euler MacLaurin formula is an asymptotic approximation valid for every value of the parameter \( \gamma \) whereas in the Strutinsky method we are obliged to take a sufficiently large smoothing value for this parameter (Eq. (41)). Thus, the second element in both parentheses in Eq. (54) must be small enough compared to the unit. For example, taking \( M = 8 \) and \( M = 30 \), we have tested numerically that:

\[
\Pi_{8,\gamma}(\lambda) \approx \frac{\pi \lambda^{1/2}}{4E_0^{3/2}} \left( 1 + 10^{-6} \left( \frac{\gamma}{\lambda} \right)^{10} \right) - \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2}\lambda^{1/2}} \left( 1 + 10^{-5} \left( \frac{\gamma}{\lambda} \right)^{10} \right)
\]

\[
\Pi_{30,\gamma}(\lambda) \approx \frac{\pi \lambda^{1/2}}{4E_0^{3/2}} \left( 1 + 10^{-9} \left( \frac{\gamma'}{\lambda} \right)^{32} \right) - \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2}\lambda^{1/2}} \left( 1 + 10^{-7} \left( \frac{\gamma'}{\lambda} \right)^{32} \right)
\]

Thus, in spite of the Strutinsky method is only an approximation of the semi classical method, it is obvious that these results are very accurate in terms of relative error. In this respect, it can be said that if Strutinsky’s method is applied correctly, it gives good results and can thus be considered as a type of semi-classical method.

It is to be noted that, in these expressions the smoothing parameter is not the same (\( \gamma' \neq \gamma \)) because this parameter increases with the order \( M \).

Appendix A: Hermite polynomials:

1. Definition

\[
H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \quad \text{with } n = 0, 1, 2, \ldots.
\]

(A1)

The degree of this polynomial is \( n \).

2. Orthogonality and norm:

\[
\int_{-\infty}^{+\infty} H_n(x)H_m(x)e^{-x^2}dx = 2^n n! \sqrt{\pi} \delta_{nm}
\]

(A2)

\[
\delta_{nm} = 0 \quad \text{if } n \neq m \quad \delta_{nm} = 1 \quad \text{if } n = m
\]

(A3)

3. Parity and special values

\[
H_n(-x) = (-1)^n H_n(x)
\]

(A4)

\[
H_n(0) = (-1)^n \frac{n!}{(n/2)!} \quad n \text{ even}
\]

(A5)

\[
H_n(0) = 0 \quad n \text{ odd}
\]

(A6)
4. Well known property:

\[ \int_{-\infty}^{+\infty} x^k H_m(x) e^{-x^2} \, dx = 0 \quad \text{for } k = 0, 1, 2, \ldots, m - 1 \]  

(A7)

In other words: \( H_m(x) \) is orthogonal to any polynomial of degree less than \( m \).

Appendix B: Christoffel-Darboux formula applied to averaging functions

\[ \sum_{m=0}^{M} \frac{H_m(x) H_m(y)}{2^m m!} = \frac{1}{2} \left( \frac{H_{M+1}(x) H_M(y) - H_{M+1}(y) H_M(x)}{2^M M! (x-y)} \right) \]  

(B1)

Application to the averaging function \( F_M(x) \), making \( y = 0 \) in the above formula:

\[ \sum_{m=0}^{M} \frac{H_m(x) H_m(0)}{2^m m!} = \frac{1}{2} \left( \frac{H_{M+1}(x) H_M(0) - H_{M+1}(0) H_M(x)}{2^M M! (x-0)} \right) \]  

(B2)

Hermite polynomial has the property that \( H_m(0) = 0 \) for odd \( m \). Consequently the sum contains only terms corresponding to even values \( m \) up to even \( M \). Furthermore Hermite polynomial \( H_m(x) \) is therefore even and the sum in Eq. (B2) is then an even function. Consequently \( H_{M+1}(0) = 0 \) and we finally conclude that \( F_M(x) \) is an even function and that \( M \) must be even otherwise that function cancels. Thus, it turns out that:

\[ F_M(x) = \left\{ \sum_{m=0}^{M} \frac{H_m(0)}{2^m m!} H_m(x) \right\} e^{-x^2} \frac{1}{\sqrt{\pi}} = \left\{ \frac{H_M(0) H_{M+1}(x)}{2^M M!} \right\} \frac{1}{2x} e^{-x^2} \frac{1}{\sqrt{\pi}} \]  

(B3)

Or using the definition of the constant \( B_M \)

\[ F_M(x) = \left\{ \sum_{m=0}^{M} \frac{H_m(0)}{2^m m!} H_m(x) \right\} e^{-x^2} \frac{1}{\sqrt{\pi}} = \left\{ B_M \right\} \frac{H_{M+1}(x)}{2x} e^{-x^2} \frac{1}{\sqrt{\pi}} \]

With (see Eq. [23]):

\[ B_M = \begin{cases} \frac{(-1)^{M/2}}{2^M (M/2)!} & \text{if } M \text{ even} \\ 0 & \text{if } M \text{ odd} \end{cases} \]

Appendix C: Demonstrations of some Formulas:

1. Integral of the averaging functions

\[ \int_{-\infty}^{+\infty} F_M(x) \, dx = 1 \]  

(C1)

Using the first form \( F_M(x) \) in Eq. (26):

\[ \int_{-\infty}^{+\infty} \left\{ \sum_{m=0}^{M} B_m H_m(x) \right\} e^{-x^2} \frac{1}{\sqrt{\pi}} \, dx = B_m \sum_{m=0}^{M} \int_{-\infty}^{+\infty} H_m(x) e^{-x^2} \, dx \]  

and since \( H_0(x) = 1 \) this can be re-written as

\[ \sum_{m=0}^{M} B_m \int_{-\infty}^{+\infty} H_0(x) H_m(x) e^{-x^2} \, dx = \sum_{m=0}^{M} B_m \int_{-\infty}^{+\infty} H_0(x) H_m(x) e^{-x^2} \, dx = \sum_{m=0}^{M} B_m \delta_{m0} = B_0 = 1 \]

We have used the orthogonality property and the fact that \( B_m = \frac{H_m(0)}{2^m m!} = \frac{(-1)^{m/2}}{2^m (m/2)!} \).
2. Orthogonality between monomials and averaging functions

This comes essentially from the property given by Eq. ([A7]),

\[ \int_{-\infty}^{+\infty} x^k F_M(x) dx = 0 \quad k = 1, 2, 3, \ldots, M \quad (M = \text{even}) \quad (C2) \]

In effect, using the second form of \( F_M(x) \) given in Eq. ([27]), we can write:

\[ \int_{-\infty}^{+\infty} x^k F_M(x) dx = \int_{-\infty}^{+\infty} x^k \left\{ B_M H_{M+1}(x) \right\} \frac{e^{-x^2}}{\sqrt{\pi}} dx = \left( B_M / 2 \right) \int_{-\infty}^{+\infty} x^{k-1} H_{M+1}(x) \frac{e^{-x^2}}{\sqrt{\pi}} dx = 0 \quad \text{if} \quad k - 1 < M + 1. \]

Due to Eq. ([A7]), the previous inequality amounts to \( k < M + 2 \) or \( k = 2, 4, 6 \ldots M \). The case \( k = 0 \) has been already proved. The case with odd \( k \) is obvious because \( F_M(x) \) is even.

3. Property of Hermite polynomials

\[ \int_{-\infty}^{+\infty} x^k H_m(x) e^{-x^2} dx = \frac{\sqrt{\pi} k!}{2^{k-m} \left( k - m \right)!} \quad \text{if} \quad k \geq m \geq 0 \quad (C3) \]

This property has been proved from combinations of the following equation [6]:

\[ \int_{-\infty}^{+\infty} x^{2w+m} H_m(x) e^{-x^2} dx = \frac{2^m \Gamma \left[ \frac{2w+m+1}{2} \right] \Gamma \left[ \frac{2w+m+2}{2} \right]}{\Gamma (w+1)} \quad w = 0, 1, 2, \ldots \]

with the well known property of the Gamma function:

\[ \Gamma (z) \Gamma (z+1/2) = 2^{1-2z} \sqrt{\pi} \Gamma (2z) \]

and

\[ \Gamma (n+1) = n! \]

4. Property of averaging functions

\[ \int_{-\infty}^{+\infty} x^k F_M(x) dx = C_{K_M} = \frac{(-1)^{M/2}}{(M/2)!} \frac{(k - 1)!}{2^{k-1} ((k - M - 2)/2)!} \quad k = M + 2, M + 4, M + 6, \ldots \ldots \infty \quad (C4) \]

Using the second form of \( F_M(x) \), i.e. Eq. ([27]), one has:

\[ \int_{-\infty}^{+\infty} x^k F_M(x) dx = \int_{-\infty}^{+\infty} x^k \left\{ B_M H_{M+1}(x) \right\} \frac{e^{-x^2}}{\sqrt{\pi}} dx = \left( B_M / 2 \right) \int_{-\infty}^{+\infty} x^{k-1} H_{M+1}(x) \frac{e^{-x^2}}{\sqrt{\pi}} dx = 0 \quad \text{if} \quad k - 1 < M + 1. \]

Thus, making \( k - 1 \rightarrow k \) and \( M + 1 \rightarrow M \) in Eq. ([C3]) one obtains the result of Eq. ([C4]).

Appendix D: Proof of formula ([53])

We calculate Eq. ([52]) by using spherical coordinates for the first integral and polar coordinates for the second:

\[ \Pi_{M, \gamma} (\lambda) = \frac{1}{8} \int_{0}^{\infty} \frac{1}{2} F_M \left( \frac{N^2 E_0 - \lambda}{\gamma} \right) 4\pi N^2 dN - \frac{3}{4} \int_{0}^{\infty} \frac{1}{2} F_M \left( \frac{N^2 E_0 - \lambda}{\gamma} \right) 2\pi n d\phi + \frac{3}{4} \int_{1}^{\infty} \frac{1}{2} F_M \left( \frac{\lambda^2 E_0}{\gamma} - \frac{5}{3} \right) d\theta - \frac{1}{8} G(1, 1, 1) \]

- In the first integral, making \( n_x^2 + n_y^2 + n_z^2 = N^2 \) and \( s = N^2 E_0 - \lambda \) we will have \( N^2 = \frac{\lambda + \gamma s}{E_0} \) and \( 2NdN = \frac{\gamma}{E_0} ds \)
- In the second integral, making \( n_x^2 + n_y^2 = n^2 \) and \( t = \frac{n^2 E_0}{\gamma} - \frac{\lambda}{\gamma} \) we will have \( n^2 = \frac{\lambda + \gamma t}{E_0} \) and \( 2ndn = \frac{\gamma}{E_0} dt \)
• In the third integral, making \( u = \frac{\gamma^2 E_0}{\lambda} - \frac{\lambda}{\gamma} \) we will have \( n_x^2 = \frac{\lambda^2 - \gamma u}{E_0} \) and \( 2n_x d\nu_x = \frac{1}{E_0} du \)

We find: \( \Pi_{M,\gamma}(\lambda) = \frac{1}{8} \int_{-\infty}^{\infty} \frac{1}{\gamma} F_M(s) 2\pi \left( \frac{\lambda + \gamma s}{E_0} \right)^{1/2} \sum_{\nu} \frac{\lambda^2 - \gamma u}{E_0} ds - \frac{3}{4} \int_{-\infty}^{\infty} \frac{1}{\gamma} F_M(t) \frac{\lambda^2 - \gamma u}{E_0} dt + \frac{3}{4} \int_{-\infty}^{\infty} \frac{1}{\gamma} F_M(u) \frac{1}{E_0^{1/2}} \left( \frac{\lambda + \gamma u}{E_0} \right)^{1/2} \frac{1}{E_0} du \)

The smoothing condition is about \( \gamma \gtrsim 3E_0 \) (which means the inter shell spacing is of the order of the zero point energy) and the asymptotic limit is \( \lambda \gg \gamma \). Because of these conditions, we obtain with a good approximation:

\[
\Pi_{M,\gamma}(\lambda) \approx \frac{1}{8} \int_{-\infty}^{\infty} \frac{1}{\gamma} F_M(s) 2\pi \left( \frac{\lambda + \gamma s}{E_0} \right)^{1/2} \frac{\lambda^2 - \gamma u}{E_0} ds - \frac{3}{4} \int_{-\infty}^{\infty} \frac{1}{\gamma} F_M(t) \frac{\lambda^2 - \gamma u}{E_0} dt + \frac{3}{4} \int_{-\infty}^{\infty} \frac{1}{\gamma} F_M(u) \frac{1}{E_0^{1/2}} \left( \frac{\lambda + \gamma u}{E_0} \right)^{1/2} \frac{1}{E_0} du
\]

Expanding the square roots in terms of \( \Pi \cdot \gamma \) and \( \Pi \cdot \gamma \), one will have:

\[
\Pi_{M,\gamma}(\lambda) \approx \frac{\pi^{\lambda/2}}{4E_0^{3/2}} \int_{-\infty}^{\infty} F_M(s) \left( 1 + \frac{\gamma s}{\lambda} \right)^{1/2} ds - \frac{3\pi}{8E_0} \int_{-\infty}^{\infty} F_M(t) dt + \frac{3}{8E_0^{1/2} \lambda^{1/2}} \int_{-\infty}^{\infty} F_M(u) \left( \frac{\gamma s}{\lambda} \right)^n du
\]

Making: \( (1 + \left( \frac{\gamma s}{\lambda} \right)^n = \sum_{n=0}^{\infty} \binom{\alpha}{n} (n - a - 2) \cdots (\alpha - a) x^n \) with \( |x| < 1 \)

This gives:

\[
\Pi_{M,\gamma}(\lambda) \approx \frac{\pi^{\lambda/2}}{4E_0^{3/2}} \int_{-\infty}^{\infty} F_M(s) \left( \frac{\gamma s}{\lambda} \right)^n ds - \frac{3\pi}{8E_0} \int_{-\infty}^{\infty} F_M(t) dt + \frac{3}{8E_0^{1/2} \lambda^{1/2}} \sum_{n=0}^{\infty} b_n \int_{-\infty}^{\infty} F_M(u) \left( \frac{\gamma s}{\lambda} \right)^n du
\]

So applying property number 9 of the table, one gets:

\[
\Pi_{M,\gamma}(\lambda) \approx \frac{\pi^{\lambda/2}}{4E_0^{3/2}} \left( 1 + a_{M+2} C_{M+2,M} \left( \frac{\gamma}{\lambda} \right)^{M+2} + a_{M+4} C_{M+4,M} \left( \frac{\gamma}{\lambda} \right)^{M+4} + \cdots \right)
\]

\[
- \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2} \lambda^{1/2}} \left( 1 + b_{M+2} C_{M+2,M} \left( \frac{\gamma}{\lambda} \right)^{M+2} + b_{M+4} C_{M+4,M} \left( \frac{\gamma}{\lambda} \right)^{M+4} + \cdots \right)
\]

(D1)

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