The logarithmic perturbation theory for bound states in spherical-symmetric potentials via the $\hbar$-expansions

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February 2, 2008

Abstract

The explicit semiclassical treatment of the logarithmic perturbation theory for the bound-state problem for the spherical anharmonic oscillator and the screened Coulomb potential is developed. Based upon the $\hbar$-expansions and suitable quantization conditions a new procedure for deriving perturbation expansions is offered. Avoiding disadvantages of the standard approach, new handy recursion formulae with the same simple form both for ground and excited states have been obtained. As examples, the perturbation expansions for the energy eigenvalues of the quartic anharmonic oscillator and the Debye potential are considered.

1 Introduction

The main task in application of the quantum mechanics is to solve the Schrödinger equations with different potentials. Unfortunately, realistic physical problems can practically never be solved exactly. Then one has to resort to some approximations. Most widely used among them is the perturbation theory. However, the explicit calculation with the Rayleigh – Schrödinger perturbation theory, described in most quantum mechanics textbooks, runs into the difficulty of the summation over all intermediate unperturbed eigenstates. To avoid this difficulty, various alternative perturbation procedures have been proposed [1–13].

Nevertheless up to now, one of the principal approximation techniques is the logarithmic perturbation theory [14–21]. Within the framework of this approach, the conventional way to solve a quantum-mechanical bound-state problem consists in changing from the wave function to its logarithmic derivative and converting the time-independent Schrödinger equation into the nonlinear Riccati equation.

In the case of ground states, the consequent expansion in a small parameter leads to handy recursion relations that permit us to derive easily the corrections to the energy as
well as to the wave function for each order. However, when radially excited states are considered, the standard technique of the logarithmic perturbation theory becomes extremely cumbersome and, practically, inapplicable for describing higher orders of expansions.

Recently, a new procedure based on specific quantization conditions has been proposed to get series of the logarithmic perturbation theory via the $\hbar$-expansion technique within the framework of the one-dimensional Schrödinger equation [22]. Avoiding the disadvantages of the standard approach, this straightforward semiclassical procedure results in new handy recursion formulae with the same simple form both for the ground state and excited states.

The object of the present work is to extend the above mentioned formalism to the bound-state problems within the framework of the three-dimensional Schrödinger equation with central potentials, such as the anharmonic scillator potential and the screened Coulomb one, which are widely used in practice.

## 2 Basic concepts of the method

We study the bound-state problem for a non-relativistic particle moving in a central potential admitted bounded eigenfunctions and having in consequence a discrete energy spectrum. Let us therefore consider the reduced radial part of the Schrödinger equation

$$\frac{\hbar^2}{2m} U''(r) + \left( \frac{\hbar^2 l(l + 1)}{2mr^2} + V(r) \right) U(r) = EU(r), \quad (1)$$

with the effective potential having only one simple minimum.

Following usual practice, we apply the substitution, $C(r) = \hbar U'(r)/U(r)$, accepted in the logarithmic perturbation theory and go over from the Schrödinger equation (1) to the Riccati equation

$$\hbar C'(r) + C^2(r) = \frac{\hbar^2 l(l + 1)}{r^2} + 2mV(r) - 2mE. \quad (2)$$

According to our assumption, we are seeking the eigenvalues and the eigenfunctions of this equation explicitly in a semiclassical manner with series expansions in powers of the Planck constant

$$E = \sum_{k=k_1}^{\infty} E_k \hbar^k, \quad C(r) = \sum_{k=k_2}^{\infty} C_k(r) \hbar^k, \quad (3)$$

where the order in $\hbar$ of these quantities, i.e. the values of $k_1$ and $k_2$, should be defined as a preliminary.

As in the standard approach, the substitution of these expansions into the Riccati equation leads to the simple recursion system. This system can be solved successively in the case of ground states, while the description of the excited states has some problems with taking into account the nodes of wave functions. For avoiding these problems, we shall attempt to use the quantization condition and the formalism of the theory of functions of a complex variable.

Remind that, in the complex plane, a number of zeros $N$ of a regular function inside a closed contour is defined by the principle of argument known from the complex analysis.
Being applied to the logarithmic derivative, \( C(r) \), it means that
\[
\frac{1}{2\pi i} \oint C(r) \, dr = \frac{1}{2\pi i} \sum_{k=0}^{\infty} \hbar^k \oint C_k(r) \, dr = \hbar N. \tag{4}
\]

This quantization condition is exact and is widely used for deriving higher-order corrections to the WKB-approximation \([23, 24]\) and the \( 1/N \)-expansions \([25–27]\). There is, however, one important point to note. Because the radial and orbital quantum numbers, \( n \) and \( l \), correspondingly, are specific quantum notions, the quantization condition \((4)\) must be supplemented with a rule of achieving a classical limit for these quantities. It is this rule that stipulates the kind of the semiclassical approximation.

In particular, within the framework of the WKB-approach the passage to the classical limit is implemented using the rule
\[
\hbar \to 0, \quad n \to \infty, \quad l \to \infty, \quad \hbar n = \text{const}, \quad \hbar l = \text{const}, \tag{5}
\]
whereas the \( 1/N \)-expansion requires the condition \([25–27]\)
\[
\hbar \to 0, \quad n = \text{const}, \quad l \to \infty, \quad \hbar n \to 0, \quad \hbar l = \text{const}. \tag{6}
\]

The proposed semiclassical treatment of the logarithmic perturbation theory involves the alternative possibility:
\[
\hbar \to 0, \quad n = \text{const}, \quad l = \text{const}, \quad \hbar n \to 0, \quad \hbar l \to 0. \tag{7}
\]

With the last rule, the right-hand side of the equation \((4)\) has the first order in \( \hbar \) and the quantization condition now takes the simple form
\[
\frac{1}{2\pi} \oint C_1(r) \, dr = N, \quad \frac{1}{2\pi} \oint C_k(r) \, dr = 0, \quad k \neq 1. \tag{8}
\]

However, this definition of the quantization condition is incomplete since we have not pointed out the path of integration. We shall now show that the suitable choice of the contour of integration and the consequent integration with application of the Cauchy residue theorem easily solves the problem of describing radially excited states.

3 The anharmonic oscillator

*Quantization conditions.* The discussion of details of the proposed technique we begin with the case of the anharmonic oscillator potential which is given by a symmetric function \( V(r) \) that can be written as a Taylor series expansion
\[
V(r) = \frac{1}{2} m \omega^2 r^2 + \sum_{i \geq 1} f_i r^{2i+2}. \tag{9}
\]

In the first place, let us consider the rule \((7)\) of achieving the classical limit from the physical point of view. Since \( \hbar l \to 0 \) as \( \hbar \to 0 \), the centrifugal term, \( \hbar^2 l (l + 1) / r^2 \), has the second order in \( \hbar \) and disappears in the classical limit that corresponds to falling a particle into the center. This means that a particle drops into the bottom of the potential
well as $\hbar \to 0$ and its classical energy becomes $E_0 = \min V(r) = 0$. Hence, the series expansions in powers of the Planck constant for the energy eigenvalues and the $C(r)$ must now read as $E = \sum_{k=1}^{\infty} E_k \hbar^k$ and $C(r) = \sum_{k=0}^{\infty} C_k(r) \hbar^k$.

Upon inserting these expansions into the Riccati equation (2) and collecting coefficients of equal powers of $\hbar$, we obtain the following hierarchy of equations

\begin{align*}
C_0^2(r) &= 2 m V(r), \\
C_0'(r) + 2 C_0(r) C_1(r) &= -2 m E_1, \\
C_1'(r) + 2 C_0(r) C_2(r) + C_1^2(r) &= \frac{l(l+1)}{r^2} - 2 m E_2, \\
\vdots
\end{align*}

\begin{align*}
C_{k-1}'(r) + \sum_{i=0}^{k} C_i(r) C_{k-i}(r) &= -2 m E_k, \quad k > 2. \quad (10)
\end{align*}

In the case of ground states, this recurrence system can be solved as straightforwardly as in the standard approach. For excited states, we intend to take into account the nodes of the wave function with the quantization condition (8) for which we must define the contour of integration.

It should be stressed that our technique is quite distinguished from the WKB method not only in the rule of achieving a classical limit but also in the choice of a contour of integration in the complex plane. With a view to elucidate the last difference let us now sketch out the WKB treatment of this bound-state problem. In the complex plane, because the potential is described by the symmetric function (9), there are two pairs of turning points, i.e. zeros of the classical momentum, on the real axis. Therefore we have two cuts between these points: in the region $r > 0$ as well as in the region $r < 0$. In spite of only one cut lies in the physical region $r > 0$, the contour of integration in the WKB quantization condition has to encircle both cuts for the correct result for the harmonic oscillator to be obtained [28].

In our approach, when a particle is dropping into the bottom of the potential well these four turning points are drawing nearer and, at last, are joining together at the origin. Consequently, all zeros of the wave function are now removed from both positive and negative sides of the real axis into the origin and our contour of integration must enclose only this point and no other singularities.

Further, let us count the multiplicity of a zero formed in the wave function at $r = 0$. Imposed by the requirement of the regularity, the behavior $r^{l+1}$ as $r \to 0$ brings the value $l + 1$. The number of nodes in the physical region $r > 0$ is equal to the radial quantum number $n$. But, because the potential (9) is a symmetric function, the same number of zeros must be in the region $r < 0$, too. Then the total number of zeros inside the contour becomes equal to $N = 2n + l + 1$.

For evaluation of the contour integrals in the quantization condition (8), let us consider the system (10) and investigate the behavior of the functions $C_k(r)$. From the first equation of this system, it follows instantly that the $C_0(r)$ can be written as

\begin{equation}
C_0(r) = -[2 m V(r)]^{1/2} = -m \omega r \left(1 + \frac{2}{m \omega^2} \sum_{i=1}^{\infty} f_i r^{2i}\right)^{1/2} = r \sum_{i=0}^{\infty} C_i^0 r^{2i}, \quad (11)
\end{equation}
where the minus sign is chosen from the boundary conditions and coefficients $C_i^0$ are defined by parameters of the potential through the relations

$$
C_0^0 = -m\omega, \quad C_i^0 = \frac{1}{2m\omega} \left( \sum_{p=1}^{i-1} C_p^0 C_{i-p}^0 - 2mf_i \right), \quad i \geq 1. \quad (12)
$$

At the origin, on account of the equality $C_0(0) = 0$, a simple pole arises for the function $C_1(r)$, while $C_k(r)$ has a pole of the order $(2k - 1)$. Thus $C_k(r)$ can be represented by the Laurent series

$$
C_k(r) = r^{1-2k} \sum_{i=0}^{\infty} C_k^i r^{2i}, \quad k \geq 1. \quad (13)
$$

Finally, with applying the residue theorem, the quantization condition (8) expressed explicitly in terms of the coefficients $C_k^i$ takes the especially simple form

$$
C_{k-1}^k = N \delta_{1,k}, \quad (14)
$$

where $N = 2n + l + 1$.

It is this quantization condition that makes possible the common consideration of the ground and excited states and permits us to derive the simple recursion formulae.

**Recursion formulae and the example of application.** The substitution of the series (12) and (13) into the system (10) in the case $i \neq k - 1$ yields the recursion relation for obtaining the Laurent-series coefficients of the logarithmic derivative of the wave function

$$
C_i^k = \frac{-1}{2C_0^0} \left[ (3 - 2k + 2i)C_i^{k-1} - \sum_{j=1}^{k-1} \sum_{p=0}^{i} C_p^j C_{i-p}^{k-j} + 2 \sum_{p=1}^{i} C_p^0 C_{i-p}^k - l(l+1)\delta_{2,k}\delta_{0,i} \right]. \quad (15)
$$

If $i = k - 1$, by equating the expression (15) for $C_{k-1}^k$ to the quantization condition (14) we arrive at the recursion formulae for the energy eigenvalues

$$
2mE_k = -C_{k-1}^{k-1} - \sum_{j=0}^{k-1} \sum_{p=0}^{k-1} C_p^j C_{k-1-p}^{k-j}. \quad (16)
$$

Derived in this way, first corrections to the energy eigenvalues of the spherical anhar-
monic oscillator take the form

$$E_1 = \frac{1 + 2N}{2} \omega, \quad E_2 = \frac{(3 - 2L + 6\eta)}{4m^2 \omega^2} f_1,$$

$$E_3 = \frac{1 + 2N}{8m^4 \omega^5} \left( (-21 + 9L - 17\eta) f_1^2 + m (15 - 6L + 10\eta) \omega^2 f_2 \right),$$

$$E_4 = \frac{1 + 2N}{16m^6 \omega^8} \left( \frac{333 + 11L^2 - 3L (67 + 86\eta) + 3\eta (347 + 125\eta)}{f_1^3} - 6m (60 + 3 (-13 + L) L + 175\eta - 42L\eta + 55\eta^2) \omega^2 f_1 f_2 + m^2 (6L^2 - 12L (6 + 5\eta) + 35 (3 + 2\eta (4 + \eta))) \omega^4 f_3 \right),$$

$$E_5 = -\frac{1 + 2N}{128m^8 \omega^{11}} \left( \frac{30885 + 909L^2 - 27L (613 + 330\eta) + \eta (49927 + 10689\eta)}{f_1^4} - 4m (11220 + 393L^2 - 6L (1011 + 475\eta) + \eta (16342 + 3129\eta)) \omega^2 f_1^2 f_2 + 16m^2 \left( \frac{33L^2 - L (501 + 190\eta) + 63 (15 + \eta (19 + 3\eta))}{f_1^4} \omega^4 f_1 f_3 + 2m^2 \left( \frac{3495 + 138L^2 + 4538\eta + 786\eta^2 - 30L (63 + 26\eta)}{f_1^6} \omega^4 f_2^2 - 4m^3 \left( \frac{30L^2 - 20L (24 + 7\eta) + 63 (15 + 2\eta (8 + \eta))}{f_1^8} \omega^6 f_4 \right) \right), \quad \quad (17)$$

where $N = 2n + l + 1$, $\eta = N (N + 1)$, $L = l(l + 1)$.

As it was expected, the obtained expansion is indeed the series of the logarithmic perturbation theory in powers of the Taylor-series coefficients for the potential function, with the first approximation being equal to the energy of the three-dimensional harmonic oscillator

$$E_1 = \left( 2n + l + \frac{3}{2} \right) \omega. \quad \quad (18)$$

Thus, the problem of obtaining the energy eigenvalues and eigenfunctions for the bound-state problem for the anharmonic oscillator can be considered solved. The equations (15)-(16) have the same simple form both for the ground and excited states and define a useful procedure for the successive calculation of higher orders of expansions of the logarithmic perturbation theory.

As an example, we examine eigenenergies for the anharmonic oscillator with the potential

$$V(r) = m\omega^2r^2/2 + \lambda r^4, \quad \lambda > 0. \quad \quad (19)$$

Then the equations (17) are rewritten as

$$E_1 = \left( \frac{1}{2} + N \right) \omega, \quad \quad E_2 = \frac{(3 - 2L + 6\eta)}{4m^2 \omega^2} \lambda,$$

$$E_3 = -\frac{(1 + 2N)(21 - 9L + 17\eta)}{8m^4 \omega^5} \lambda^2,$$

$$E_4 = \frac{(333 + 11L^2 - 3L (67 + 86\eta) + 3\eta (347 + 125\eta))}{16m^6 \omega^8} \lambda^3,$$

$$E_5 = -\frac{(1 + 2N)(30885 + 909L^2 - 27L (613 + 330\eta) + \eta (49927 + 10689\eta))}{128m^8 \omega^{11}} \lambda^4. \quad \quad (20)$$

We recall that here $N = 2n + l + 1$, $\eta = N (N + 1)$, $L = l(l + 1)$. 
It is readily seen that the use of the $\hbar$-expansion technique does lead to the explicit perturbation expansion in powers of the small parameter $\lambda$.

In the case of ground states, obtained expansions for the energy eigenvalues coincide with those listed in Ref. [29]. In the case of excited states, our corrections coincide with corrections up to the second order which are just only calculated in Ref. [30].

As it is known, the expansions for the anharmonic oscillator are asymptotic and diverge for any finite value of the parameter $\lambda$ that requires the use of some procedures of improving the convergence (for references see [31]). It should be noted, that the proposed technique is easily adapted to apply any scheme of the series renormalization [32].

4 The screened Coulomb potential

Quantization conditions. Now let us consider the case of the screened Coulomb potential which in common practice has a form

$$V(r) = \frac{1}{r} F(\kappa, r).$$  \hspace{1cm} (21)

where $\kappa$ is a small parameter.

In what following, we do not single out explicitly the screening parameter, but incorporate it into coefficients $V_i$ of the Taylor series expansion of this potential

$$V(r) = \frac{1}{r} \sum_{i=0} V_i r^i.$$  \hspace{1cm} (22)

Note, that after performing the scale transformation $r \rightarrow \hbar^2 r$ powers of the screening parameter appear in common with powers of Planck’s constant squared. Hence, the perturbation series must be, as a matter of fact, not only $\kappa$-expansions but also the semiclassical $\hbar^2$-expansions, too.

In the classical limit, when a particle falls into the center, its energy eventually approaches infinity. Hence, the expansions (23) must be represented as $E = \hbar^{-2} \sum_{k=0}^{\infty} E_k \hbar^{2k}$ and $C(r) = \hbar^{-1} \sum_{k=0}^{\infty} C_k(r) \hbar^k$ that results in the recurrent system

$$C_0^2(r) = -2mE_0,$$

$$C_0(r)C_1(r) = m \left[ V(r) - E_1 \right],$$

$$C'_1(r) + 2C_0(r)C_2(r) + C_1^2(r) = \frac{l(l+1)}{r^2} - 2mE_2,$$

$$\cdots$$

$$C'_{k-1}(r) + \sum_{j=0}^{k} C_j(r)C_{k-j}(r) = -2mE_k, \ k > 2.$$  \hspace{1cm} (23)

which changes only in the first two equations in comparison with (10).

Now, let us consider the choice of the contour of integration in the quantization relation. Since in the classical limit a particle falls into center, the classical turning points again draw to the origin and the nodes of the wave function are joined together at $r = 0$. Then, as well as in the anharmonic oscillator case, the contour of integration must enclose
only the origin. However, now the nodes of the function come into the origin only from
the positive region of the real axis. Thus, with the number of nodes and the value \( l + 1 \)
included, the total number of zeros in the quantization condition (14) becomes equal to
\( N = n + l + 1 \).

Further, from (23) it appears that \( C_0(r) \) is the constant and its Taylor-series coefficients
are
\[
C_0^0 = -\sqrt{-2mE_0}, \quad C_0^i = 0,
\]
(24)
Owing to the Coulomb behavior of the potential at the origin, the \( C_1(r) \) has a simple pole
at this point, while the function \( C_k(r) \) has a pole of the order \( k \) and may be represented
as
\[
C_k(r) = r^{-k} \sum_{i=0}^{\infty} C_k^i r^i,
\]
(25)
that leads to the known quantization condition
\[
C_{k-1}^k = N \delta_{1,k},
\]
(26)
where \( N = n + l + 1 \).

Recursion formulae and the example of application. After substitution (24)-(25) into
(23), when \( (i \neq k) \), we have:
\[
C_i^1 = \frac{m}{C_0^0} \left[V_i - E_1 \delta_{1,1}\right],
\]
\[
C_i^k = -\frac{1}{2C_0^0} \left[(i-k+1)C_{i-1}^{k-1} + \sum_{j=1}^{k-1} \sum_{p=0}^{i} C_p^j C_{i-p}^{k-j}
+ 2mE_k \delta_{i,k} - l(l+1) \delta_{i,0} \delta_{k,2}\right], \quad k > 1.
\]
(27)

In the case \( i = k \), from (26) and (27), we obtain
\[
E_0 = -\frac{mV_0^2}{2N^2}, \quad E_1 = V_1,
\]
\[
E_k = -\frac{1}{2m} \left[C_{k-1}^{k-1} + \sum_{j=1}^{k-1} \sum_{p=0}^{k} C_p^j C_{k-p}^{k-j} + 2C_0^0 C_k^k\right], \quad k > 1,
\]
(28)
that, through the the Taylor-series coefficients for the potential function, is
\[
E_0 = -\frac{mV_0^2}{2N^2}, \quad E_1 = V_1, \quad E_2 = (L - 3N^2) \frac{V_2}{2 m V_0},
\]
\[
E_3 = \frac{N^2}{2 m^2 V_0^2} (1 - 3L + 5N^2) V_3,
\]
\[
E_4 = \frac{N^2}{8 m^3 V_0^4} \left((3L^2 - 5N^2 - 7N^4) V_2^2 + (3L(2 - L) - 5N^2(5 - 6L) - 35N^4) V_0 V_4\right),
\]
\[
E_5 = \frac{N^4}{8 m^4 V_0^5} \left((-5L(2 + 3L) + 7N^2(9 - 2L) + 45N^4) V_2 V_3 + (12 - 50L + 15L^2 + 35N^2(3 - 2L) + 63N^4) V_0 V_5\right),
\]
(29)
where \( N = n + l + 1 \) and \( L = l(l + 1) \).

We see that the zero approximation gives the exact solution for the Coulomb problem.

As an example of application, we consider the case of the Debye potential, which is widely used in many branches of physics:

\[
V(r) = -\frac{\alpha}{r}\exp(-\kappa r).
\]  

(30)

For this potential, the first corrections to the energy eigenvalues take the form

\[
E_0 = -\frac{m\alpha^2}{2N^2}, \quad E_1 = \alpha \kappa, \quad E_2 = \frac{(L - 3N^2)}{4m} \kappa^2, \\
E_3 = \frac{N^2}{12m^2\alpha} (1 - 3L + 5N^2) \kappa^3, \\
E_4 = \frac{N^2}{192m^3\alpha^2} (3L(2 + 5L) - 5(11 - 6L)N^2 + 77N^4) \kappa^4, \\
E_5 = \frac{N^4}{320m^4\alpha^3} (4 - 50L - 45L^2 + 35(7 - 2L)N^2 + 171N^4) \kappa^5, 
\]  

(31)

where \( N = n + l + 1 \), and \( L = l(l + 1) \).

And again we recognize the explicit perturbation expansion in powers of the small parameter \( \kappa \).

Typical results of the calculation with these formulae are presented in the Table I where the sequences of the partial sums of \( K \) corrections to the energy eigenvalues for the Debye potential \( V(r) = -\alpha \exp(-\kappa r)/r \) is compared with results of the numerical integration, \( E_{\text{num}} \), in Coulomb units \( \hbar = m = \alpha = 1 \). It is seen that for small values of the screening parameter, the convergence of the series is quite sufficient for the use them without any renormalization. However, the results become gradually worse when the screening parameter increase, as it was pointed for such potentials in [33].

| \( K \) | \( n = 0, \ l = 0, \ \kappa = 0.2 \) | \( n = 1, \ l = 0, \ \kappa = 0.04 \) | \( n = 1, \ l = 1, \ \kappa = 0.02 \) |
|---|---|---|
| 0 | 0.5000000000 | 0.1250000000 | 0.0555555556 |
| 1 | 0.3000000000 | 0.0750000000 | 0.0355555556 |
| 2 | 0.3300000000 | 0.0825000000 | 0.0380555556 |
| 3 | 0.3260000000 | 0.0816250000 | 0.0378155556 |
| 4 | 0.3271000000 | 0.0818140625 | 0.0378614556 |
| 5 | 0.3266800000 | 0.0817559375 | 0.03784969436 |
| 10 | 0.3268179839 | 0.081715528 | 0.03785241171 |
| 15 | 0.3268059572 | 0.081711705 | 0.03785238868 |
| 20 | 0.3268100537 | 0.081711991 | 0.03785238922 |
| 25 | 0.3268067333 | 0.081711951 | 0.03785238920 |
| \( E_{\text{num}} \) | 0.3268085112 | 0.0817711958 | 0.03785238920 |

5 Summary

In conclusion, a new useful technique for deriving results of the logarithmic perturbation theory has been developed. Based upon the \( h \)-expansions and suitable quantization con-
ditions, new handy recursion relations for solving the bound-state problem for a spherical anharmonic oscillator and a static screened-Coulomb potential have been obtained. These relations can be applied to excited states exactly in the same manner as to ground states providing, in principle, the calculation of the perturbation corrections of large orders in the analytic or numerical form. Besides this remarkable advantage over the standard approach to the logarithmic perturbation theory, our method does not imply knowledge of the exact solution for the zero approximation, which is obtained automatically. And at last, the recursion formulae at hand, having the same simple form both for the ground state and excited states, can be easily adapted to applying any renormalization scheme for improving the convergence of obtained series, as it is described in [32].

This research was supported by a grant N 0106U000782 from the Ministry of Education and Science of Ukraine which is gratefully acknowledged.

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