The Milne problem and higher orders of the WKBJ approximation

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A linear third-order equation, which is equivalent to the Milne equation, is derived. This equation is used to formulate a new version of the WKBJ approximation, in which the expansion has an extremely simple structure. A condition for the applicability for the higher-order corrections of the WKBJ expansion is found.

The general solution of the one-dimensional Schrödinger equation,

$$-\frac{h^2}{2m}\frac{d^2\psi}{dx^2} + (V(x) - E)\,\psi = 0\,, \tag{1}$$

can be written[1]

$$\psi(x) = aw(x)\sin\left\{\frac{1}{h}\int_{x_0}^{x}\frac{dx'}{w^2(x')} + b\right\},$$

where a and b are arbitrary constants, and $w(x)$ is the solution of the Milne equation,

$$-\frac{h^2}{2m}\frac{d^2 w}{dx^2}+(V(x)-E)w=-\frac{1}{2mw^3}\ . \tag{2}$$

Several recent studies have dealt with the use of this transformation both for numerical calculations and for deriving various analytic results (study of the Thomas-Fermi model, construction of the WKBJ approximation, calculations of scattering phase shifts and density matrices, etc.). These studies are reviewed in Ref. 2, for example. A serious disadvantage of the Milne equation is its nonlinearity, which makes it difficult to use it to derive analytic results. In this letter we derive a linear third-order equation which is equivalent to Eqs. (1) and (2) simultaneously and which can be used, in particular, to formulate a new version of the WKBJ expansion with an extremely simple structure.

A linear equation can be derived from the Milne equation by multiplying Eq. (2) by w^3, transforming to the new, unknown function $f=w^2$, and differentiating the resulting equation with respect to x. As a result, we find the following equation for $f(x)$:

$$-\frac{h^2}{4m}\frac{d^3 f}{dx^3}+2(V(x)-E)\frac{df}{dx}+\frac{dV}{dx}f=0. \tag{3}$$

The same equation can be found from the Schrödinger equation by transforming from ψ to ψ^2 ($f=\psi^2$). Three linearly independent solutions of Eq. (3) can be chosen in such a manner that two are related to solutions of the Schrödinger equation (solutions of the ρ type: $\rho_1=\psi_1^2$, $\rho_2=\psi_2^2$), and one is related to a solution of the Milne equation (a solution of the λ type: $\lambda=w^2$). In the WKBJ approximation, the solutions of the ρ type have an essential singularity at $h\to 0$, so that the expansion in h is constructed for the logarithmic derivative of ρ, as is the standard expansion for the wave function, and we will not discuss it further here. The solutions of the λ type, which do not have this singularity, can be expanded directly in a power series in h.

Let us examine the WKBJ expansion for the solutions of the λ type. The zeroth approximation λ_0 is found by discarding the third derivative from Eq. (3): $\lambda_0=1/p(x)(p(x)=\sqrt{2m(E-V)})$. To find the following approximations we substitute λ into Eq. (3) in the form

$$\lambda(x)=\sum_{n=0}^{\infty} h^{2n}\lambda_n(x). \tag{4}$$

Equating the coefficients of the various powers of h to zero, we find

$$-\frac{1}{4m}\frac{d^3\lambda_{n-1}}{dx^3}+2(V(x)-E)\frac{d\lambda_n}{dx}+\frac{dV}{dx}\lambda_n=0\ . \tag{5}$$

Recurrence relation (5) has a very simple structure. It relates the corrections of orders n and $n-1$ in a manner linear in λ_i, and it does not depend explicitly on n. We express λ_n in terms of λ_{n-1} using (5):

$$\lambda_n = \hat{L}\lambda_{n-1} + \frac{c_n}{p(x)}; \quad \hat{L} \equiv -\frac{1}{4p(x)}\int_{x_0}^{x} dy \frac{1}{p(y)}\frac{d^3}{dy^3}. \tag{6}$$

It can be seen from (6) that in the calculation of a correction λ_n an undetermined constant c_n arises; this constant is associated with the uncertainty in the lower integration limit, x_0. To determine c_n we must substitute the expansion for λ into a nonlinear Milne equation and find these constants from it. At first glance, it would appear that we should again have to solve nonlinear recurrence relations, but in this case for the coefficients c_n, so that we would lose the basic advantage of this approach. However, as we will now show, this problem can be solved in a simple way, and it does not create any further difficulties. We denote by λ_n^0 the calculated corrections for the case in which $c_n = 0$ for all n; i.e., $\lambda_n^0 = \hat{L}\lambda_{n-1}^0 = \hat{L}^n\lambda_0$. In general, the corrections λ_n can be expressed in terms of λ_n^0 and c_n in the following way:

$$\lambda_n = \lambda_n^0 + \sum_{l=0}^{n-1} c_{n-l}\lambda_l^0. \tag{7}$$

Substituting (7) into (4), we easily find that for each coefficient $h^{2n}c_n$ we find the same series, and the dependence on λ_n^0 and c_n in the expansion for λ is factorized

$$\lambda = C\lambda^0, \; C \equiv \sum_{n=0}^{\infty} h^{2n} c_n, \quad \lambda^0 \equiv \left(\sum_{n=0}^{\infty} h^{2n}\hat{L}^n\right)\lambda_0. \tag{8}$$

Substituting $w(x)$ into Eq. (2) in the form $w = (C\lambda^0)^{1/2}$, we find C:

$$C = \left\{\frac{h^2}{2}\left[\lambda^0\frac{d^2\lambda^0}{dx^2} - \frac{1}{2}\left(\frac{d\lambda^0}{dx}\right)^2\right] + 2m(E - V)(\lambda^0)^2\right\}^{-1/2}. \tag{9}$$

Generally speaking, the right side of (9) can be expanded in powers of h, and all the coefficients c_n can be singled out explicitly, but this is not the best approach. Accordingly, if the expansion of λ^0 has already been found, then essentially no further calculations are required to determine the coefficients c_n.

In other approaches, when the WKBJ expansion is constructed for the action $S = ih\ln\psi$ or for w, the original equation for these functions turns out to be nonlinear, and the recurrence relation for the correction of order n is a tangled combination of all the preceding corrections. Several papers have been devoted to classifying these corrections systematically and developing a diagram technique for such complicated expansions (see, for example, Ref. 3, and the bibliography there). It can be seen from the results above that all these problems disappear if we construct an expansion for the quantity λ, which represents the wavelength of the particle in the limit $h \to 0$. This expansion has an extremely simple structure: It contains only even powers of h and is a geometric progression of the operator $\hat{L}$ [Eq. (8)].

As an example, we consider the WKBJ expansions for a particle with a zero energy in a power-law potential $V = -\alpha^2 x^{2\nu}/2m$. This is an interesting case in that it describes all types of violations of the WKBJ approximation because of power-law singularities. The value $\nu = 1/2$ corresponds to an ordinary turning point. From recurrence relation (6) we easily find a general term of the expansion:

$$\lambda_n = \frac{(-1)^n \Gamma\left(n + \frac{\nu}{2(\nu+1)}\right)\Gamma\left(n + \frac{1}{2}\right)\Gamma\left(n + \frac{\nu+2}{2(\nu+1)}\right)}{\alpha n!\,\Gamma\left(\frac{\nu}{2(\nu+1)}\right)\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{\nu+2}{2(\nu+1)}\right)} \cdot \left(\frac{\nu+1}{\alpha x^{\nu+1}}\right)^{2n} x^{-\nu}. \qquad (10)$$

It can be seen from expression (9) that at $\nu < -1$ the WKBJ approximation breaks down as $x \to \infty$, while at $\nu > -1$ it breaks down at the point $x = 0$; correspondingly, the semiclassical approximation becomes exact at $x = 0$ in the first case and in the limit $x \to \infty$ in the second. When $\nu = -1 \pm 1/(2q+1)$ $(q = 0,1,2,...)$, the expansion is cut off at $n = q$, and the first q terms of the WKBJ expansion give the exact solution. Expansion (10) is an asymptotic expansion and diverges $[\lambda_n \sim (n!)^2]$, so that the corrections λ_n can be taken into account only until they begin to grow. The index N of the order at which the expansion should be truncated is determined by setting the derivative of λ_n with respect to n equal to zero. At large values of n, using (10), we find the condition $N = \alpha x^{\nu+1}/h(\nu+1)$, which may be rewritten as

$$N = \frac{1}{h}\left|\int_{x_0}^{x} p(x')dx'\right|, \qquad (11)$$

where x_0 is the point at which the WKBJ approximation breaks down ($x_0 = 0$ if $\nu > -1$ or $x_0 = \infty$ if $\nu < -1$). The number of terms in the WKBJ expansion, N, is thus determined by the magnitude of the classical action before the singularity is reached. The condition for the applicability of the WKBJ expansion, (11), is invariant in form and is found for a broad range of potentials, so it presumably is valid in a more general case.

This analysis simplifies in a fundamental way the study of the higher orders of the WKBJ approximation. All the transformations are exceedingly simple, and it is surprising that this method for constructing the WKBJ expansion was not discovered previously. Linear equation (3) may also prove useful for other problems involving a Milne transformation. It can be used, for example, to obtain simple integral representations for $\psi^2(x)$ when the solution of the Schrödinger equation is expressed in terms of the hypergeometric function.

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