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Abstract

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MATHEMATICAL PHYSICS

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APPLICATION OF THE WKB METHOD IN THE ASYMPTOTIC SOLUTION OF EQUATIONS

(Presented by Academician N. N. Bogolyubov, 21 XII 1964)

1. It is known that the W.K.B. method ⁽¹⁾ makes it possible to find the asymptotics of solutions and the eigenvalues λ_n of the Sturm-Liouville equation

$$\frac{d}{dx} \left[p(x) \frac{dy}{dx} \right] + [-q(x) + \lambda \rho(x)] y = 0 \quad (1)$$

for $n \gg 1$. (In particular, such problems often arise in quantum mechanics.) For this equation (1) it is necessary to reduce it to the form

$$d^2u/dt^2 + Q(t)u = 0, \quad (2)$$

which is achieved by the substitution

$$t = \chi(x), \quad y = u/\sqrt{p(x)\chi'(x)}, \quad (3)$$

where $\chi(x)$ is an arbitrary monotone function.

The asymptotic solution corresponding to the W.K.B. method, for the former function of the former argument, has the form

$$y = C [r(x)p(x) - \sigma(x)]^{-1/4} \exp \left\{ \pm i \int_{x_0}^x \frac{dx}{p(x)} \sqrt{r(x)p(x) - \sigma(x)} \right\}, \quad (4)$$

where

$$r(x) = -q(x) + \lambda \rho(x); \quad \sigma(x) = [p(x)\chi'(x)]^2 (1/2 s' + 1/4 s^2);$$

$$s = -p(x) \frac{d}{dx} \frac{1}{p(x)\chi'(x)}; \quad s' = \frac{1}{\chi'(x)} \frac{d}{dx} s.$$

Since $\chi(x)$ is an arbitrary function, the form of the asymptotic solution (4) depends on the choice of $\chi(x)$ ⁽²⁾. In the present paper we wish to show that this arbitrariness can be used to obtain the best (within the W.K.B. method) asymptotic solutions. One of the results of such an approach will be the justification of certain known empirical rules previously applied to improve the W.K.B. method, as well as the derivation of new asymptotic formulas for certain special functions.

2. Let us eliminate the arbitrariness in the choice (3) by requiring that the asymptotic solutions always have the correct behavior at the singular points of the equation. We shall find the form of $\chi(x)$ on the basis of this condition. If, as usual, $p(x) > 0$ inside the domain of definition and has simple zeros only at the endpoints of the interval of the boundary-value problem, then this condition is satisfied by the transformation*

$$t = \chi(x) = \int \frac{dx}{p(x)}, \quad y(x) = y(x(t)) = u(t). \quad (5)$$

Indeed, if near a singular point $p(x) \sim p_0 x$ and $r(x) = r_0/x + r_1 + \dots$ (the regularity condition for a singular point), then the solution of the equa—

* The condition $p(x) \geq 0$ ensures the monotonicity of $\chi(x)$ and the uniqueness of the inverse transformation.

of (1) in a neighborhood of the singular point $x = 0$ has the form

$$y \sim x^\rho (1 + c_1 x + \dots), \quad \rho = \pm \sqrt{-r_0/p_0}. \quad (6)$$

It is easy to see that the solution (4) has the same characteristic exponents at the singular point, if transformation (5) is used. This, in turn, is a consequence of the fact that transformation (5), carrying the singular points to $\pm\infty$, ensures the exact satisfaction there of the boundary conditions for the asymptotic solutions.

3. In problems of quantum mechanics one usually applies the transformation (3)

$$t = \chi(x) = x, \quad y = u/\sqrt[4]{p(x)}. \quad (7)$$

However, it was observed long ago ⁽³⁾ that, in order to improve the results obtained in equations with potentials $V(x)$ that admit separation of variables in parabolic and spheroidal coordinates (the Stark effect in the hydrogen atom, the problem of the hydrogen molecular ion), it is necessary to make the replacement $m^2 - 1 \rightarrow m^2$. (Without the indicated replacement, the phase integrals for

σ -terms ⁽⁴⁾ are inconsistent, and an incorrect phase of the wave function is obtained far from the turning points.)

The indicated difficulties are essentially caused by the fact that, at the singular point, transformation (7) for the solution (4) leads to incorrect characteristic exponents $\rho = -1/2 \pm \sqrt{-r_0/p_0 - 1/4}$. Transformation (5) can serve as a justification for the replacement $m^2 - 1 \rightarrow m^2$, since it leads directly to such expressions for the quasimomenta (which, incidentally, coincide with their classical analogues), where this replacement is already contained.*

4. Using (4) and (5), one can immediately write the general form of the asymptotic solutions of the three-dimensional Schrödinger equation (or Helmholtz equation—when $V(\xi) = 0$, $\varepsilon_1 = k^2$)

$$\Delta\psi + [\varepsilon_1 - V(\xi)]\psi = 0 \quad (8)$$

in all coordinate systems in which it separates. This is possible if the product of the Lamé coefficients is representable in the form ⁽⁶⁾:

$$h_1 h_2 h_3 = f_1(\xi_1) f_2(\xi_2) f_3(\xi_3) |\varphi_{ij}(\xi_i)|, \quad i = 1, 2, 3 \quad (9)$$

($|\varphi_{ij}(\xi_i)|$ is the Stäckel determinant), and the potential $V(\xi)$ in the form:

$$V(\xi) = \sum_i \frac{v_i(\xi_i)}{h_i^2}. \quad (10)$$

In this case the problem reduces to solving the system of equations

$$\frac{1}{f_i} \frac{d}{d\xi_i} \left(f_i \frac{dX_i}{d\xi_i} \right) + \left(\sum_j \varphi_{ij}(\xi_i) \varepsilon_j - v_i \right) X_i = 0 \quad (11)$$

(ε_2 and ε_3 are separation constants: $\psi = CX_1(\xi_1)X_2(\xi_2)X_3(\xi_3)$). Denote

$$\sum_j \varphi_{ij}(\xi_i) \varepsilon_j - v_i(\xi_i) = r_i(\xi_i). \quad (12)$$

Taking also into account that for transformation (5) $\sigma(x) = 0$, we obtain asymptotic solutions, for example in the region where $r_i(\xi_i) > 0$:

$$X_i = \frac{C_i}{\sqrt{f_i(\xi_i)} \sqrt[4]{r_i(\xi_i)}} \cos \left(\int_{\xi_i^0}^{\xi_i} d\xi \sqrt{r_i(\xi_i)} - \frac{\pi}{4} \right) \quad (13)$$

(ξ_i^0 is the corresponding root (“turning point”) of the equation $r_i(\xi_i) = 0$). The eigenvalue ε_1 (for the Schrödinger equation) and the separation constants ε_2 and ε_3 are found from the quasiclassical quantization conditions—

* In an analogous manner Langer ⁽⁵⁾ justified the empirical replacement $l(l+1) \rightarrow (l+1/2)^2$ in the Schrödinger equation for a centrally symmetric potential. In doing so he used the transformation $t = \chi(r) = \ln r$, $R(r) = u/\sqrt{r}$, which, as is easy to see, in the case of the zero of second order in $p(r)$ also leads to the correct characteristic exponents for the solution (4).

tions, which are different depending on the sign of ε_1 and the form of the effective potentials $r_i(\xi_i)$ (see, for example, ^(1, 3)).

5. The associated Legendre polynomials (the angular function of the Schrödinger equation in a centrally symmetric field) satisfy the equation

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial y}{\partial \theta} + \left(-A - \frac{m^2}{\sin^2 \theta} \right) y = 0. \quad (14)$$

The separation constant A must be determined from the condition

$$\oint d\theta \sqrt{-A - \frac{m^2}{\sin^2 \theta}} = 2\pi \left(n_\theta + \frac{1}{2} \right) \quad (15)$$

(the integral over both edges of the cut around the branch points of the root under the integral). Hence ($l = n_\theta + |m|$) we obtain

$$A = -(l + 1/2)^2 \quad (16)$$

and the asymptotic form of the associated Legendre polynomials, normalized to unity*:

$$P_{lm}(\theta) = \sqrt{\frac{2l+1}{\pi}} \frac{1}{\sqrt{\sin \theta}} \left[\left(l + \frac{1}{2} \right)^2 - \frac{m^2}{\sin^2 \theta} \right]^{-1/4} \times \\ \times \cos \left(\int_{\theta_1}^{\theta} d\theta \sqrt{\left(l + \frac{1}{2} \right)^2 - \frac{m^2}{\sin^2 \theta} - \frac{\pi}{4}} \right). \quad (17)$$

For the asymptotic solution of Bessel' s equation

$$(xy')' + (k^2x - m^2/x)y = 0 \quad (14')$$

we obtain in exactly the same way (normalization to $\delta(k - k')$)

$$J_m(kx) = \sqrt{\frac{2}{\pi x}} \left(1 - \frac{m^2}{k^2 x^2}\right)^{-1/4} \cos\left(\int_{m/k}^x dx \sqrt{k^2 - \frac{m^2}{x^2}} - \frac{\pi}{4}\right). \quad (17')$$

Formulas (17) and (17'), for

$$\frac{1}{\sin^2 \theta} \left(\frac{m}{l + 1/2}\right)^2 \ll 1 \quad \text{and} \quad \left(\frac{m}{kx}\right)^2 \ll 1,$$

pass into the known ones.

6. The Schrödinger equation for an electron in the field of two fixed charges Z_1 and Z_2 (the two-center problem, see, for example, (7)) separates in prolate elliptic coordinates. If the relations between the parameters satisfy the quasiclassical conditions (8), then for the wave functions of the discrete spectrum we have**:
- a) for $p^2 \gg 1$, $(p^2 - A)/p \gg 1$, $p^2 \gg A$ (the approximation of distant centers)

$$\begin{aligned} \psi(\xi, \eta, \varphi) = & \frac{2}{\pi^{3/2}} \frac{\varepsilon^{3/4}}{\sqrt{n}} \left[\cos\left(\int_{\xi_1}^{\xi} R(\xi) d\xi - \pi/4\right) / \sqrt{(\xi^2 - 1)R(\xi)} \right] \times \\ & \times \left[\cos\left(\int_{\eta_1}^{\eta} Q(\eta) d\eta - \pi/4\right) / \sqrt{(1 - \eta^2)Q(\eta)} \right] e^{im\varphi}; \end{aligned} \quad (18)$$

- b) for $p^2 \ll 1$, $A/p^2 \gg 1$ (the approximation of close centers)

$$\begin{aligned} \psi(\xi, \eta, \varphi) = & \frac{2}{\pi^{3/2}} \frac{\varepsilon^{3/4} (-A)^{1/4}}{\sqrt{R(Z_1 + Z_2)}} \left[\cos\left(\int_{\xi_1}^{\xi} R(\xi) d\xi - \pi/4\right) / \sqrt{(\xi^2 - 1)R(\xi)} \right] \times \\ & \times \left[\cos\left(\int_{\eta_1}^{\eta} Q(\eta) d\eta - \pi/4\right) / \sqrt{(1 - \eta^2)Q(\eta)} \right] e^{im\varphi}. \end{aligned} \quad (19)$$

* Use of (7) leads to the phase integral

$$\oint d\theta \sqrt{-A + \frac{1}{4} - \frac{m^2 - \frac{1}{4}}{\sin^2 \theta}},$$

which diverges for $m = 0$.

** If one uses transformation (7), then instead of $R(\xi)$ and $Q(\eta)$ one obtains expressions differing from (19) by the replacement $m^2 \rightarrow m^2 - 1$.

Here

$$\begin{aligned}
 R(\xi) &= [(-p^2\xi^2 + b'\xi + A)/(\xi^2 - 1) - m^2/(\xi^2 - 1)^2]^{1/2}; \\
 Q(\eta) &= [(p^2\eta^2 + b\eta - A)/(1 - \eta^2) - m^2/(1 - \eta^2)^2]^{1/2}; \\
 p^2 &= \frac{1}{4}R^2\varepsilon = -\frac{1}{2}R^2E; \quad b' = R(Z_2 + Z_1); \quad b = R(Z_2 - Z_1);
 \end{aligned} \tag{20}$$

R is the distance between the charges; E is the electron energy; A is the separation constant; n is the principal quantum number. Series for A in powers of p^2 in these limiting cases are given, for example, in ⁽⁹⁾.

If the electron is in the continuous spectrum, then $-p^2 \rightarrow \chi^2 = \frac{1}{4}R^2k^2$, where k is the electron momentum. For the radial wave function (normalized to the δ -function of k) we have:

$$X(\xi) = \sqrt{\frac{2\chi}{\pi}} \frac{2}{R} \cos \left(\int_{\xi_1}^{\xi} R(\xi) d\xi - \pi/4 \right) / \sqrt{(\xi^2 - 1)R(\xi)}, \tag{21}$$

for the angular function

$$Y(\eta) = \sqrt{\frac{2}{\pi}} (-A)^{1/4} \cos \left(\int_{\eta_1}^{\eta} Q(\eta) d\eta - \pi/4 \right) / \sqrt{(1 - \eta^2)Q(\eta)} \tag{22}$$

(the relation between A and k^2 , see ⁽⁹⁾). As $R \rightarrow 0$, $\xi \rightarrow 2r/R$, $\eta \rightarrow \cos \theta$, (21) and (22) pass into the normalized wave functions of the continuous spectrum of an electron in a Coulomb field.

For $Z_1 = Z_2 = 0$, formulas (21) and (22) give the asymptotics of spheroidal functions, i.e., solutions of the Helmholtz equation in ellipsoidal coordinates*. All integrals (18)–(22) are expressed in terms of elliptic integrals.

7. Transformation (5) is also of methodological interest, since it gives a simple and practically convenient method for obtaining the asymptotics of solutions of certain self-adjoint equations. For example, for Laguerre polynomials, i.e., solutions of the equation $(x^{m+1}e^{-x}y')' + \lambda x^m e^{-x}y = 0$, after the substitution $t = \chi(x) = \ln x$ we obtain the asymptotic representation

$$\begin{aligned}
 L_n^m(x) &= \frac{1}{\sqrt{\pi}} x^{-m/2} e^{x/2} \left[x \left(n + \frac{m+1}{2} \right) - \frac{x^2}{4} - m^2 \right]^{-1/4} \times \\
 &\times \cos \left(\int_{x_1}^x dx \sqrt{\frac{2n+m+1}{2x} - \frac{m^2}{4x^2} - \frac{1}{4} - \frac{\pi}{4}} \right).
 \end{aligned} \tag{23}$$

We note that (in a somewhat different formulation) the problem of applying the W.K.B. method to finding the asymptotics of certain special functions and orthogonal polynomials was considered in ⁽¹¹⁾.

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* The asymptotics of the functions corresponding to the normalization adopted in the tables of Stratton et al. ⁽¹⁰⁾ are obtained from (21), for $b = b' = 0$, by division by $\sqrt{2/\pi k}$.

Note: Figure translations are in progress. See original paper for figures.

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